

**Institute of Solid State Physics  
University of Latvia**



# **ANNUAL REPORT**

**2010**

Riga 2011

**Annual Report 2010, Institute of Solid State Physics, University of Latvia.**

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**2011**

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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:**

- studies of electronic and ionic processes in wide-gap materials with different degrees of structural ordering;
- development of new inorganic materials (single crystals, glasses, ceramics, thin films) for optics and electronics;
- vision research, development of new technologies for psycho-physical testing and primary vision care;
- design and manufacturing of scientific instruments and instruments for analytical tasks and environmental monitoring.

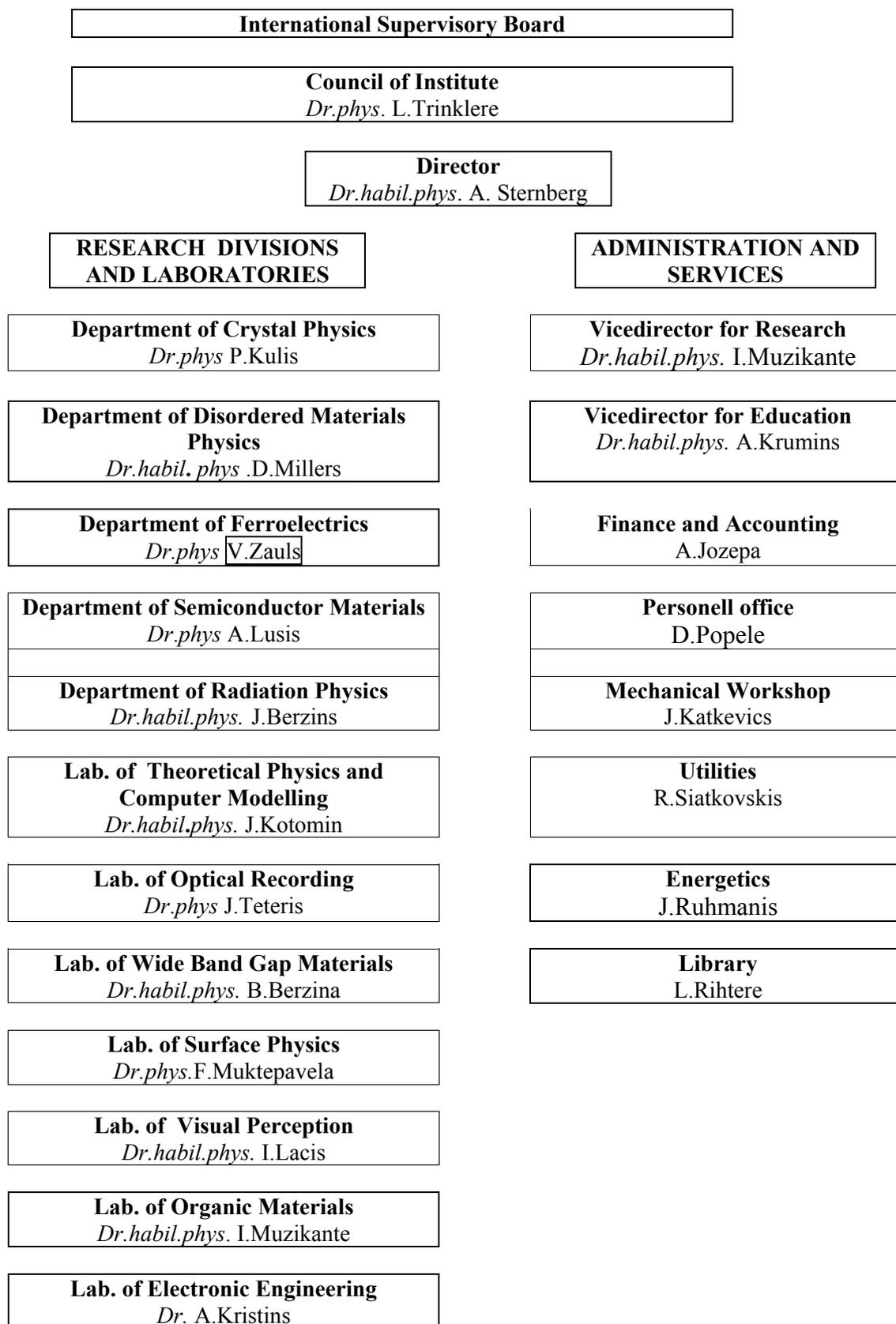
The highest decision-making body of the Institute is the **Scientific Council** of 21 members elected by the employees of the Institute (Table 2). Presently Dr. phys. L.Trinklere is the elected chairperson of the ISSP Council. The Council appoints director and its deputies.

**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 performed 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..."

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff**. At present there are 150 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 2010 there were 21 PhD students and 46 undergraduate and graduate students in physics and optometry programmes working at the ISSP.

*Table 1*

**ORGANIZATIONAL STRUCTURE OF THE ISSP IN 2009**



### **The Scientific Council of the Institute**

1. Laima Trinklere, Dr.phys., chairperson of the Council
2. Marcis Auzins, Dr.habil.phys.
3. Larisa Grigorjeva, Dr.habil.phys.
4. Anastasija Jozepa
5. Andris Krumins, Prof., Dr.habil.phys.
6. Peteris Kulis, Dr.phys.
7. Aleksejs Kuzmins, Dr.phys.
8. Donats Millers, Dr.habil.phys.
9. Inta Muzikante, Dr.habil.phys.
10. Daina Riekstina, Dr.phys.
11. Uldis Rogulis, Dr.habil.phys.
12. Andrejs Silins, Prof., Dr.habil.phys.
13. Linards Skuja, Dr.habil.phys.
14. Maris Springis, Dr.habil.phys.
15. Anatolijs Sharakovskis, PhD student
16. Andris Sternbergs, Dr.habil.phys.
17. Janis Teteris, Dr.phys.
18. Anatolijs Truhins, Dr.habil.phys.
19. Aivars Vembris, PhD student
20. Vismants Zauls, Dr.phys.
21. Guntars Zvejnieks, Dr.phys.

### **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. Prof. Dr.M.Kirm, University of Tartu, Estonia
7. Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia
8. Prof. Sergei Tuituinnikov, Joint Institute for Nuclear Research, Dubna, Russia
9. Prof. Juris Upatnieks, Applied Optics, USA
10. Prof. M. Van de Voorde, Max – Planck – Institute, Stuttgart, Germany
11. Prof. Harald W.Weber, Atomic Institute of Austrian Universities, Vienna, Austria

The annual report summarizes the research activities of the ISSP in 2010. 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 286.9 thous. Ls budget in 2010. The infrastructure financing for ISSP in 2010 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 2010:

No	Author	Award
1.	Dr.habil.phys. A.Shluger	Foreign Member of Latvian Academy of Science
2.	Dr.habil.phys. J.Purans	The correspondent member of Latvian Academic of Science
3.	Dr.phys. O.Dumbrajs	Author of the best scientific achievement (from Latvian Academic of Science)
4.	Dr.phys.J.Kleperis, Dr.phys.G.Bajars, J.Šmits, G.Kučinskis	Author of the best scientific achievement (from Latvian Academic of Science)

At the end of 2010, 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 2010 **three international conferences** have been organised at the Institute:

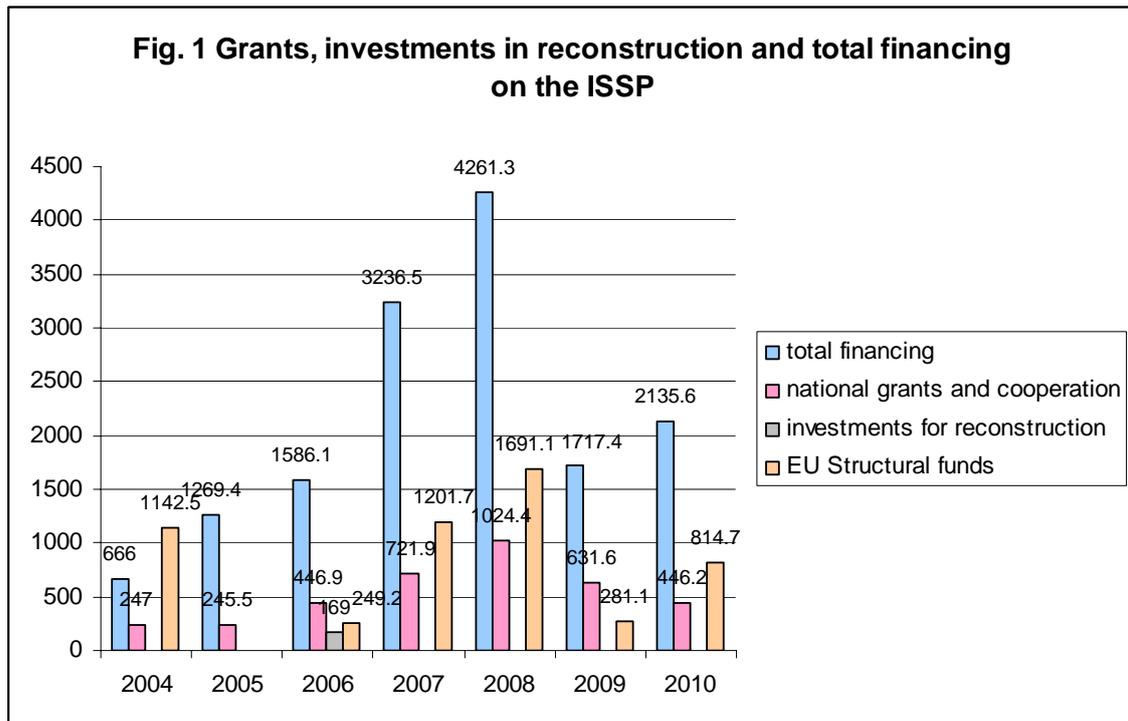
- Annual International conference “Functional materials and nanotechnologies”, March 16 - 19, 2010, Riga, Latvia;
- International Student Conference “Developments in Optics and Communications 2010”, April 23 – 25, 2010, Riga, Latvia;
- The 9<sup>th</sup> International Symposium on Systems with Fast Ionic Transport, June 1 - 5, 2010, Riga, Latvia

*Table 4*

**INCOME OF ISSP, THOUSAND Ls, FROM 2004 - 2010**

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Structural funds from EU
2004	1 809	246.7	123.5	166.5	121.8	1142,5
2005	1 269,4	245,5	358,8 + 120)*	172,8	387,6	
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

\*) – investment for building reconstruction



The main source for **international funding** were 10 EC 7<sup>th</sup> Framework Programme contracts:

- F-Bridge – 6.3 thous. EUR
- Catherine – 12.6 thous. EUR
- 4 EURATOM projects – 70.7 thous. EUR
- CACOMEL project – 10.8 thous. EUR
- Karlsruhe project – 14.0 thous. EUR

#### **Main achievements in 2010**

1. 79 SCI papers published by the staff of Institute.
2. 3 patent applications
- 3 9 B.sc. thesis and 15 M.Sc. thesis in physics were defended under the supervision of our scientists
4. A.Sharakovskis, K.Smits, G.Ikaunieks, E.Sledevskis and A.Gerbreders were acquired degree of doctor of physics (PhD)

Many thanks to everybody who contributed to this report as well as to the organizations that supported the Institute financially: Science Department of the Latvian Ministry of Education and Science, Latvian Council of Science, University of Latvia, EC 7<sup>th</sup> 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

Head of Department Dr. phys. P. Kulis

### Research Area and Main Problems

1. Magnetic resonance (EPR, optically detected EPR) investigations of the structure of the intrinsic and radiation defects, and their recombination process in some actual wide gap scintillator, x-ray storage phosphor and dosimeter materials. The scientific cooperation with other magnetic resonance groups, especially with the University of Paderborn, Germany. A contribution to the better understanding of the defects and processes in luminescent detector materials is expected.
2. Synthesis and investigation of oxyfluoride nanocomposite materials prospective for the light emitters, detectors and visualization systems with enhanced quantum efficiency. Oxyfluoride compounds activated with lanthanide ions may exhibit emission of photons of greater energy than those absorbed during the excitation (up-conversion of energy). The glass and glassceramics samples were synthesized using conventional methods. Several chemical methods were tried for the synthesis of oxyfluoride nanostructures. The energy relaxation mechanisms were studied during up-conversion processes by means of spectral and time-resolved luminescence measurements both in glass and glass ceramics containing  $\text{NaYF}_4:\text{Er}$ ,  $\text{LaF}_3:\text{Er}$  and in chemically synthesized oxyfluorides.
3. Technology of Al-Ga nitride semiconductor heterostructures for light-emitting and laser diodes for violet and ultraviolet spectral regions - the goal of the project is the development of light-emitting diodes and laser diodes for violet and ultraviolet spectral region. The project involves synthesis and design of corresponding new materials on the basis of the third group nitrides, elaboration of the thin film heterostructures and further development of production of multifunctional photonic devices in joint stock company "Alfa".
4. Investigation and characterization of the impurity content in fusion plasmas and reactor hot wall are the main goals of EURATOM project. The objectives of this project require study of the influence of the liquid metal limiter on the main plasma parameters, including concentration of evaporated metal atoms in plasma. Laser spectroscopy techniques are proposed for development of procedures for research of impurities in plasma and plasma facing materials. According to the objectives emission of Ga metal vapours in plasmas during the evaporation of the metal gush has been considered. Density of metal vapours in plasma can be obtained using two spectroscopic methods: the steady state emission of the multiple ionised metal ions and the charge exchange emission during ionization of evaporated metal ions.
5. Laser-induced ablation for analysis of the impurities in plasma facing components as the method for the detection of any chemical element is used for the remote analysis. The major tasks of the present investigation are setting up and testing the equipment for laser ablation spectroscopy and developing the methodology for impurity depth profiling. The investigation is carried out using the plasma facing materials of ASDEX Upgrade tokamak by means of laser-induced ablation spectroscopy and profilometry of the corresponding ablation craters. The experimental set-up for the laser-induced ablation spectroscopy was developed and manufactured. The optimal conditions of the laser-induced ablation of the samples of ASDEX Upgrade divertor plates were found. Plasma emission spectra of these plasma facing components showing a substantial number of impurities were recorded. The impurity elements were determined, and the possible sources of the impurities suggested. The depth of the accumulation of basic impurities (hydrogen, boron) in the surface of the ASDEX Upgrade divertor plates (carbon R6710 tiles) is estimated using plasma emission

spectra. Obtained results allows considering the method of the laser-induced ablation spectroscopy to be feasible for rapid analysis of plasma facing materials. With minor modifications, this method can be suggested as an *in situ* technique for determination the state of the plasma facing components inside the chamber of a thermonuclear fusion reactor.

### **Scientific Staff**

1. Dr. phys. J. Butikova
2. Dr. phys. L. Dimitrocenko
3. Dr. phys. A. Fedotovs
4. Dr. phys. P. Kulis
5. Dr. phys. B. Polyakov
6. Prof., Dr. habil. phys. U. Rogulis
7. Dr. phys. A. Sarakovskis
8. Dr. habil. phys. M. Springis
9. Prof., Dr. habil. phys. I. Tale
10. Dr. phys. J. Trokss
11. Mg. E. Elsts
12. Mg. phys. J. Jansons

### **PhD Students**

1. Dz. Berzins
2. J. Grube
3. A. Petruhins
4. G. Marcins
5. A. Voitkans

### **Students**

1. M. Cubarovs
2. G. Doke

### **Scientific visits abroad**

1. I.Tale, 11th Europhysical Conference on Defects in Insulating Materials „EURODIM 2010”, PÉCS, Hungary 12-16 July 2010.
2. M.Cubarov, 11th Europhysical Conference on Defects in Insulating Materials „EURODIM 2010”, PÉCS, Hungary 12-16 July 2010.
3. A.Sarakovskis, 11th Europhysical Conference on Defects in Insulating Materials „EURODIM 2010”, PÉCS, Hungary 12-16 July 2010.
4. J.Grube, 11th Europhysical Conference on Defects in Insulating Materials „EURODIM 2010”, PÉCS, Hungary 12-16 July 2010.
5. A.Fedotovs, 11th Europhysical Conference on Defects in Insulating Materials „EURODIM 2010”, PÉCS, Hungary 12-16 July 2010.
6. G. Marcins, 12-th International Conference-School, Advanced Materials and Technologies, August 27 - 31, 2010, Palanga, Lithuania.
7. G. Marcins, E-MRS 2010 Fall Meeting, September 13-17, Warsaw, Poland
8. I.Tale, Spain, Barcelona, 28.04.-30.04.; 20.10.-23.10.
9. I.Tale, Germany, 29.03.-01.04.; 20.07.-23.07.; 03.09.-11.09.
10. I.Tale, Austria, 02.11-07.11.
11. L. Dimitrocenko, Finland, Helsinki, 2 days
12. A.Voitkans, Japan, 03.01.-15.03.

## Cooperation

### Latvia

Joint stock company “Alfa”

### Germany

1. University of Rostock, Germany (Prof. H.-J. Fitting).
2. “Aixtron” Aachen, Germany
3. Max Plank Institute of Plasma Physics, Garching, Germany

## Main results

### LOCALIZATION DYNAMICS OF EXCITON LUMINESCENCE IN $\text{In}_x\text{Ga}_{1-x}\text{N}$ EPITAXIAL FILMS

I Tale, L Dimitrocenko, P Kulis, G Marcins, A Sarakovskis and A Voitkans

Picosecond time resolved photoluminescence (PL) spectroscopy of excitonic processes in MOCVD grown  $\text{In}_x\text{Ga}_{1-x}\text{N}$  mixed films with the In concentration in range from  $x=0.1$  to  $0.18$  under the band-to-band excitation are considered. It is stated that by an In content in alloy up to 12% the band-band photo excitation at 8 K results in creating of localized excitons and biexcitons represented by close overlapping Gaussian shape luminescence bands having FWHM 27 and 8.7 meV, respectively. PL decay kinetics of both bands involves two exponential decay stages. Excitons and biexcitons in unperturbed lattice positions causes fast decay with  $\tau \sim 10$  ps, whereas their transfer to the metastable state due to relaxation of In – Ga local configuration causes slow decay  $\tau \sim 90$  ps. At increased In content up to 19% both the localized excitons and biexcitons are represented by Gaussian type luminescence bands being non-uniform broadened to the high energy side. The continuous distribution of excitons and biexcitons in transition energies is stated by analysis of the red-shift of luminescence bands during the spectra decay. An additional new narrow low energy PL band arises at low energy side expected to be caused by excitons at InN clusters.

### OBJECT SIZE EFFECT ON THE CONTACT POTENTIAL DIFFERENCE MEASURED BY SCANNING KELVIN PROBE METHOD

B.Polyakov, R.Krutokhvostov, A.Kuzmin, E.Tamanis, I.Muzikante, I.Tale

Contact potential difference (CPD) was measured by macroscopic Kelvin probe instrument and scanning Kelvin probe microscope on Al, Ni and Pt on ITO substrates at ambient conditions. CPD values measured by scanning Kelvin probe microscope and macroscopic Kelvin probe are close within the error of about 10-30 % for large studied objects, whereas scanning Kelvin probe microscope signal decreases, when the object size becomes smaller than  $1.4 \mu\text{m}$ . CPD and electric field signals measured using many-pass technique allowed us to estimate the influence of electrostatic field disturbance, especially, in the case of small objects.

## **LASER-INDUCED BREAKDOWN SPECTROSCOPY FOR DETERMINING IMPURITY CONTENT AND DEPTH PROFILE IN PLASMA FACING MATERIALS**

J. Butikova, A. Sarakovskis, I. Tale

Appropriate methods for investigating the effects of plasma exposure are required in order to improve and develop new plasma-facing components. Particle fluxes from plasma result in complex plasma-wall interactions causing phenomena such as erosion and migration of materials, retention, co-deposition and diffusion. Several methods of analyzing the surface and impurity content in the near-surface layers are currently employed. An alternative method of establishing the impurity content in solid materials is laser-induced breakdown spectroscopy. This powerful tool for spectro-chemical analysis provides both impurity content analysis and layer-by-layer depth profiling. We present spectral information and discuss questions regarding the depth profiles of the impurities.

## **SOME ASPECTS OF PULSED LASER DEPOSITION OF Si NANOCRYSTALLINE FILMS**

B. Polyakov, A. Petruhins, J. Butikova, A. Kuzmin, I. Tale

Nanocrystalline silicon films were deposited by a picosecond laser ablation on different substrates in vacuum at room temperature. A nanocrystalline structure of the films was evidenced by atomic force microscopy (AFM), optical and Raman spectroscopy. A blue shift of the absorption edge was observed in optical absorption spectra, and a decrease of the optical phonon energy at the Brillouin zone centre was detected by Raman scattering. Early stages of nanocrystalline film formation on mica and HOPG substrates were studied by AFM. Mechanism of nanocrystal growth on substrate is discussed.

## **CATHODOLUMINESCENCE OF TERBIUM- AND YTTERBIUM-ACTIVATED OXYFLUORIDE GLASSES AND GLASS CERAMICS**

E. Elsts, U. Rogulis, J. Jansons, A. Sharakovskis

Cathodoluminescence (CL) spectra and decay times have been studied for oxyfluoride glasses and glass ceramics of the system:  $\text{SiO}_2\text{Al}_2\text{O}_3 - \text{Na}_2\text{O} - \text{LaF}_3 - \text{NaF}$ , activated by terbium and ytterbium.

The CL spectra of the glasses and glass ceramics show characteristic Tb<sup>3+</sup> luminescence bands: blue ( $^5\text{D}_3 \rightarrow ^7\text{F}_1$ ) and green ( $^5\text{D}_4 \rightarrow ^7\text{F}_1$ ) groups. With increasing terbium concentration the blue- to green-group ratio decreases.

The CL decay curves can be sufficiently well approximated by two exponents – fast and slow. Decay times for the blue-group CL bands are faster than for those of green group.

As the terbium concentration increases, the lifetimes for the lines of the blue group shorten, while for the green group they remain unchanged. This could be explained by the cross-relaxation between the transitions  $^5\text{D}_3 \rightarrow ^5\text{D}_4$  and  $^7\text{F}_6 \rightarrow ^7\text{F}_0$  of two terbium ions.

## **EPR OF RADIATION DEFECTS IN LITHIUM-OXYFLUORIDE GLASS CERAMICS**

A. Fedotovs, U. Rogulis, A. Sarakovskis, L. Dimitrocenko

We studied oxyfluoride composites based on lithium silicate glasses with yttrium fluorides and rare-earth dopants. The electron paramagnetic resonance (EPR) has been used to obtain information about radiation induced defects in these materials. Spectra have been measured before and after X-ray irradiation at room temperature and at liquid nitrogen temperature. Fluoride crystallites within samples were created by means of thermal treatment at specific temperatures. EPR spectra of radiation induced defects in oxyfluoride glass ceramics, in which crystallites have not been yet created, show no explicit hfs interaction of fluorine nuclei. However, in glass ceramics, which already contains fluoride crystallites, the hfs characteristic to fluorine nuclei appears in the EPR spectra. EPR hyperfine structure could be explained within a model of an F-type centre in  $YF_3$  crystalline phase.

## **EPR STUDIES OF THE OXYFLUORIDE GLASS CERAMICS USING $Mn^{2+}$ AS A PARAMAGNETIC PROBE**

A. Fedotovs, Dz. Berzins, A. Sarakovskis, U. Rogulis and G. Doke

In this work, we used  $Mn^{2+}$  as a dopant in the oxyfluoride glasses with various fluoride compounds. Electron paramagnetic resonance (EPR) measurements were carried out before and after a heat treatment of the material. In both cases, a well pronounced hyperfine (hf) structure of the EPR spectra characteristic to the  $Mn^{2+}$  ion have been observed. EPR measurements have also been studied for the separate fluoride counterparts of the oxyfluoride glasses. EPR spectra of the  $LaF_3:Mn^{2+}$  and  $CaF_2:Mn^{2+}$  powders show that  $Mn^{2+}$  ion has a strong superhyperfine (shf) interaction with surrounding fluorine nuclei, and this shf structure could be observed also in the heat treated glass samples.

## **EXCITED STATE ABSORPTION AND ENERGY –TRANSFER MECHANISMS OF UP-CONVERSION LUMINESCENCE IN $Er^{3+}$ DOPED OXYFLUORIDE GLASS CERAMICS AT DIFFERENT TEMPERATURES**

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

Oxyfluoride silicate glass  $SiO_2-Al_2O_3-NaCO_3-NaF-LaF_3-ErF_3$  was synthesized. The glass transitions and crystallization temperatures were determined by differential thermal analysis. Glass ceramics containing  $LaF_3:Er^{3+}$  crystallites of size  $\sim 20$  nm were formed in glass matrix after the heat treatment of the precursor glass in the vicinity of the crystallization temperature. Up-conversion luminescence, excitation spectra as well as time-resolved up-conversion luminescence of the glass and glass ceramics was studied at different temperatures. The up-conversion transients showed that at room temperature the dominant mechanism of the up-conversion luminescence in the glass ceramics is excited state absorption while at lower temperatures energy-transfer mechanism prevails. The origins of these differences are discussed in terms of the transitions between Stark manifolds of  $^4I_{15/2}$ ,  $^4I_{11/2}$  and  $^4F_{7/2}$  states in  $Er^{3+}$  ions.

# SELECTIVE EXCITATION OF UP-CONVERSION LUMINESCENCE BY $\text{Yb}^{3+}$ - $\text{Er}^{3+}$ ENERGY TRANSFER IN GLASS AND CRYSTALLINE PHASE OF OXYFLUORIDE GLASS CERAMICS

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

Up-conversion luminescence of oxyfluoride glass and glass ceramics containing  $\text{LaF}_3$  crystallites doped with  $\text{Yb}^{3+}$  and  $\text{Er}^{3+}$  was investigated at low temperature. Excitation of  $\text{Yb}^{3+}$  in the IR region revealed the fast and the slow components of  $\text{Er}^{3+}$  up-conversion luminescence originating from both glass and crystalline phases. The temporal differences of the both kinds of the luminescence allowed reconstructing the excitation spectra of the up-conversion luminescence related to the glass and crystalline phases in the glass ceramics.

## Scientific publications

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2. A. Fraile Rodríguez, A. Kleibert, J. Bansmann, A. Voitkans, L. J. Heyderman, and F. Nolting, Size-dependent spin structures in iron nanoparticles, - Phys. Rev. Lett. 2010, 104, 127201.
3. A. Kleibert, A. Voitkans, K-H Meiwes-Broer, Reflection high energy electron diffraction as a tool in cluster deposition experiments, phys. stat. sol. B, 2010, Volume 247, Issue 5, pages 1048–1055.
4. K. Fauth, G.E. Ballentine, C. Praetorius, A. Kleibert, N. Wilken, A. Voitkans, K.-H. Meiwes-Broer, Magnetic properties of Fe nanoclusters on Cu(111) studied with X-ray magnetic circular dichroism, phys. stat. sol. B, 2010, Volume 247, Issue 5, pages 1170–1179.
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7. I. Tale, L. Dimitrocenko, P.Kulis, G. Marcins, A. Sarakovskis, A.Voitkans, Localization dynamics of exciton luminescence in  $\text{In}_x\text{Ga}_{1-x}\text{N}$  epitaxial films, - 11<sup>th</sup> Europhysical Conference on Defects in Insulating Materials (EURODIM2010) IOP Publishing, IOP Conf. Series: Materials Science and Engineering 15 (2010) 012059 doi:10.1088/1757-899X/15/1
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9. A. Fedotovs, Dz. Berzins, A. Sarakovskis, U. Rogulis, G. Doke, EPR studies of the oxyfluoride glass ceramics using  $\text{Mn}^{2+}$  as a paramagnetic probe, IOP Conference Series: Materials and Engineering, 2010, vol. 15, 012068 [doi:10.1088/1757-899X/15/1/012068].
10. A. Sarakovskis, J.Grube, G. Doke, M. Springis, Excited state absorption and energy –transfer mechanisms of up-conversion luminescence in  $\text{Er}^{3+}$  doped oxyfluoride

glass ceramics at different temperatures, - Journal of Luminescence, 2010, 130, p.805-811.

11. A. Sarakovskis, J.Grube, G. Doke, M. Springis, Selective excitation of up-conversion luminescence by  $\text{Yb}^{3+}$ - $\text{Er}^{3+}$  energy transfer in glass and crystalline phase of oxyfluoride glass ceramics, - Optical Materials, 2010, 32, p.832-835.

### Lectures on Conferences

#### 26th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 17-19, 2010

1. J. Jansons, Professor Kurt Schwartz – 80<sup>th</sup> anniversary, - Abstracts of the 26<sup>th</sup> Scientific Conference ISSP LU, 2010, p. 4-6.
2. A. Petruhins, B. Polakov, E.Tamanis, I. Tale, P. Kulis, Optical properties of sulfide nanostructures, - Ibid., p. 7
3. A.N. Trukhin, A. Sharakovski, J. Grube, d.L. Griscom, Luminescence of localized states in  $\text{SiO}_2$ -Si and  $\text{SiO}_2$ -Al glasses, -. Ibid., p. 8.
4. G. Doke, J.Grube, A Sarakovskis, M. Springis, Synthesis and luminescence properties of  $\text{NaLaF}_4$  activated with  $\text{Er}^{3+}$  ions, - Ibid., p. 10.
5. E. Elsts, U. Rogulis, J. Jansons, A. Sarakovskis, Cathodoluminescence of terbium and ytterbium activated oxyfluoride glasses and glass ceramics, - Ibid., p. 11.
6. J. Grube, G. Doke, A Sarakovskis, M. Springis, Mechanisms of “up-conversion” luminescence in silicate glass and glass ceramics doped with  $\text{Er}^{3+}$  ions, - Ibid., p. 45.
7. A. Fedotovs, Dz. Berzins, A.Sarakovskis, U. Rogulis, -  $\text{Mn}^{2+}$  as paramagnetic probe for studies of glass and ceramics, -Ibid., p. 46.

#### International conference “Functional materials and nanotechnologies” FM&NT, Riga, 2010, 16 - 19 march

1. J. Butikova, D. Jakovlevs, I. Tale, Aspects of SEM analysis of ablated tiles in ASDEX upgrade tokamak, - International conference „Functional materials and nanotechnologies” FM&NT 2010, Book of abstracts, ISSP LU, Riga, 16-19. march, p. 47.
2. A. Voitkans, A. Kleibert, K.-H. Meiwes-Broer, Reflection high energy electron diffraction as a tool for nanoparticle deposition studies, - Ibid, p. 48...;
3. G. Doke, A. Sarakovskis, J. Grube, M. Springis, Synthesis and up-conversion luminescence in erbium doped  $\text{NaLaF}_4$ , - Ibid., p.74.
4. J.Grube, A. Sarakovskis, G. Doke, M.Springis, Up-conversion luminescence in erbium and ytterbium doped silicate glass ceramics, - Ibid., p. 77.
5. A. Fedotovs, Dz. Berzins, A.Sarakovskis, U. Rogulis, Paramagnetic probes for studies of crystallization in the oxyfluoride glass ceramics, - Ibid., p. 78.
6. G. Marcins, M. Chubarov, J. Butikova, I. Tale, B. Poyakov, R. Kalendarjov, A. Muhin, Structure and characteristics of laser crystallized thin amorphous Si films, - Ibid., p. 88.
7. M. Chubarov, G. Marcins, I. Tale, L. Dimitrocenko, Thermoactivated spectroscopy of defect levels in GaN thin films -, Ibid., p. 89.
8. A. Petruhins, B. Polyakov, E. Tamanis, I. Tale, P.kulis, Sulphide nanostructure fabrication using pulsed laser deposition, - Ibid., p. 123.
9. A. Voitkans, J. Butikova, I. Tale, Laser induced ablation analysis of post-mortem tiles of ASDEX upgrade tokamak, - Ibid., p. 124.
10. L. Grigorjeva, J. Grube, A. Sarakovskis, Near-band luminescence of ZnO crystals in subnanosecond range, - Ibid., p.167.

11. K. Smits, L. Grigorjeva, D. Millers, A.Sarakovskis, D. Jankovica, J. Grabis, UP-conversion luminescence in ZrO<sub>2</sub> nanocrystals, - *ibid.*, p. 169.

### **11th Europhysical Conference on Defects in Insulating Materials „EURODIM 2010”, PÉCS, Hungary 12-16 July 2010**

1. M. Chubarov, L. Dimitroenco, G. Marcins, I. Tale, Thermally activated electronic transport and donor-acceptor recombination in Al<sub>x</sub>Ga<sub>1-x</sub>N alloys, - 11th Europhysical conference on defects in insulating materials, EURODIM 2010, Book of abstracts, Pecs, Hungary, p.1.4.
2. A. Fedotovs, Dz. Berzins, A. Sarakovskis, U. Rogulis, G. Doke, EPR studies of the oxyfluoride glass ceramics using paramagnetic probes, Abstracts of the 11th Europhysical Conference on defects in Insulating Materials, Eurodim'2010, PECS, Hungary, B7.
3. L. Dimitroenco, A. Sarakovskis, I. Tale, A. Voitkans, Photoluminescence of In<sub>x</sub>Ga<sub>1-x</sub>N epitaxial film, - 11th Europhysical conference on defects in insulating materials, EURODIM 2010, Book of abstracts, Pecs, Hungary, p.A98
4. J. Grube, A. Sarakovskis, G. Doke, M. Springis, Er<sup>3+</sup> concentration impact on up-conversion properties of NaLaF<sub>4</sub>:Er<sup>3+</sup>, - *Ibid.*, p. A102.
5. A. Sarakovskis, J. Grube, G. Doke, K. Smits, M. Springis, Influence of oxygen impurities on up-conversion luminescence of erbium doped NaLaF<sub>4</sub>, - *Ibid.*, A103

### **The 12-th international Conference-school ”Advanced materials and technologies” Palanga, Lithuania, 27-31 August, 2010**

G. Marcins, M.Chubarov, J. Butikova, I. Tale, R. Kalendarjov, Structure and characteristics of laser crystalized amorphous Si films, - The 12-th international Conference”Advanced materials and technologies, Book of Abstracts, Palanga, Lithuania, 27-31 August, 2010

### **FANAS 2010 Conference: Friction and Adhesion in Nanomechanical Systems, October 25-28, 2010, Saarbrücken, Germany**

B.Polyakov, S.Vlassov, L.Dorogin, A.Lohmus, R.Lohmus, In situ manipulation of ZnO nanowires inside scanning electron microscope, - FANAS 2010 Conference: Friction and Adhesion in Nanomechanical Systems, , October 25-28, 2010, Saarbrücken, Germany

### **E-MRS 2010 Fall Meeting, Warsaw, Poland**

G. Marcins, M.Chubarov, J. Butikova, I. Tale, A. Muhin, R. Kalendarjov, Structure and characteristics of laser crystalized amorphous Si films, - E-MRS 2010 Fall Meeting, Book of Abstracts, Warsaw, Poland, Symposium C, p. 21.

### **Popular Science Articles (in Latvian)**

1. J. Jansons. Fizikas profesors Kurtam Švarcam – 80 gadi. – „Zvaigžņotā Debess”, 2010. g. pavasaris (207), 34. – 38. lpp.
2. J. Jansons. Vladimirs Afanasjevs – Baikonuras kosmodroma virsniēks 1970. gados. – „Zvaigžņotā Debess”, 2010. g. vasara (208), 20. – 24. lpp. un nobeigums 2010. g. rudens (209), 13. – 16. lpp.
3. J. Jansons. LU fizikas docents Ojārs Šmits (24.04.1930.–14.03.1993.). – „Zvaigžņotā Debess”, 2010./11. g. ziema (210), 14. – 21. lpp.

## DEPARTMENT OF DISORDED MATERIAL PHYSICS

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

<b>Solid state radiation physics Laboratory</b> <b>Head of laboratory</b> <b>Dr.habil.phys.L.Grigorjeva</b>	<b>Laboratory of amorphous materials spectroscopy</b> <b>Head of laboratory</b> <b>Dr.habil.phys. L.Skuja</b>	<b>Laboratory of Solid state optics</b> <b>Head of laboratory</b> <b>Dr.habil.phys. A.Trukhin</b>
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### Research area and experimental setups

The electronic properties of advanced materials for scintillators, light transformers, gas sensors, radiation detectors, photocatalysis, persistent luminofors are studied by means of spectroscopic methods including time-resolved spectroscopy.

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

For luminescence excitation a pulsed electron beam accelerator (10 ns, 270 keV,  $10^{12}$  electrons/pulse), YAG:Nd and nitrogen lasers (266 nm, 337 nm, 532 nm), excimer lasers (248, 193 and 157 nm) were used.

Vacuum ultraviolet spectroscopy: McPherson 234/302 200mm monochromator with  $\text{D}_2$  lamp with  $\text{MgF}_2$ -window serving as light source (120-250 nm).

Raman and luminescence 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, detected elements from Na to U, spatial resolution 50  $\mu\text{m}$ ).

<b>Laboratory of solid state radiation physics</b>  Dr.habil.phys.S.Chernov Dr.habil.phys. L.Grigorjeva Dr.habil.phys. D.Millers Dr.K.Smits <b>Technical staff</b> Eng. A.Sitdikov <b>Ph.D students</b> M.Shorokhov <b>Students</b> L.Bukonte; J.Rikveilis Z.Alute; V.Liepina	<b>Laboratory of amorphous materials spectroscopy</b>  Dr.habil.phys. A.Silins Dr.habil. L.Skuja <b>Students</b> L.Tiļuga
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### Scientific Visits Abroad

1. Dr.habil.phys.L.Grigorjeva, Estonia (5 days)
2. Dr.habil.phys. D.Millers, Poland (3 days)
3. Dr.K.Smits, Hungary, (7 days)
4. Dr.K.Smits, France (14 days)
5. Dr.K.Smits, France (15 days)
6. Dr.habil.phys. D.Millers, France (14 days)
7. Dr.Habil.phys. L.Grigorjeva, France (14 days)
8. Dr.Habil.phys. L.Grigorjeva, Greece (7 days)
9. Dr.Habil.phys. L.Grigorjeva, Germany (6 days)

10. Dr.habil. L.Skuja, Japan, (2 month)

11. Dr.habil. L.Skuja, Italy (7 days)

## Cooperation

### Latvia

SIA "Baltic Scientific Instruments (Dr.V.Gostilo, M.Shorohov)

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

Riga Technical University, Institute of Silicate Materials ( Prof.A.Medvids, Prof.M.Knite))

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

### Estonia

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

### Russia

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

Burjatia State University, (Dr.A.V.Nomoev)

### Poland

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

Institute of Low Temperatures and Structure Researchs, PAS Wroclaw (Prof.W.Strek)

### France

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

Université Jean Monnet Of Saint-Etienne (France) (Prof. Y Ouerdane).

### Japan

Tokyo Institute of Technology (Prof. H.Hosono, M.Hirano)

Tokyo Metropolitan University (Dr. K. Kajihara)

### Israel

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

## Scientific publications

1. L.Grigorjeva, A.Krasnikov, V.V.Laguta, M.Nikl, S.Zazubovich. Luminescence and creation of electron centers in UV-irradiated  $\text{YAlO}_3$  single crystals. *J.of.Appl.phys.* 108(5) (2010) 053509.
2. L.Grigorjeva, D.Millers, K.Smits, J.Grabis, J.Fidelus, W.Lojkowski, T.Chudoba, K.Bienkowski. The luminescence of ZnO ceramics. *Radiat.Measur.*, 45 (3-6) (2010) 441-443.
3. K.Smits, L.Grigorjeva, D.Millers, A.Sarakowskis, A.Opalinska, J.Fidelus, W.Lojkowski. *Optical Mater.*, 32 (8), (2010) 827-831.
4. R.Zabels, F.Muktepavela, L.Grigorjeva, E.Tamanis, M.Mishels-Piesins. *Optical Mater.*, Nanoindentation and photoluminescence of ZnO thin films and single crystal., 32 (8) (2010) 818-822.
5. V.Pankratov, L.Shirmane, T.Chudoba, P.Gluchowski, D.Hreniak, W.Strek, W.Lojkowski. Peculiarities of luminescent properties of cerium doped YAG transparent ceramics. *Radiat.Meas.*, 46( 2010) 392-394.

6. K.Kajihara, T.Miura, H.Kamioka, M.Hirano, L.Skuja, H.Hosono, Diffusion of oxygen molecules in fluorine-doped amorphous SiO<sub>2</sub>. Materials Science and Engineering, B173 (2010) 158-161

### Lectures in Conferences

#### **International Baltic Sea Region Conference "Functional materials and nanotechnologies 2010 (FM&NT)", March-16-18, Riga, Latvia**

1. W.Lojkowski, K.Galazka, T.Chudoba, A.Opalinska, J.D.Fidelus, K.Smits, L.Grigorjeva, D.Millers, E.Wolska, M.Godlewski. Investigation of luminescence of zirconia nanopowders during change of oxygen content in the gas over the sample. Book of abstracts, p.64.
2. L.Grigorjeva, J.Grube, A.Sarakovskis, D.Millers. Near-band luminescence of ZnO crystals in subnanosecond range. Book of abstracts, p.167.
- 3.J.Grabis, D.Jankovica, L.Grigorjeva, D.Millers. Photoluminescent and photocatalytic activity of nanosized zink tungstate prepared by combustion synthesis. Book of abstract, p.168.
4. K.Smits, L.Grigorjeva, D.Millers, A.Sarakovskis, D.Jankovica, J.Grabis. Up-conversion luminescence in ZrO<sub>2</sub> nanocrystals. Book of abstracts, p.169.
5. L.Skuja, K.Kajihara, M.Hirano, H.Hosono Defects in the bulk and on the surfaces of amorphous silicon dioxide. Book of abstracts, p. 30.

#### **Transparent Conductive Materials (TCM-2010) 17-21 Oct. Crete, Greece**

L.Grigorjeva, D.Millers, F.Muktepavela, R.Zabels. Luminescence and mechanical properties of Al, In and Ti doped ceramics. Transparent Conductive Materials (TCM-2010) 17-21 Oct. Crete, Greece, ref.N.316 (oral).

#### **LU CFI 26<sup>th</sup> Scientific Conference, 2010, 17-19 Febr., Riga, Latvia**

1. M.Shorohov, L.Grigorjeva. Properties of TlBe crystals: dependence on growth methods. Abstracts, p.38 (oral).
2. Z.Alute, L.Grigorjeva, D.Millers. Luminescence of titanium, indium and zinc oxides doped with Eu<sup>3+</sup>. Abstracts, p.44. (poster).
3. V.Liepina. The synthesis and the study of luminescent properties of phosphorescent materials. Abstracts, p.50 (poster).
4. L. Tiļuga, J. Latvels, I. Muzikante, L. Skuja, Kārīņu sastāva un biežuma noteikšana nanometru diapazonā ar rentgenfluorescences metodi

#### **6<sup>th</sup> Laser Ceramic Symposium. International Symposium on Transparent Ceramics for Photonic Applications, 6-8 December, 2010, Munster, Germany**

L.Grigorjeva, D.Millers, K.Smits, W.Lojkowski, A.Swidarska-Stroda, W.Strek. Time-resolved luminescence characteristics of Ce and Nd doped YAG ceramics obtained by high pressure technique. Technical Digest, p.7 (oral).

#### **11th Europhysical Conference on Defects in Insulating Materials (EURODIM 2010). 12-116 July, 2010, Pecs, Hungary**

K.Smits, D.Millers, L.Grigorjeva. Short-lived defects in yttrium stabilized zirconia. Book of abstracts, p.84 (poster).

L.Grigorjeva, A.Krasnikov, V.V.Laguta, M.Nikl, S.Zazubovich. Luminescence and creation processes of electron centers in UV-irradiated YAlO<sub>3</sub> single crystals. Book of abstracts, p. 87.

**8th Internat Symposium "SiO<sub>2</sub>, Advanced dielectrics and related devices" 21-23  
June, 2010, Varenna, Italy**

K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono Lattice-interstitial oxygen exchange in amorphous SiO<sub>2</sub> studied by photoluminescence of <sup>18</sup>O-labeled interstitial oxygen molecules (Keynote talk). Abstract K-ESP1026.

**Doctoral thesis**

K.Smits. Luminescence of zirconia nanocrystals. LU, 2010

**Master thesis**

Z.Alute. Cinka oksīda, titāna oksīda un indija oksīda cieto šķīdumu optiskās īpašības. LU, 2010

L.Tiļuga. Daudzkanālu un vienkanāla metožu salīdzinājums rentgenfluorescences un optiskajā spektroskopijā., LU, 2010.

## SOLID STATE OPTICS LABORATORY

**Head of Laboratory, Professor, Dr. hab. phys. Anatoly Trukhin**

### Research area and Main Problems

The electronic excitations, intrinsic and impurity defect of the ordered materials (crystals) and the disordered material (optical glasses) are the main object of Solid State Optics Laboratory of DMP. Electronic structure and electronic processes of crystalline and glassy materials was studied. The localized states are studied in details. The properties of such “static” localized states determine almost all properties of glassy materials in their application in modern optoelectronics and telecommunication.

### Scientific staff

1. senior researcher, Dr. hab. Phys. A. Trukhin

### Cooperation

#### Russia

1. State University of Irkutsk, Institute of Geochemistry (Professors E.A. Radzhabov, A.I. Nepomnyaschikh)
2. L.F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia (Dr. T. Dyuzheva)
3. Fiber Optics Research Center of the Russian Academy of Sciences, 119333, Moscow, Russia (Prof. K. M. Golant)

#### Germany

University of Rostock, Germany (Professor, Dr. H.-J. Fitting)

#### USA

1. impactGlass research international, 3938 E. Tucson, AZ 85712, USA (Ph.D. D.L. Griscom)
2. Solid State Division, Oak Ridge National Laboratory. Oak-Ridge, TN. 37831 (Ph.D. Lynn A. Boatner)
3. University of Central Florida, CREOL (Professor, Dr.L.B.Glebov)

#### France

1. Universite Paris Sud, Orsay, Lab. Labo. Physico-Chimie des Solides UMR8648, (Dr.B. Poumellec)
2. Laboratoire H. Curien, UMR-CNRS 55516, Rue du Pr. B. Lauras, 42000 Saint-Etienne, France (Prof. Y. Ouerdan, Prof. A. Boukenter)

#### Italy

University of Palermo, Prof. Roberto Boscaino, Inst. Nazionale di Fisica della Mat.and Dipartimento di Scienze Fisiche ed Astronomiche dell 'Università,via Archirafi, 36, I-90123 Palermo,Italy

#### Estonia

Institute of Physics, University of Tartu, Estonia (Prof.C. Luschchik, Dr. R.Kink, Dr. Yu. Maksimov)

### Main results

#### LOCALIZED STATES IN SiO<sub>2</sub>-Si AND SiO<sub>2</sub>-Al GLASSES

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\*\*impactGlass research international, 3938 E. Grant Rd. #131, Tucson, AZ 85712, USA

Silica glass samples with extra silicon (artificial oxygen deficiency) and with aluminum (not accompanied with alkali ions) were studied. The luminescence properties are

compared in the range of temperature 15 -290 K of these two samples under excitation of ArF excimer laser (193 nm). In both samples the luminescence of oxygen deficient centers is detected. At 290 K in SiO<sub>2</sub>-Si the luminescence of lone twofold-coordinated silicon was detected with exponential decay for blue ( $\tau=10.3$  ms) and UV ( $\tau=4.5$  ns). Cooling of the sample leads to strong increase of luminescence intensity up to 80 K with little changes for lower temperatures. The component of exponential decay of the blue band is covered with much more stronger non-exponential decay of the blue band. In SiO<sub>2</sub>-Al the luminescent properties are identical to that of SiO<sub>2</sub>-Si with exception of exponential component with  $\tau=10.3$  ms. In the cases of both samples the decay of the blue band is faster than 10 ms, showing that living time of the center is limited in some way. However the decay of the UV band is much slower than 4.5 ns and it ranged in time of 2-5  $\mu$ s. Prolongation of the time of UV band is explained with recombination processes. Diminishing of the luminescence intensity with acceleration of decay time with increase of the temperature is correlated with thermally activated jumping of the self-trapped hole. So, the electronic processes of recombination luminescence are related to creation of a pair electron trapped on oxygen deficient center and nearest STE, after excitation of localized state with photon, and following recombination with emitting of the light corresponding to oxygen deficient center of luminescence. Al impurity, not accompanied with alkali ions increase concentration of localized states in the range of 6.4 eV on the same level as provide extra silicon.

### **LUMINESCENCE OF SILICON DIOXIDE- SILICA GLASS, $\alpha$ -QUARTZ AND STISHOVITE. A SHORT REVIEW**

A. N.Trukhin, K.Smits<sup>a</sup>, A. Sharakosky<sup>a</sup>, G. Chikvaidze<sup>a</sup>,  
T. I. Dyuzheva<sup>b</sup>, L. M.Lityagina<sup>b</sup>

<sup>a</sup>*Institute of Solid State Physics, University of Latvia, LV-1063 Riga, Latvia*

<sup>b</sup>*L.F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia*

Luminescence of different modifications of silicon dioxide – silica glass,  $\alpha$ -quartz crystal and dense, octahedron structured stishovite crystal are compared. Under x-ray irradiation of pure silica glass and pure  $\alpha$ -quartz crystal only luminescence of self-trapped exciton is detected, excitable only in the range of intrinsic absorption. Different luminescence was detected in stishovite. That luminescence is excitable also below optical gap and could not be ascribed to a self-trapped exciton. Under ArF laser excitation of pure  $\alpha$ -quartz crystal only luminescence of self-trapped exciton was detected under two-photon excitation. In silica glass and stishovite mono crystal spectrally mutually similar luminescence was detected under single-photon excitation of ArF laser. In silica glass that is luminescence of oxygen deficient center presented by so called twofold coordinated silicon center (L.N.Skuja et al, Solid State Commun., 50 (1984) 1069) as well as this center modified with unknown surrounding or localized states of silica glass (A.N.Trukhin, et al, J. Non-Crystalline Solids, 248 (1999) 49). In stishovite that luminescence was ascribed to some defect existing after crystal growth. For  $\alpha$ -quartz crystal similar to silica and stishovite luminescence could be obtained only by irradiation with lattice damaging source – dense electron beam at temperature below 80 K as well as neutron or  $\gamma$ -irradiation at 290 K. In spite of similarity between luminescence of these three materials – as received silica glass and stishovite mono crystal and irradiated  $\alpha$ -quartz crystal there are differences explained with specific of different materials.

The nature of luminescence excited in the transparency range of stishovite is ascribed to a defect existing in the crystal after growth. Similarity of the stishovite luminescence

with that of oxygen-deficient silica glass and induced by radiation luminescence of  $\alpha$ -quartz crystal presumes similar nature of centers in those materials.

## LUMINESCENCE OF LOCALIZED STATES IN SILICON DIOXIDE GLASS

A.N.Trukhin

*Solid State Physics Institute, University of Latvia*

The target is description of the properties of localized states in silica glass. It has been observed that laser light interaction with localized states of silica glass leads to creation of luminescence centers. Created luminescence centers, excited with laser light, provide intra-center luminescence of oxygen deficient centers (ODC). Beside these processes laser light can give rise to charge separation. Recombination of created electrons and holes leads to recombination luminescence, a cause of the prolongation of some fast in intra-center process luminescence. Evidence has been given that center of recombination at ODC sites involves an electron trap at the defect, whereas the hole is created as a self-trapped hole center. Recombination results in the localized state recovering its initial state with disappearance of the transiently created luminescence center. Such recombination is of luminescence of long duration in contrast with intra-center processes which are limited in time and we observe a shortened duration of such luminescence. Studies of temperature dependences of recombination luminescence intensity and decay show that intensive changes in these parameters take place in the known range of temperatures of self-trapped hole liberation. Decrease of measured intra-center luminescence duration is followed with less rapid decrease of recombination luminescence intensity. In some times the luminescence intensity even grows with heating, when decay kinetics is accelerated. As a rule, luminescence decay curves are non-exponential well described with stretched exponential function, showing first order fractal-kinetics.

It is argued that discovered localized states of silica glass are connected with structure other than tetrahedrons. In dense silicon dioxide crystal with rutile structure (stishovite) luminescence similar to ODC luminescence of silica glass has been found.

### Presentation at conferences

1. A.N.Trukhin, K.Smits, A. Sharakovsky, G. Chikvaidze, T. I. Dyuzheva , L. M.Lityagina, Luminescence of dense, octahedral structured crystalline silicon dioxide (stishovite). In: the International conference "Functional materials and nanotechnologies" 2010, Institute of Solid State Physics, University of Latvia, Riga, Latvia, p. 29.
2. A.N. Trukhin, Luminescence of localized states in silicon dioxide glasses, a short review, Book of Abstracts: 8 Symposium SiO<sub>2</sub> Advanced Dielectrics and Related Devices, Villa Monastero, Varenna (Lecco, Italy), June 21-23 , 2010, p.11.

### Scientific publication

3. A.N. Trukhin, A. Sharakovski, J. Grube and D.L. Griscom, Sub-band-gap-excited luminescence of localized states in SiO<sub>2</sub>-Si and SiO<sub>2</sub>-Al glasses, Journal of Non-Crystalline Solids, 356 (2010) 982-986.

## DEPARTMENT OF FERROELECTRIC PHYSICS

Head of Department Dr. phys. **V. ZAULS**

The Department of Ferroelectric Physics is engaged in basic and applied research and education activities focused on studies of functional ferroelectric oxide materials including theoretical modelling, synthesis, processing, and characterization. Synthesis and processing of bulk ceramics samples is based on solid state reactions of oxides and carbonates exploiting two-stage hot pressing technologies. Characterization methods include X-ray diffraction, atomic force microscopy, piezo-response force microscopy, electron scanning microscopy with EDX option, dielectric impedance and hysteresis measurement tools, ellipsometry and reflectometry techniques, adaptive optics, generation and measuring of wavefront errors in piezo-electric materials. Phase transitions and ordering effects in “ordinary” ferroelectrics and ferroelectric relaxors are studied along with new compositions, including multi-component systems containing admixtures and materials based on niobates and tantalates of alkaline and earth-alkaline elements without lead.

Theoretical research is focussed on quantum theories and computer simulations addressing the nano-meter scale structure of advanced complex oxides.

The main problems of research:

- Synthesis of ferroelectric ceramics and investigation of microstructure;
- Synthesis and characterization of piezoelectric ceramics without lead;
- Synthesis and properties of optical materials;
- Dielectric properties of ferroelectric perovskite relaxors;
- Polarization mechanisms and stability of the relaxor state in complex solid solutions;
- Dielectric response in lead ferrotantalate ceramics;
- Microstructure, dielectric and elastic properties of sodium-lithium niobate-tantalate ceramics;
- Elastic properties of ceramics derived from barium titanate;
- Intrinsic localized excitations in nonlinear lattices: heuristic explanation of the nature of polar nano-regions.

### Scientific staff: Doctors

1. Dr. phys. Eriks Birks
2. Dr. phys. emeritus Karlis Bormanis
3. Dr. habil. phys. Vilnis Dimza
4. Dr. phys. Eriks Klotins
5. Dr. habil. phys. Andris Krumins
6. Dr. phys. Maris Kundzins
7. Dr. phys. Anatoly Mishnev
8. Dr. habil. phys. Maris Ozolins
9. Dr. habil. phys. Andris Sternberg
10. Dr. phys. **Vismants Zauls**
11. Dr. habil. phys. Juris Zvirgzds

### Scientific staff: Magisters

1. Mg. chem. Maija Antonova
2. Mg. chem. Anna Kalvane
3. Mg. phys. Karlis Kundzins
4. Mg. Sc. ing. Ilze Smeltere

### PhD Students

1. Mg. phys. Marija Dunce
2. Mg. phys. Sergejs Fomins
3. Mg. phys. Varis Karitans

### Graduate Students

1. B. sc. Davis. Engers
2. B. sc. Eriks Klotins (junior)

### Technical staff

1. Ing. Maris Livins
2. Ing. Modris Logins
3. Ing. Alberts Tupulis

## Scientific Visits Abroad

Dr. phys. emeritus **Karlis Bormanis**

1. 2010 IEEE International Conference on Solid Dielectrics: Potsdam, Germany, July, 6 days.
2. 6<sup>th</sup> International Conference on Microwave Materials and their Applications „MMA-2010”: Warsaw, Poland, September, 8 days.
3. Lithuanian – Ukrainian – Polish Meeting on Ferroelectrics Physics: Vilnius, Lithuania, September, 5 days.

Mg. phys. **Marija Duncė**

1. Faculty of Physics, University of Vienna, Functional Materials, COST program: Vienna, Austria, April, 1 month.
2. International Conference Electroceramics XII: Trondheim, Norway, June, 6 days.
3. The 12-th International Conference „Advanced Materials and Technologies” and Summer School “European Doctorate in Physics and Chemistry of Advanced Materials”: Palanga, Lithuania, August, 5 days.
4. Lithuanian – Ukrainian – Polish Meeting on Ferroelectrics Physics: Vilnius, Lithuania, September, 5 days.

Mg. phys. **Sergejs Fomins**

1. SPIE / COS Meeting on Photonics Asia: Beijing, China, October, 3 days.

Mg. phys. **Varis Karitāns**

1. 5th European Meeting on Visual and Physiological Optics (*EMVPO*): Stockholm, Sweden, August, 3 days.

Dr. phys. **Maris Kundzins**

1. EFDA: Public Information Group Meeting: Riso National Laboratory for Sustainable Energy, Denmark, May, 2 days.

Dr. habil. phys. **Maris Ozolinsh**

1. 5th European Meeting on Visual and Physiological Optics (*EMVPO*): Stockholm, Sweden, August, 3 days.

Mg.Sc.ing. **Ilze Smeltere**

1. Scientists Exchange to Laboratory of Applied Physics, Pedagogical University of Krakow: Krakow, Poland, May, 15 days.
2. International Conference Electroceramics XII: Trondheim, Norway, June, 6 days.
3. The 12-th International Conference „Advanced Materials and Technologies” and Summer School “European Doctorate in Physics and Chemistry of Advanced Materials”: Palanga, Lithuania, August, 5 days.
4. Lithuanian – Ukrainian – Polish Meeting on Ferroelectrics Physics: Vilnius, Lithuania, September, 5 days.

Dr. habil. phys. **Andris Sternberg**

1. Meetings of the Consultative Committee for the EURATOM Specific Research and Training Programme in the Field of Nuclear Energy (Fusion), (CCE-FU): Brussels, January, 3 days; April, 3 days; September, 2 days; Barcelona, October, 3 days.
2. Nanotechnologies Safety for Success Dialogue: Brussels, February, 2 days; Berlin, September, 3 days.

3. The European Joint Undertaking for ITER and the Development of Fusion for Energy, Meeting of the Governing Board: Barcelona, January, 2 days; March, 2 days; June, 2 days; October, 4 days; December, 3 days.
4. Meetings of the High Level Group of EU Member States and FP7 Associated States on Nanoscience and Nanotechnologies: Brussels, July, 2 days; December, 2 days.
5. Russia/CIS/Baltic/Japan Symposium on Ferroelectricity RCBJSF-10: Yokohama, Japan, June, 5 days.
6. I Lithuanian – Ukrainian – Polish Meeting on Ferroelectrics Physics: Vilnius, Lithuania, September, 2 days.
7. Seminar “Synchrotron Radiation in Science and Technology- Bright Future at MAX-IV”: Otepa, Estonia, October, 3 days.
8. 36<sup>th</sup> International Conference on Micro & Nano Engineering: Genoa, Italy, September, 4 days.
9. Meeting of the EFDA Steering Committee: Madrid, March, 3 days; Lisbon, October, 2 days.
10. COST Domain Committee Meetings: Materials, Physics and Nanosciences: Brussels, March, 2 days; Berlin, September, 4 days.
11. MATERA: WP4+WP1&WP2 Board and Working Group Meetings: Rome, 3 days; Luxembourg, 3 days; Istanbul, 3 days.

Dr. phys. **Vismants Zauls**

1. MIND Project Review Meeting: Ljubljana, Slovenia, January, 3 days.
2. MIND Project Meeting at IEEE Conference: Brussels, Belgium, February, 3 days.
3. International Conference Electroceramics XII: Trondheim, Norway, June, 6 days.
4. I Lithuanian – Ukrainian – Polish Meeting on Ferroelectrics Physics: Vilnius, Lithuania, September, 5 days.

## **Cooperation**

### **Latvia**

1. Riga Technical University, Faculty of Material Science and Applied Chemistry (Prof. M. Knite, Juris Zavickis, Prof. A. Ozols, I. Timma).
2. Daugavpils University, Innovative Microscopy Centre (Dr. E. Tamanis).
3. University of Latvia, Institute of Chemical Physics (Dr. D. Erts).
4. Company “GroGlass SIA”.

### **Austria**

1. Faculty of Physics, University of Vienna, Functional Materials (Prof. Armin Fuith).

### **Czech Republic**

1. Institute of Physics, Academy of Sciences of the Czech Republic, Prague (Dr.phys. A. Dejneka, Prof. J. Petzelt, Dr. I. Hlinka, Dr. S. Kamba).

### **Denmark**

1. Ferroperm Piezoceramics A/S (Dr. W. Wolny).

### **Finland**

1. University of Oulu (Dr. M. Tyunina).

## **Italy**

1. Italian Institute of Technology, Corso Trento 21, Turin, Italy (Dr. Ilze Aulika).

## **Lithuania**

1. Vilnius University, Vilnius (Prof. J. Banys, Dr. R. Grigalaitis).

## **Poland**

1. Institute of Physics, Krakow Pedagogical University, Krakow (Prof. Cz.Kus, Dr. B.Garbarz – Glos, Prof. J.Suchanich).

## **Portugal**

1. University of Aveiro, Department of Ceramic and Glass Engineering Research Unit on Ceramic Materials, Aveiro (Prof. A. Kholkina).

## **Russia**

1. Ural State University, Ekaterinburg (Prof. V. Shur).
2. Volgograd State Architectural and Engineering University, Volgograd (Prof. A. Burkhanov).
3. Institute of Chemistry and Technology of Rare Elements and Minerals, Apatity (Prof. N.V. Sidorov, Dr. M.N. Palatnikov).
4. Russian Academy of Science, Dagestan Research Centre, Institute of Physics (Prof. Z.M. Omarov, Prof. S.N. Kallaev).
5. Dagestan State University (Prof. S.A. Sadikov).
6. Laboratory of Adaptive Optics, Moscow State University (Dr. A.Larichev).

## **Slovenia**

1. Jozef Stefan Institute, University of Ljubljana (Dr. M. Kosec, Dr. B. Malic).

## **Spain**

1. Laboratory of Optics, University of Murcia (Prof. P.Artal).

## **Main results**

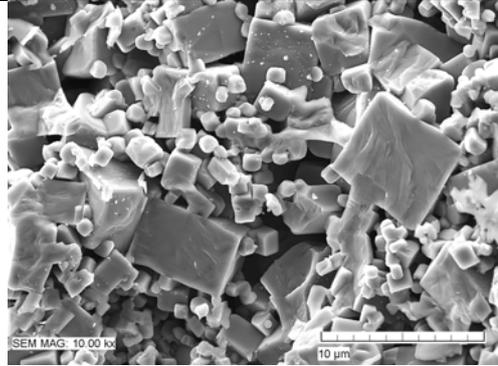
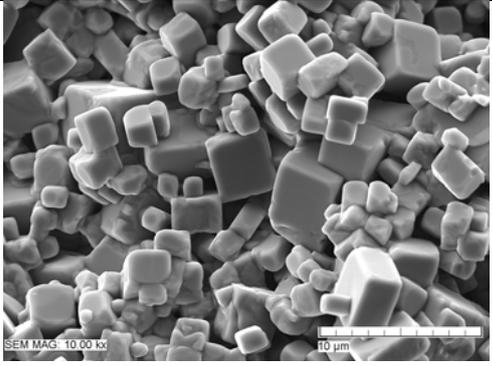
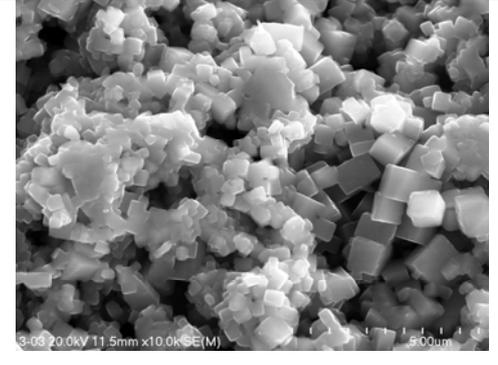
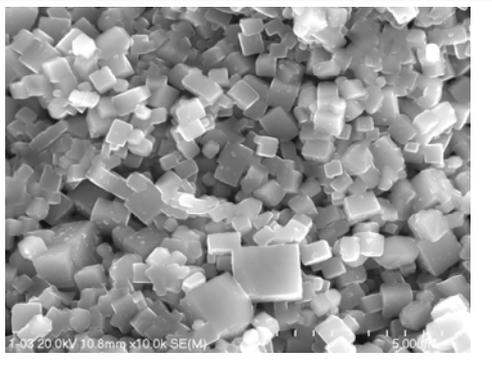
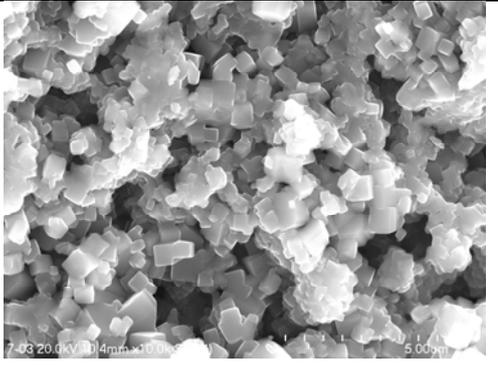
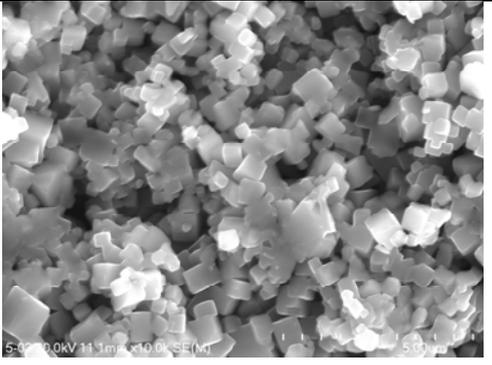
### **SYNTHESIS AND CHARACTERIZATION of MODIFIED $(K_{0.5}Na_{0.5})NbO_3$ LEAD-FREE PIEZOELECTRIC CERAMICS**

I.Smeltre, M.Antonova, A.Kalvane, and M.Livinsh

In the present work modified lead-free piezoelectric ceramics  $(1-x)(K_{0.5}Na_{0.5})Nb_{1-y}Sb_yO_3-xBaTiO_3$  ( $x=0.01, 0.02, 0.04$ ;  $y=0.04, 0.07$ ) were produced by conventional solid state sintering method. Manganese oxide  $MnO_2$  of 0.5 mol% was added as a sintering aid in order to promote the densification of the ceramic body. Ceramics were sintered at temperatures  $1150^\circ - 1240^\circ C$  for 4 h depending on x and y. The optimal temperature was determined from the temperature resulting in the highest sintering density as well as by taking into consideration sintering shrinkage of ceramic sample, and the highest values of dielectric permittivity. Density measurements detected by Archimedes method showed that  $BaTiO_3$  addition to the original composition increased the density of the ceramic sample reaching  $4.51 g/cm^3$  for KNNs4-1BT.

The fracture microstructure of the  $(1-x)(K_{0.5}Na_{0.5})Nb_{1-y}Sb_yO_3-xBaTiO_3$  ( $x=0.02, 0.04$ ;  $y=0.04, 0.07$ ) was investigated by SEM. Sb-substituted KNN ceramics have inhomogeneous microstructure with bimodal grain size distribution, the presence of

voids can be observed. Solid solutions with BaTiO<sub>3</sub> addition have smaller average grain sizes; the shape of grains is a little rounded. MnO<sub>2</sub> addition suppresses the grain growth even more. A little amount of liquid phase is also detected. The EDS made in the chosen microregions of the sample surface analysis confirmed the purity and experimentally assumed qualitative composition.

	
$(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3$	$(K_{0.5}Na_{0.5})Nb_{0.93}Sb_{0.07}O_3$
	
$0.98(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3-$ $0.02BaTiO_3$	$0.98(K_{0.5}Na_{0.5})Nb_{0.93}Sb_{0.07}O_3-$ $0.02BaTiO_3$
	
$0.96(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3-$ $0.04BaTiO_3$	$0.96(K_{0.5}Na_{0.5})Nb_{0.93}Sb_{0.07}O_3-$ $0.04BaTiO_3$

Dielectric measurements revealed that those complex solid solutions have diffuses phase transition and maximum values of dielectric permittivity  $\epsilon$  are lower than for starting material  $(K_{0.5}Na_{0.5})(Nb_{1-y}Sb_y)O_3$  ( $y=0.04, 0.07$ ) although  $\epsilon$  values at room temperatures are higher.

## **POLARIZATION MECHANISMS AND STABILITY OF RELAXOR STATE IN $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3\text{-PbTiO}_3$ SOLID SOLUTIONS**

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

Detailed research of dielectric polarization was done for two groups of solid solutions –  $0.4\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-(}0.6\text{-}x\text{)SrTiO}_3\text{-}x\text{PbTiO}_3$  (NBT-ST-PT 0.4/0.6- $x/x$ ) and  $(0.4\text{-}x)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-}0.6\text{SrTiO}_3\text{-}x\text{PbTiO}_3$  (NBT-ST-PT 0.4- $x/0.6/x$ ) – in concentration range from  $x=0.00$  to  $x=0.25$  and from  $x=0.00$  to  $x=0.35$  correspondingly. Electric field dependences of polarization  $P(E)$  (polarization hysteresis loops) were measured at different temperatures. From these dependences, temperature dependences of maximal polarization (at 20 kV/cm), remanent polarization and spontaneous polarization were obtained. For compositions with high concentrations of PT ( $x$ ), the observed remanent polarization reached values till  $\sim 25 \mu\text{C}/\text{cm}^2$ . In case of solid solutions NBT-ST-PT 0.4/0.6- $x/x$  in the concentration range from  $x=0.08$  to  $x=0.15$  and in case of solid solutions NBT-ST-PT 0.4- $x/0.6/x$  in the concentration range from  $x=0.08$  to  $x=0.30$  double hysteresis loops were observed in a definite temperature region, which indicates that it is possible to induce phase transitions between ferroelectric (FE) and relaxor states by applying electric field. For these compositions, temperature dependences of critical electric fields  $E_{k1}$  and  $E_{k2}$  were studied and corresponding phase transition temperatures were obtained.

The obtained results indicate that at low PT concentrations  $x$  the relaxor state persists in the whole temperature range and phase transition to FE state can't be induced. At higher concentrations (beginning from  $x=0.08$ ) there appears a possibility to induce phase transition to FE state by applying electric field. On further increasing of the concentration  $x$  FE state appears spontaneously at a definite temperature. These results are in good agreement with earlier studies of temperature-frequency dependences of dielectric  $\varepsilon(T,\omega)$  permittivity.

In order to extend the concept of stability of the relaxor state, phase diagrams of NBT-ST-PT-PMN and NBT-ST-PT-NN quadruple solid solutions were studied. Despite the complicated substitution structure in  $A^{2+}$  and  $B^{4+}$  sublattices of  $A^{2+}B^{4+}O_3$  perovskite, the increasing of NN ( $\text{NaNbO}_3$ ) and PMN ( $\text{PbMn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ ) concentration clearly demonstrates transfer from FE to relaxor state. Together with the published studies about the relaxor state in other compositions with perovskite structure, these results indicate that appearance of the relaxor state is connected with the ratio of energies of FE state and pearly inhomogeneous state.

## **STRUCTURE AND PHYSICAL PROPERTIES of $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-CdTiO}_3$ SOLID SOLUTIONS**

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

Crystallographic structure, dielectric and electro-mechanical properties, as well as thermal expansion of  $(1\text{-}x)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-}x\text{CdTiO}_3$  solid solutions were studied in concentration range till 80% of  $\text{CdTiO}_3$ .

It was observed that the structure of the solid solutions changes from rhombohedral to pseudocubic, tetragonal and orthorhombic as concentration of  $\text{CdTiO}_3$  increases. Thus there are three morphotropic phase boundaries in  $(1\text{-}x)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-}x\text{CdTiO}_3$ . The behaviour of ferroelectric properties is different in concentration ranges with different lattice symmetry. However there is still some overlapping. The dispersion of dielectric permittivity, characteristic for relaxor ferroelectrics, is observed not only in concentration range of macroscopically cubic, but also in the range of tetragonal phase. The relaxor ferroelectrics behaviour of the

composition  $x=0.40$  can be related to the observed weak tetragonality ( $c/a=1.001$ ) of this composition. The declining of thermal expansion temperature dependence  $dl/l(T)$  above the dielectric permittivity maximum temperature, which is characteristic for relaxor ferroelectrics, is also observed in composition range from  $x=0.40$  till  $x=0.60$ . At the same time, for compositions  $x=0.50$  and  $x=0.60$ , this declining results in phase transition to ferroelectric state at temperatures, which correspond to maximum of dielectric permittivity. Similarly, the composition  $x=0.60$ , located in the concentration range of orthorhombic structure, preserves phase transition behaviour, characteristic for compositions with tetragonal phase.

## ELASTIC PROPERTIES OF BARIUM ZIRCONATE TITANATE CERAMICS

B. Garbarz-Glos\*, K. Bormanis, A. Kalvane, A. Budziak\*\*, and W. Śmiga\*

The barium zirconium titanate samples  $BaZr_xTi_{1-x}O_3$  were prepared by conventional ceramic technology. Microstructure and material constants of polycrystalline ferroelectric materials  $BaZr_xTi_{1-x}O_3$  for  $0 \leq x \leq 0.35$  were investigated to determine their dependence on zirconium concentration. The performed measurements show that the material is chemically homogeneous. The examined samples are good quality, the grains are well shaped and there is a very small amount of a glassy phase. Material constants: the Young's modulus  $E$ , the shear modulus  $G$  and the Poisson's ratio  $\nu$  were determined by ultrasonic method. The measurements were carried out with the INCO -VERITAS Ultrasonic Measuring Set UZP-1. Material constants were calculated from the longitudinal and transverse ultrasonic wave propagation velocity and the apparent density of the samples, using the following formulas:

$$E = V_L^2 \cdot \rho (1 + \nu) (1 - 2\nu) / (1 - \nu), \quad (1)$$

$$G = V_T^2 \rho, \quad (2)$$

$$\nu = (V_L^2 - 2V_T^2) / (2V_L^2 - 2V_T^2), \quad (3)$$

where  $E$  is Young's modulus,  $G$  – shear modulus,  $\nu$  - Poisson's ratio,  $\rho$  - density,  $V_L$  – velocity of the longitudinal wave,  $V_T$  - velocity of the transverse wave.

The investigation of elastic properties was performed in order to determine the effect of the load of material on its properties, thus on the durability of the devices made of this material.

The ultrasonic wave velocity and the values of both Young's modulus and the shear modulus are the highest for  $BaZr_{0.30}Ti_{0.70}O_3$  sample ( $V_L = 5980.9$  m/s,  $V_T = 3550.6$  m/s,  $E = 163.88$  GPa and  $G = 66.73$  GPa). It has been shown that the Young's modulus value increases with the increase of zirconium concentration in  $BaTiO_3$ . The dependence of shear modulus  $G$  on sample composition is similar to the respective dependences of Young's modulus  $E$  whereas the Poisson's ratio  $\nu$  decreases with the increase in zirconium concentration. The lowest value has been found for  $BaZr_{0.275}Ti_{0.725}O_3$ .

\*Institute of Physics, Pedagogical University, Podchorążych 2, 30-084 Krakow, Poland

\*\*The H.Niewodniczanski Institute of Nuclear Physics Polish Academy of Sciences

## DESCRIPTION OF RELAXOR STATE in $Na_{1/2}Bi_{1/2}TiO_3$ - $SrTiO_3$ - $PbTiO_3$ SOLID SOLUTIONS

M. Dunce, E. Birks, M Kundzinsh, and M. Antonova

Traditionally, for description of dielectric properties of ferroelectric relaxors there is assumed temperature dependence of static dielectric permittivity, which is characterized by its continuous increasing, if temperature is decreased. Another traditional assumption

is continuous distribution function of relaxation times  $g(\ln\tau)$  in range between  $\tau_{\min}$  and  $\tau_{\text{cut-off}}$ , where temperature dependence of  $\tau_{\text{cut-off}}$  follows Vogel-Fulcher law, diverging at a definite temperature  $T_f < T_m$  ( $T_m$  – temperature of maximum of dielectric permittivity).

This interpretation is based on relaxation of polar microregions in multiwell potential in presence of external electric field. The divergence of relaxation times or freezing is explained as result of unlimited increasing of interaction between these microregions. Among behaviour, inherent for such concept, there are appearance of maximum in temperature dependence of dielectric permittivity and its temperature shift, depending on frequency of measuring field. Since such the relaxation mechanism does not contribute to dielectric permittivity at  $T < T_f$ , other mechanisms are needed to explain the experimentally stated relaxation at low temperatures.

In this work a detailed study of temperature-frequency dependences of dielectric permittivity was done for  $(1-x-y)\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3-x\text{SrTiO}_3-y\text{PbTiO}_3$  system of solid solutions, as well as for  $(1-x)\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3-x\text{PbTiO}_3$  ( $x=0.1$ ),  $\text{Pb}_{1-x}\text{La}_x(\text{Zr}_{0.65}\text{Ti}_{0.35})_{1-x/4}\text{O}_3$  ( $x=0.09$ ), which exhibit relaxor properties. It was shown that the behaviour of relaxation is the same both above, and below  $T_f$ . From such a point of view it follows that real freezing in ferroelectric relaxors does not occur, instead continuous increasing of  $\tau_{\text{cut-off}}$  is expected, if temperature decreases in all temperature range below maximum of dielectric permittivity. Temperature dependence of the parameters, describing relaxation, introduced earlier for low temperature region, contains information about static dielectric permittivity and  $\tau_{\text{cut-off}}$ . As well as previously developed models, this concept for the present time does not explain the nature of distribution of relaxation times.

## **MICROSTRUCTURE, DEFECTS AND ELASTIC PROPERTIES OF SODIUM NIOBATE CERAMIC HIGH-PRESSURE SOLID SOLUTIONS**

K. Bormanis, M. Palatnikov\*, O. Shcherbina\*, V. Efremov\*, N. Sidorov\*, and A. Salak\*\*

The structure of perovskite  $\text{Li}_x\text{Na}_{1-x}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$  solid solutions (SS) allow for different structural deformations, defects determining complexity and diversity of properties, numerous phase transitions including those of ferroelectric and antiferroelectric nature, and presence of morphotropic regions, all that, particularly in ceramic samples, being the reason of internal stress manifested by elastic properties of polycrystalline specimens. Elastic properties reflecting atomic interactions and macroscopic anisotropy are important in solid state studies.

Synthesis of perovskite sodium niobate solid solutions under high pressure increases microscopic homogeneity and broadens the range of solubility of the components of restricted solid solutions. At hot-pressing synthesis of  $\text{Li}_{0.17}\text{Na}_{0.83}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$  ceramics the increase of temperature is found to lower the value of the elasticity modulus regardless to the content of tantalum.

The reason is likely related to features of recrystallisation of disordered hot-pressed  $\text{Li}_{0.17}\text{Na}_{0.83}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$  SS under high pressures and, consequently, spoiling adhesion between grain boundaries because of a large number of micro-fractures being created.

The features of microstructure of hot-pressed perovskite solid solution ceramics of  $\text{Li}_x\text{Na}_{1-x}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$  ( $x = 0.12, 0.17$ ;  $y = 0, y \geq 0.5$ ) have not been earlier studied as functions of the temperature of synthesis and composition. The  $\text{Li}_x\text{Na}_{1-x}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$  SS are mainly comprised of isomorphous grains the shape elements of which complying with the perovskite structure allow for existence rhombic and rhombohedral symmetry of the elementary cell.

The observed decrease of the modulus of elasticity of high-pressure  $\text{Li}_{0.17}\text{Na}_{0.83}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$  solid solutions with increasing the baking temperature is assumed

to be related to conditions of re-crystallisation of disordered solid solutions at synthesis under high pressure.

\* Institute of Chemistry, Kola Science Centre RAS, Apatity, Murmansk Region, Russia.

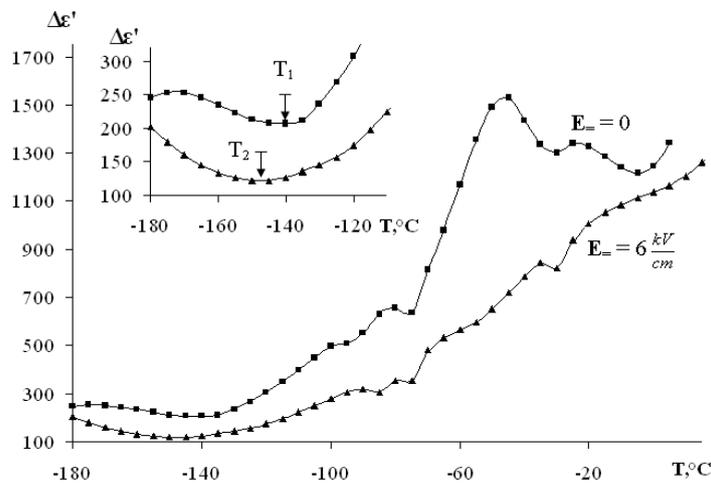
\*\* Department of Ceramics and Glass Engineering / CICECO, University of Aveiro, Aveiro, Portugal.

## THE EFFECT OF BIAS FIELD ON DIELECTRIC RESPONSE IN LEAD FERROTANTALATE CERAMICS

K. Bormanis, A.I. Burkhanov\*, A.I. Vaingolts\*, and A. Kalvane

Lead ferrotantalate  $\text{PbFe}_{1/2}\text{Ta}_{1/2}\text{O}_3$  is known as ferroelectric with a broad phase transition an anti-ferromagnetic ordering in which may occur at low temperatures [1].

The presently reported study of dielectric properties of the  $\text{PbFe}_{1/2}\text{Ta}_{1/2}\text{O}_3$  ceramics at low and infra-low frequencies is made a wide range of temperatures under a bias field.



Behaviour of the effective depth of dielectric permittivity  $\Delta\epsilon(T)$  ( $\Delta\epsilon' = \epsilon'_{1\text{Hz}} - \epsilon'_{1\text{kHz}}$ ) over a range of temperatures is illustrated in Figure. The inset shows behaviour of the parameter in the thermal range where anti-ferromagnetic ordering occurs (the Neel temperature  $T_N$ ).

Applied field of  $E = 6$  kV/cm enhances broadening of  $\epsilon'(T)$  maximums and shifts the maximums to higher temperatures.

Additional anomalies of the dielectric response are revealed at  $T < T_m$ . At bias field of 6 kV/cm applied to the sample the minimum of the  $\Delta\epsilon'(T)$  curve shifts considerably to a lower temperature ( $T_1$  and  $T_2$  respectively). Such anomalous behaviour of the dielectric response around  $T_N$  most likely is due to magneto-electric interaction rather than “freezing” of the domain structure as often observed in ordinary ferroelectrics at low temperatures in which case  $T_1$  would shift to a higher temperature.

[1] Yu.N. Venevtsev, V.V. Gagulin, and V.N. Ljubimov. Ferrimagnetics. Moscow, Science, 1982 (in Russian).

\* Volgograd State Architectural and Engineering University, Volgograd, Russia.

## METHODS OF COMPENSATING EYE MOVEMENTS IN ADAPTIVE OPTICS SYSTEMS

Varis Karitans\*, and Maris Ozolinsh\*

Optical distortions or aberrations are inherent to both atmosphere of the Earth and a human eye. What regards to vision science, these aberrations significantly contribute to lowered quality of retinal imaging. However, the aberrations aren't the only obstacle preventing sharp retinal imaging. Eye movements must also be taken into account. Eye movements prevents the computer from calculating aberrations correctly. Secondly, retinal images are viewed under large magnification thus sharpness of small retinal

features is subject to tiny movements of an eye. Thus it is necessary to track eye movements and apply some methods in order for eye movements to be compensated.

Current methods for compensation of eye movements involve use of retinal scanners which track direction of the reflected laser beam dithered to a specific retinal structure. Galvanometric mirrors are then driven by error signals generated according to measurements of retinal scanners. Principle of working has been widely described already [1]. We work on developing novel methods for compensating eye movements. Basics of our method is use of linear profile sensor s9226 provided by *Hamamatsu* [2] (see Fig. 1). The sensor measuring the reflection from the anterior surface of a cornea. Microcontroller then calculates the direction of the incident beam and the necessary corrections in optical set-up to compensate these eye movements. Shortcoming of this system is that corrections are made by stepper motors working at low speed only few deg/s. To avoid optical noise very narrow band-pass optical filter must be placed in front of the sensor.

We design another method which is essentially the same as that described previously except that eye position is calculated from the measured electrooculography (EOG) signals. A significant problem in this case would be electrical noises generated within the human body and the environment thus requiring filtering noises at different frequencies. In addition, EOG is a rough method of estimating position of an eye (few tenths of degree).

[1] D. X. Hammer, R.D. Ferguson, N.V. Iftimia, T. Ustun, S.A. Burns. Tracking Adaptive Optics Scanning Laser Ophthalmoscope (TAOSLO). – Invest Ophthalmol Vis Sci E-abstract, 46, pp. 3550.

[2] Internet: [http://sales.hamamatsu.com/assets/pdf/parts\\_S/s9226-03\\_kmpd1121e01.pdf](http://sales.hamamatsu.com/assets/pdf/parts_S/s9226-03_kmpd1121e01.pdf)

\* ISSP and Department of Optometry and Vision Science, University of Latvia

## **INFLUENCE OF OCULAR ABERRATIONS ON THE DIAMETER OF RETINAL BLOOD VESELS**

Varis Karitans, Maris Ozolinsh, Sergejs Fomins,  
Aiga Svede\*, Gunta Krumina\*, and Nikita Georgievich Iroshnikov\*\*

Lower-order and higher-order ocular aberrations influence not only visual perception but also appearance of retinal images. We suggest that the diameter of blood vessels may differ for various patterns of aberrations based on how the maps of point spread functions are orientated to these vessels. We test our hypothesis by a star chart simulation method and by using simulating aberrations in a real image of a living retina. We observed that broadening of the blood vessels due to ocular aberrations depend not only on the relative orientation of the wavefront but also on the actual width of them. The change in the diameter ratio is clinically significant and is comparable to changes in the A/V ratio due to various retinal and systemic pathologies.

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## **MULTISPECTRAL COLOR ANALYSIS FOR QUANTITATIVE EVALUATION OF PSEUDOISOCROMATIC COLOR DEFICIENCY TESTS**

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Multispectral color analysis was used for spectral scanning of Ishihara and Rabkin color deficiency test book images. It was done using tunable liquid-crystal LC filters

built in the Nuance II analyzer. Multispectral analysis keeps both, information on spatial content of tests and on spectral content. Images were taken in the range of 420-720nm with a 10nm step. We calculated retina neural activity charts taking into account cone sensitivity functions, and processed charts in order to find the visibility of latent symbols in color deficiency plates using cross-correlation technique. In such way the quantitative measure is found for each of diagnostics plate for three different color deficiency carrier types - protanopes, deutanopes and tritanopes. Multispectral color analysis allows to determine the CIE xyz color coordinates of pseudoisochromatic plate design elements and to perform statistical analysis of these data to compare the color quality of available color deficiency test books.

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## Lectures on Conferences

**LU Cietvielu fizikas institūta 26. Zinātniskā konference.**

**Rīga, 2010. gada 17. - 19. februāris.**

**26<sup>th</sup> Scientific Conference, Institute of Solid State Physics, University of Latvia.**

**Riga, Latvia, February 17–19, 2010.**

1. D. Engers, Ē. Klotiņš. Temperatūras ietekme uz ķīmiski sakārtotiem polāriem nanoapgabaliem relaksoru segnetoelektriķu  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$  (PMN) kristālos. Temperature Development of Chemically Ordered Polar Nanoregions in Relaxor Ferroelectric  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$  (PMN). Tēzes, 33. lpp.
2. I. Smeltere, M. Antonova, A. Kalvāne, M. Līviņš, V. Zauls. Modificēta KNN cietā šķīduma sintēze un dielektriskās īpašības. Synthesis and Dielectric Properties of Modified KNN Solid Solution. Tēzes, 39. lpp.
3. M. Dunce, M. Antonova, M. Kundziņš, Ē. Birks. Relaksoru stāvokļa apraksts PMN-ST-PT cieto šķīdumu sistēmā. Description of Relaxor State in PMN-ST-PT System of Solid Solutions. Tēzes, 40. lpp.
4. R. Taukulis, V. Zauls, M. Kundziņš. Submikrometru pārvietojumu mērīšanas sensora uzbūve un pielietojums pjezodeformāciju pētījumiem. Sub-Micron Accuracy Displacement Probe for Direct Piezoelectric Response Measurements. Tēzes 54. lpp.
5. S. Fomins, U. Atvars. Subjektīvā oponento krāsu noteikšana. Opponency in Subjective Adjustment Experiment. Tēzes 61. lpp.
6. I. Gvardina, A. Kristiņš, J. Melderis, G. Pikurs, J. Zvirgzds. Gaisa kompresoru stacijas attālinātas vadīšanas un kontroles sistēma. System for Remote Management and Control of Air Compressor Station. Tēzes 62. lpp.
7. A. Šternbergs. Mūsdienu materiālzinātnes problēmas un risinājumi. Challenging Trends and Cutting-Edge Issues in Materials Sciences. Tēzes 68. lpp.
8. V. Karitāns, M. Ozoliņš. Lineārs profila sensors acs stāvokļa detektēšanai. Linear Profile Sensor for Detecting Position of an Eye. Tēzes 83. lpp.
9. S. Fomins, M. Ozoliņš. Krāsu redzes testu multispektrālā analīze. Multispectral Analysis of Colour Deficiency Tests. Tēzes 84. lpp.

**Functional Materials and Nanotechnologies 2010.**

**Riga, Latvia, March 16-19, 2010.**

1. E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, and D. Engers. Temperature Development of Chemically Ordered Nanoregions in Relaxor Ferroelectric  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$  (PMN). Book of Abstracts, p. 41.
2. M. Dunce, E. Birks, M. Antonova, and M. Kundzins. Description of Relaxor State in  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - $\text{SrTiO}_3$ - $\text{PbTiO}_3$  System of Solid Solutions. Book of Abstracts, p. 53.

3. G. Chikvaidze, V. Zauls, M. Gadzyra, V. Osokin, V. Panibratskiy, and V. Solonenko. The Influence of Nonstoichiometric Silicon Carbide Nanopowder on the Reducing Efficiency of Silicon for Solar Cells. Book of Abstracts, p. 67.
4. J. Suchanicz, A. Finder, K. Konieczny, I. Jankowska-Sumara, B. Garbarz-Glos, R. Bujakiewicz-Koronska, K. Pytel, M. Antonova, I. Smeltere, and A. Sternberg. Electric Properties of  $\text{Na}_{0.5}\text{K}_{0.5}(\text{Nb}_{1-x}\text{Sb}_x)\text{O}_3+0.5\text{MnO}_2$  Ceramics ( $x=0.04, 0.05$  and  $0.06$ ). Book of Abstracts, p. 96.
5. I. Smeltere, M. Antonova, M. Livinsh, and B. Garbarz-Glos. Synthesis and Characterization of Lead-Free  $1-x(\text{K}_{0.5}\text{Na}_{0.5})\text{Nb}_{1-y}\text{Sb}_y\text{O}_3-x\text{BaTiO}_3$ . Book of Abstracts, p. 97.
6. W. Smiga, A. Budziak, M. Antonova, M. Livinsh, and B. Garbarz-Glos. Effects of Axial Pressure on the Electrical Properties of  $\text{Li}_{0.06}\text{Na}_{0.94}\text{NbO}_3$  Ceramic. Book of Abstracts, p. 104.
7. S. Bagdzevicius, R. Grigalaitis, J. Banyns, A. Sternberg, and K. Bormanis. Broadband Dielectric Investigation of Sodium Potassium Niobate With 10% Antimony Substitution. Book of Abstracts, p. 107.
8. I. Smeltere, K. Bormanis, A.V. Sopit, and A.I. Burkhanov. Dielectric Response in  $(\text{K}_{0.5}\text{Na}_{0.5})(\text{Nb}_{1-x}\text{Sb}_x)\text{O}_3+0.5\text{mol}\%\text{MnO}_2$  Ceramics to Weak Sinusoidal Fields of Low and Infra-Low Frequencies. Book of Abstracts, p. 108.
9. K. Bormanis, A.I. Burkhanov, A.I. Vaingolts, and A. Kalvane. The Effect of Bias Field on Dielectric Response in Lead Ferrotantalate Ceramics. Book of Abstracts, p. 109.
10. B. Garbarz-Glos, K. Bormanis, A. Kalvane, A. Budziak, and W. Šmiga. Elastic Properties of Barium Zirconate Titanate Ceramics. Book of Abstracts, p. 110.
11. M.N. Palatnikov, V.A. Sandler, V.V. Efremov, N.V. Sidorov, and K. Bormanis. Dielectric Properties and Conductivity of Ferroelectric  $\text{Li}_x\text{Na}_{1-x}\text{Ta}_{0.1}\text{Nb}_{0.9}\text{O}_3$  Solid Solutions. Book of Abstracts, p. 111.
12. M. Palatnikov, V. Efremov, O. Makarova, N. Sidorov, and K. Bormanis. Dielectric and Elastic Parameters of  $\text{Li}_x\text{Na}_{1-x}\text{Ta}_{0.1}\text{Nb}_{0.9}\text{O}_3$  Ferroelectric Solid Solution Ceramics. Book of Abstracts, p. 112.
13. M. Palatnikov, N. Sidorov, I. Biryukova, and K. Bormanis. Growth of Lithium Niobate Single Crystals from Granulated Charge. Book of Abstracts, p. 113.
14. M. Palatnikov, O. Shcherbina, A. Frolov, P. Chufyrev, N. Sidorov, and K. Bormanis. Physical Properties and Structure of Niobium Pentoxide Ceramics Treated by Concentrated Light Flow. Book of Abstracts, p. 114.
15. N.V. Sidorov, E.A. Antonicheva, A.V. Syuy, M.N. Palatnikov, and K. Bormanis. Kinetics of Photorefractive Light Scattering in  $\text{LiNbO}_3:\text{Cu}[0.015\% \text{ mass}]$  and  $\text{LiNbO}_3:\text{Zn}[0.5\% \text{ mass}]$  Single Crystals. Book of Abstracts, p. 115.
16. V.M. Voskresenskiy, O.R. Starodub, N.V. Sidorov, M.N. Palatnikov, and K. Bormanis. Modelling of Cluster Formation in Optically Nonlinear Lithium Niobate Crystal. Book of Abstracts, p. 116.
17. V. Zauls, G. Chikvaidze, M. Gadzyra, A. Viksna, V. Osokin, V. Panibratskiy, and V. Solonenko. Electron Beam Refining of Solar Silicon. Book of Abstracts, p. 136.
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1. V. Karitans, and M. Ozolinsh. Methods of Compensating Eye Movements in Adaptive Optics Systems. Abstract book, p. 35.

2. A. Stepanovs, G. Ikaunieks, K. Ozola, and M. Ozolinsh. Influence of Tinted Spectacle Lenses on Intraocular Stray Light. Abstract book, p. 18.

### **Electroceramics XII**

#### **Trondheim, Norway, June 14-16, 2010.**

1. Ilze Smeltere, Maija Antonova, Maris Livinsh, Marija Duncce, Vismants Zauls. Effect of  $\text{MnO}_2$  and  $\text{WO}_3$  Addition on Sintering and Properties of Lead-Free KNN Ceramics. Abstract No 144.
2. Marija Duncce, Reinis Taukulis, Eriks Birks, Ilze Aulika, Armin Fuith. Thermal Expansion and Electromechanical Properties in  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - $\text{SrTiO}_3$ - $\text{PbTiO}_3$  Solid Solutions. Abstract No 156.

### **Russia/CIS/Baltic/Japan Symposium on Ferroelectricity RCBJSF-10.**

#### **Yokohama, Japan, June 20-24, 2010.**

1. Marija Duncce, Eriks Birks, Maija Antonova, and Andris Sternberg. Phase Transitions in Modified  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - $\text{SrTiO}_3$  Solid Solutions. Abstract book, Oa-02, 20.

### **34th European Conference on Visual Perception,**

#### **Lausanne, Switzerland, June 22-26, 2010.**

1. S. Fomins, N. Rileyeva-Piskura, and M. Ozolinsh. Strength Judgment of Filling-in Color Aftereffect Illusion for Different Shapes. Abstracts: Perception 39, p. 86.
2. G. Ikaunieks, A. Stepanovs, and M. Ozolinsh. Effect of Yellow Tinted Spectacle Lenses on Intraocular Straylight. Abstracts: Perception 39, p. 169.

### **International Conference „Laser – 50”, Daugavpils, Latvia, June 28 – 29, 2010.**

1. V. Karitans, and M. Kuibida. Influence of Optical Aberrations of an Eye on Resolution of Dichoptic Images. Abstract book, p. 23.

### **2010 IEEE International Conference on Solid Dielectrics.**

#### **Potsdam, Germany, July 4-9, 2010.**

1. K. Bormanis, A. Kalvane, A.I. Burkhanov, and Y.V. Kochergin. Low Frequency Nonlinearity in Layered Ferroelectrics  $\text{BaBi}_2\text{Nb}_2\text{O}_9$  and  $\text{SrBi}_2\text{Ta}_2\text{O}_9$ . Proceedings, p. 805-807.

### **11th Europhysical Conference on Defects in Insulating Materials (EURODIM 2010). Pecs, Hungary, July 12-16, 2010.**

1. K. Bormanis, A.I. Burkhanov, S.V. Mednikov, Luu Thi Nhan, and A. Kalvane. Relaxor Properties of Barium-Strontium Niobate Ceramics. Book of Abstracts, p. 94.
2. M. Palatnikov, O. Shcherbina, V. Efremov, N. Sidorov, A. Salak, and K. Bormanis. Microstructure, Defects and Elastic Properties of Sodium Niobate Ceramic High-Pressure Solid Solutions. Book of Abstracts, p. 133.
3. M. Palatnikov, O. Shcherbina, A. Frolov, N. Sidorov, and K. Bormanis. Formation of Micro- and Nano-Defects of Fractal Type in Niobium Pentoxide Ceramics and Their Effects on Thermal Expansion. Book of Abstracts, p. 134.
4. E.A. Antonicheva, A.V. Syuy, N.V. Sidorov, M.N. Palatnikov, and K. Bormanis. Kinetics of Photorefractive Light Scattering in Stoichiometric  $\text{LiNbO}_3$  Single Crystals Grown From Melt Containing 58.6 Mole % of  $\text{Li}_2\text{O}$ . Book of Abstracts, p. 198.

### **19<sup>th</sup> International Symposium on the Applications of Ferroelectrics;**

#### **10<sup>th</sup> European Conference on the Applications of Polar Dielectrics (ISAF-ECAPD-2010). Edinburgh, UK, August 9-12, 2010.**

1. M. Palatnikov, N. Sidorov, and K. Bormanis. Mechanisms of Solid Phase Interaction at Synthesis of the Mixture for Lithium Niobate. Abstracts, p. 110.

2. K. Bormanis, A.I. Burkhanov, Y.V. Kochergin, and A. Kalvane. Dielectric Response of Barium-Strontium Niobate-Tantalate Ferroelectric Ceramics. Abstracts, p. 111.
3. S.N. Kallaev, Z.M. Omarov, K. Bormanis, and S.A. Sadikov. Features of Thermal Properties of Ferroelectric PLZT Ceramics in the Region of Phase Transition. Abstracts, p. 111.

**5th European Meeting on Visual and Physiological Optics (EMVPO), Stockholm, Sweden, August 22 – 24, 2010.**

1. V. Karitans, and M. Ozolinsh. Simulating Retinal Vascular Disorders by Imposing Different Types of Higher-order Aberrations on Retinal Images. Abstract book, p.58.
2. M. Ozolinsh, I. Martín, D. Lauva, and R. Kashtaljana. Colour Vision Hyperacuties. Abstract book, p.36.

**The 12-th International Conference „Advanced Materials and Technologies” and Summer School “European Doctorate in Physics and Chemistry of Advanced Materials”.**

**Palanga, Lithuania, August 27-31, 2010.**

1. S. Fomins, and M. Ozolinš. Multispectral Analysis of Color Deficiency Tests and Modeling of Cones Influence on Perception of Color. Abstract book, p. 38.
2. K. Luse, M. Ozolins, and V. Karitans. Influence of Location of Retro Reflective Signs on Recognition of Pedestrian in Reduced Visibility Conditions. Abstract book, p. 41.
3. M. Duce, E. Birks, M. Antonova and M. Kundzinsh. Phase Transitions in Modified  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3$  Solid Solutions. Abstracts, p. 80.
4. Ilze Smeltere, Maija Antonova, Anna Kalvane, Oskars Grigs, and Maris Livinsh. The Effect of Dopants on Sintering and Microstructure of Lead-Free KNN. Abstracts, p. 84.
5. M. Ozolinsh, R. Kashtaljana, and I. Martín. Eye Optical Power Dispersion Impact on Colour Stimuli Perception. Abstract book, p. 108.

**6<sup>th</sup> International Conference on Microwave Materials and their Applications „MMA-2010”. Warsaw, Poland, September 1-3, 2010.**

1. N. Sidorov, M. Palatnikov, D. Evstratova, and K. Bormanis. Impact of Laser Radiation on Photo-Refractive Lithium Niobate Single Crystal. Book of Abstracts, p. 126.

**I Lithuanian – Ukrainian – Polish Meeting on Ferroelectrics Physics. Vilnius, Lithuania, September 12-16, 2010.**

1. J. Suchanicz, K. Pytel, K. Konieczny, M. Sokolowski, A. Finder, M. Antonova, and A. Sternberg. Influence of Electromechanical Fields on Dielectric Properties of PLZT-x/65/35 Ceramics (x=6 and 7). Programme & Abstracts, p. 45.
2. M. Palatnikov, O. Shcherbina, N. Sidorov, and K. Bormanis. Effects of VTE Treatment on Composition of Lithium Tantalate Single Crystals. Programme & Abstracts, p. 52.
3. K. Bormanis, A.I. Vaingolts, A.I. Burkhanov, and A. Kalvane. Dielectric Response in Lead Ferrotantalate With Respect to Bias Field Effect. Programme & Abstracts, p. 53.
4. W. Šmiga, B. Garbarz-Glos, M. Livinsh, and A. Kalvane. Structural and Electric Properties of Sodium Lithium Niobate Ceramic Solid Solution  $\text{Li}_{0.08}\text{Na}_{0.92}\text{NbO}_3$ . Programme & Abstracts, p. 54.
5. J. Suchanicz, G. Stopa, K. Pytel, K. Konieczny, A. Finder, M. Antonova, and A. Sternberg. Electrical Transport Properties of Lead-Free  $(\text{Na}_{0.5}\text{Bi}_{0.5})_{(1-x)}\text{Ba}_x\text{Zr}_{0.04}\text{Ti}_{0.96}\text{O}_3$  Ceramics (x=0, 0.06, 0.085, 0.1). Programme & Abstracts, p. 55.
6. R. Bujakiewicz-Koronska, L. Hetmanczyk, B. Garbarz-Glos, A. Budziak, J. Koronski, J. Hetmanczyk, M. Antonova, and A. Kalvane. Investigations of Low Temperature

- Phase Transitions in BiFeO<sub>3</sub> Ceramic by Infrared Spectroscopy. Programme & Abstracts, p. 58.
7. M. Duce, E. Birks, M. Antonova, K. Kalnins, and M. Kundzinsh. Structure and Physical Properties of Na<sub>1/2</sub>Bi<sub>1/2</sub>TiO<sub>3</sub>-CdTiO<sub>3</sub> Solid Solutions. Programme & Abstracts, p. 69.
  8. Barbara Garbarz-Glos, Karlis Bormanis, and Dorota Sitko. Effect of Zr<sup>+4</sup> Doping on the Electrical Properties of BaTiO<sub>3</sub> Ceramics. Programme & Abstracts, p. 71.
  9. Ilze Smeltere, Anna Kalvane, Maija Antonova, Maris Livinsh, Barbara Garbarz-Glos, and Vismants Zauls. Effect of Tantalum Content on Synthesis of Lead-Free Piezoelectric KNN Ceramics. Programme & Abstracts, p. 91.
  10. R. Grigalaitis, J. Banys, E. Tornau, K. Bormanis, A. Sternberg, D. Kiselev, I. Bdikin, and A. Kholkin. The Structure and Evolution of Nanodomains in (1-x)PbMg<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub>-(x)PbTiO<sub>3</sub> Ceramics Visualized by Piezoresponse Force Microscopy. Programme & Abstracts, p. 95.
  11. Sarunas Bagdzevicius, Robertas Grigalaitis, Juras Banys, Andris Sternberg, and Karlis Bormanis. Broadband Dielectric Investigation of Sodium Potassium Niobate Ceramics With 8% Antimony Substitution. Programme & Abstracts, p. 99.
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Voronezh, Russia, September 14-17, 2010.**

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Beijing, China, October 18 – 20, 2010.**

M, Ozolinsh, and S. Fomins. Multispectral Colour Analysis for Quantitative Evaluation of Pseudoisochromatic Color Deficiency Tests. Abstract Summaries, p. 33.

**VII Международная научно-техническая конференция INTERMATIC-2010,  
МИРЭА, Москва, Россия, 23.-27. ноября 2010. года.**

1. А.И. Бурханов, А.В. Алпатов, К. Борманис, А. Калване. Низко- и инфранизкочастотные диэлектрические свойства в сегнетоэлектрическом твердом растворе (Pb,Sr,Bi)TiO<sub>3</sub> в области фазового перехода. Материалы конференции, часть 1, стр. 119-122.

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1. В.Т. Калинин, Н.В. Сидоров, М.Н. Палатников, А. Штернберг. Материалы электронной техники на основе кислородно-октаэдрических монокристаллов и керамик с общей формулой Li<sub>x</sub>Na<sub>1-x</sub>Ta<sub>y</sub>Nb<sub>1-y</sub>O<sub>3</sub>. Материалы научной конференции, стр. 7-8.

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1. Sarunas Bagdzevicius, Juras Banys, Robertas Grigalaitis, Andris Sternberg, and Karlis Bormanis. Dipolar Glass-Like Perovskite  $\text{Sr}_{0.8}\text{Bi}_{0.2}\text{TiO}_3$  Ceramic. *Ferroelectrics*, 2010, 400, 1, 434 - 440.
2. E. Birks, M. Duce, and A. Sternberg. High Electrocaloric Effect in Ferroelectrics. *Ferroelectrics*, 2010, 400, 336-343.
3. K. Bormanis, A.I. Burkhanov, Y.V. Kochergin, and A. Kalvane. Low Frequency Nonlinearity in Layered Ferroelectrics  $\text{BaBi}_2\text{Nb}_2\text{O}_9$  and  $\text{SrBi}_2\text{Ta}_2\text{O}_9$ . Proceedings of the 2010 IEEE International Conference on Solid Dielectrics. 4-9 July, 2010, Potsdam, Germany, 805-807.
4. M. Duce, M. Antonova, E. Birks, and A. Sternberg. Phase Transitions in  $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - $\text{SrTiO}_3$ - $\text{PbTiO}_3$  Solid Solutions. *Ferroelectrics*, 2010, 405, 57-61.
5. S. Fomins, and N. Rileyeva-Piskura. Strength Judgment of Filling-in Color Aftereffect Illusion for Different Shapes. *Perception*, 2010, 39, 86.
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8. G. Ikaunieks un M. Ozoliņš. Testi redzes žilšanas stipruma novērtēšanai un to pielietojums klīniskajā praksē. *Oftalmoloģijas žurnāls*, 2010, 14, 23-25.
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15. А.И. Бурханов, А.В. Алпатов, К. Борманис, А. Калване. Низко- и инфранизкочастотные диэлектрические свойства в сегнетоэлектрическом твердом растворе  $(\text{Pb,Sr,Bi})\text{TiO}_3$  в области фазового перехода. Материалы VII Международной научно-технической конференции 23-27 ноября 2010 г., INTERMATIC-2010, Москва, МИРЭА, 1, 119-122.
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## DEPARTMENT OF SEMICONDUCTOR MATERIALS

### SEMICONDUCTOR MATERIALS AND SOLID STATE IONICS

#### SEMICONDUCTOR MATERIALS DIVISION

Head of Division 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
- Material characterization by spectroscopic methods (Raman scattering, optical and X-ray 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);
- Lithium thin film batteries;
- Gas sensors and sensor arrays; odour recognition and removal with adsorbent and ozone 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
- 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.
- Investigations of tritium release properties of neutron multiplier beryllium materials for fusion reactor development. Analysis of tritium distribution in plasma-facing carbon-based components.
- The technologies for hydrogen production, storage, transportation, applications in traffic, energy storage and production; synthesis and research of new materials for hydrogen technologies (electrodes in electrolyzers 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 recognition and removal with adsorbents and ozone technologies; development of technologies .
- Investigations of tritium release properties of neutron-irradiated beryllium.

### Scientific staff:

- |                            |                           |
|----------------------------|---------------------------|
| 1. Dr.chem. G. Bajars      | 8. Dr.phys. J.Klavins     |
| 2. Dr.phys. G.Chikvaidze,  | 9. Dr.phys A.Kuzmins      |
| 3. Dr.phys. J.Gabrusenoks  | 10. Dr.phys. A.Lusis      |
| 4. Dr.phys. L.Grīnberga    | 11. Dr.phys. E.Pentjuss   |
| 5. Dr.phys. R.Kalendarjovs | 12. Dr.hab.phys. J.Purans |
| 6. Dr.phys. U.Kanders      | 13. Dr.phys. V.Ogorodņiks |
| 7. Dr.phys. J.Kleperis     | 14. Dr.chem. G.Vaivars    |
|                            | 15. Dr.chem. A.Vitins     |

### Technical staff:

1. K. Alsbergs
2. J. Balodis
2. L. Jēkabsons
4. A. Kursitis
5. V. Nēmcovs

### Postgraduate students: Students:

- |                  |                  |
|------------------|------------------|
| 1. A. Anspoks    | 1. J. Blūms      |
| 2. J. Dimants    | 2. I. Dirba      |
| 3. J. Hodakovska | 3. A. Gruduls    |
| 4. A. Kalinko    | 4. L. Kazule     |
| 5. P. Nazarow    | 5. I. Klepere    |
| 6. L.Pētersone   | 6. G. Kucinskis  |
| 7. A. Šivars,    | 7. Z. Lapina     |
| 8. J. Timoshenko | 9. J.Linītis     |
| 9. Ģ.Vēveris     | 10. E. Rancans   |
| 10. M.Vanags     | 11. J. Timošenko |
|                  | 12. J. Smits     |
|                  | 13. A. Zīle      |

### Laboratories of Semiconductor Material Department

- |  |   |
|--|---|
| Laboratory of Solid State Ionics             | – Head of Laboratory Dr. phys. A.Lusis          |
| Laboratory of EXAFS Spectroscopy<br>J.Purans | – Head of Laboratory Dr. hab. phys.<br>J.Purans |
| Laboratory of Hydrogen and Gass Sensors      | – Head of Laboratory Dr.J.Klepers               |

### Cooperation

#### Latvia

1. University of Latvia - Department of Chemistry (Dr. G. Kizane, Dr. A.Vīksna)
2. University of Latvia, Faculty of Biology (Prof. I.Muiznieks) and Faculty of Economics and Management (Prof. B.Sloka)
3. Riga Technical University (RTU) – Institute of Biomaterials and Biomechanics (Dr. I.Lasenko)
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 Industrial Electronics and Energetic (Prof. L. Ribickis).
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. SIA „EMU PRIM”,
13. JSC „Riga Electric Machine Building Works”,
14. IC „Plazma PL”,
15. SIA “Adviser Union”

#### **France**

1. CRMC-N, Universite de la Mediterranee (Aix-Marseille II) (Marseille, France) – Prof. D.Tonneau, Eng. D. Pailharey,.
2. SETARAM Instrumentation, Caluire – France (Dr. Stéphan MOREAU)

#### **China**

Institute of High Energy Physics, Chinese Academy of Science (Beijing, China) – Prof. Z.Y. Wu.

#### **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)

#### **Norway**

Institute for Energy Technology, Kjeller

#### **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.

#### **South Africa**

West Cape University, Institute of Advanced Material Chemistry, Porous Media Laboratory (Cape Town, Dr. Linkov).

#### **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 coatings, 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 & No.6 “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. Grant from Investment and Development Agency of Latvia “Development and pilot-project implementation on eco-effective transport system in Latvia”
8. Grant from Riga City Council and SwedBank “Hydrogen based heater for vehicle salon and engine”
9. Grant from Student Council of University of Latvia “Comparative Study of bio-hydrogen production and storage methods”
10. "Structure of nano-oxide materials and self-organization in stochastic media" Latvian Government Grant Nr.09.1580 (2010-2012).
11. ESF Project "Nanomaterials for perspective energy effective solutions", No. 2009/0202/1DP/1.1.1.2.0/09/APIA/VIAA/141 (2009-2012).
12. Latvian National Research Program IMIS (2010-2013).

### ***International:***

1. MNT ERA-NET Matera Project "Functional materials for resistive switching memories" (FMRSM) (2009-2011).
2. 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. Gunta Ķizāne).

### ***Didactic work at the University of Latvia***

1. Master degree course "Solid State Ionics" – 4 credit points (A.Lusis)
2. Course Fizi5028 "Structure and Description of Nanomaterials" at the Latvian University (A.Kuzmin).
3. Course Fizi7009 „Solid State Structure” at the Latvian University (A.Kuzmin).

## Main results

### DEVELOPMENT OF NANOSTRUCTURED AND FUNCTIONAL MATERIALS BASED ON GLASS AND NATURAL FIBERS

A. Lūsis, E. Pentjušs, J. Gabrusenoks, G. Bajārs, A. Vitiņš, J. Balodis

The leaching technology and sonochemistry have been used for nanostructuring and functionalization of technical silicate glass and natural (flax, hemp) fibers and fabrics (F). The materials for functionalization are used technical silicate glass fibers from A/S VŠŠ: **E** and **K** glasses fibers. **E** glass is based on calcium aluminoborosilicates and **K** glass is based on sodium aluminosilicates. The metal vacuum coatings for functionalization of leached glass fabrics are used.

Two phenomena in acid media are going on: dissolving and leaching of glass. Both are involved in formation of nano porous functional structure in the fibers. The leaching process is changing a surface morphology of glass fibers as well as internal nanostructure of glass fibers by forming pores.

The influences of ultrasound on leaching process versus temperature and time have been studied. The pore size 2-15 nm with specific 0,1-300 m<sup>2</sup>/g for leached fibers have been obtained. The shrinking of glass fibers leached at 80 °C with and without ultrasound are 13% and 11% accordingly. The pore area of leached glass fibers is 10-100 m<sup>2</sup>/g and can absorb 10-15 wt% water. The ultrasound shifted pores distribution to micropores direction and reduced volume of mesopore.

The functionalization of technical glass fibers and fabrics with metal coatings have practical interest. The plasma treatment and thin film coatings in combination with sonochemical processes are used for nanostructuring and functionalization of fibers and fabrics. The leached K-glass fiber fabric (GFF) had been coated with Ni or Al by DC magnetron sputtering in 100% Ar and studied electrical and electrochemical properties..

The glass fiber fabrics (GFF) coated with metal (Ni and Al) films had been studied by cyclic voltammetry and impedance spectroscopy. The graphical data and some values are presented below.

Dielectric permittivity  $\epsilon$  and electrical conductivity  $s$  of the GFF coated with metal are depended of absorbed water content and metal properties. The measured values of  $\epsilon$  and  $s$  at 100 kHz are:

- 1) Al /GFF/Al  $\epsilon = 4 - 5$ ,  $s = 10^{-8} - 10^{-4}$  S/cm
- 2) Ni /GFF/Ni  $\epsilon = 7 - 60$ ,  $s = 10^{-4} - 10^{-3}$  S/cm
- 3) Ni /GFF/Al  $\epsilon = 7 - 50$ ,  $s = 10^{-7} - 10^{-4}$  S/cm

The impedance spectra of metal coated fabrics (system M/F/M) are complicated due to the heterogeneous and nonhomogeneous constitution of system. The methodic based on impedance spectroscopy for investigation metal coated fabrics is in development stage.

There are problems with the interpretation of impedance data. One of ways is to find relations between system M/F/M constitution, pore and metal type and content of moisture. The impedance spectra of such samples are complicated due to heterogeneous and nonhomogeneous constitution. For that we need physical models.

Functionalization of nanostructured technical glass fibers and fabrics with metal coatings requires deeper studies to explain how adsorbed H<sub>2</sub>O change the impedance spectra. The resistances of metal coated samples depend on amounts of deposited metal and adsorbed water and are in the range 10-1-105 Ohm. The samples, which as prepared have  $|Z| = 10^{-1} - 10^2$  Ohm, have metallic like conduction and changed to ionic like after adsorption of water. Good fitting of EIS for wet M/F/M samples had been obtained with CPE equivalent circuits.

Further more detailed studies for functionalization of nanostructured technical glass, flax and hemp fibers and fabrics with metal coatings are required to explain how adsorbed H<sub>2</sub>O change impedance spectra.

Hierarchical pore structures on macro, micro and nano level, from one side, and interpenetrating electronically and ionically conducting networks, from other side, can be used to explain impedance data.

## LATTICE DYNAMICS AND STRUCTURAL PHASE TRANSITIONS

J. Gabrusenoks

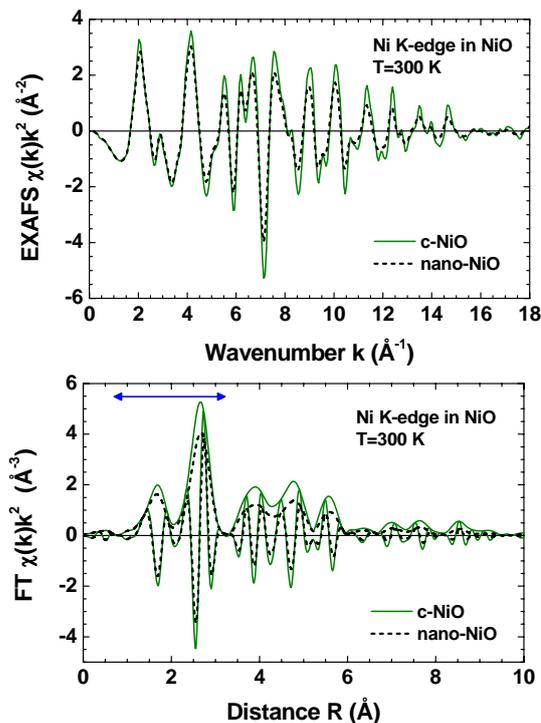
**Symmetry Properties of Lattice Dynamics of W-O Network.** The tungsten-oxygen compounds have crystalline lattices with different topology. It determines dynamic behaviour of lattice. WOCl<sub>4</sub>, WO<sub>2</sub>Cl<sub>2</sub> and WO<sub>3</sub> form crystals lattices with one-, two- and three-dimensional network of W-O bonds respectively. In case of WOCl<sub>4</sub> octahedron are linked by oxygen and form one dimensional chains –W-O-W-O-. In the two and three dimensional lattice –W-O-W-O-W-O- chains are placed in two or three directions and are mutually perpendicular.

**Dynamical properties of AlF<sub>3</sub>.** The vibrational modes of cubic and rhombohedral AlF<sub>3</sub> phases have been investigated. Calculations have been performed by using hybrid exchange density functional theory as implemented within the CRYSYAL06 program to determine the equilibrium geometries and phonon frequencies in high symmetry directions of the Brillouin zone. The calculated phonon frequencies are used to adjust the parameters of a rigid ion model. The longitudinal-transverse splitting of optical modes at  $k=0$  has been determined directly by ab initio in the directions  $\Gamma$ -X,  $\Gamma$ -M and  $\Gamma$ -R calculated phonon dispersions. The phonon dispersion curves show large instability region around the M-R direction.

## STRUCTURE RELAXATION IN NANOCRYSTALS: THE CASE OF NiO

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

The structure relaxation in nanocrystalline NiO (nano-NiO, 13 nm crystallite size) has been studied by X-ray absorption spectroscopy at the Ni K-edge at 300 K. Conventional single-scattering analysis of the EXAFS signals from the first two coordination shells showed a lattice volume expansion by about 1% and a contraction of the Ni–O bonds by about 0.5% in nano-NiO compared to microcrystalline NiO.



Experimental Ni K-edge EXAFS  $\chi(k)k^2$  signals and their Fourier transforms for c-NiO (solid lines) and nano-NiO (dashed lines) at 300 K.

A more sophisticated approach, based on a combination of classical molecular dynamics and ab initio multiple-scattering EXAFS theory, allowed us to interpret both static relaxation and lattice dynamics in nano-NiO. Such approach requires less parameters than conventional EXAFS analysis and allows accounting explicitly for thermal effects and many-atom distribution functions. The agreement between the experimental and calculated EXAFS signals can be used as a criterion to optimize the parameters of the force-field model.

**MNT ERA-NET Matera Project**  
**"FUNCTIONAL MATERIALS FOR RESISTIVE SWITCHING MEMORIES"**  
**(FMRS) –**  
**XAS STUDIES -CONTRIBUTION OF ISSP**

J. Purans, A. Kuzmin, R. Kalendarev and A. Kalinko  
R. Dittmann\*, C. Larsen\*

*\*Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany*

Since a variety of binary and ternary oxides can be reversely switched between two resistive states by applying an appropriate threshold voltage, these materials are under consideration for the use as resistive random access memory (RRAM). Doped ABO<sub>3</sub>-perovskites are suitable functional materials for storage devices with a density in the terabit range since extended defects as dislocations or defect clusters with nanoscale dimensions are considered to be the single resistive switching units. By employing LC-AFM measurements the Jülich group was able to show a clear correlation between conducting filaments and dislocations in SrTiO<sub>3</sub> single crystals. They developed a model to explain resistive switching in SrTiO<sub>3</sub> single crystals as a redox process-driven local metal-to-insulator transition within a network of dislocations. Similar experiments on SrTiO<sub>3</sub> thin films confirm that this model holds for resistive switching thin film

devices. Nevertheless, devices based on these materials are still in the early stage of development. Up to now, their performance does not fulfil the requirements for future RRAM and the basic physical and chemical mechanisms are not understood.

In earlier work from the Riga group, x-ray absorption near-edge spectroscopy (XANES) and extended x-ray absorption fine structure (EXAFS) experiments were performed on  $\text{SrFe}_x\text{Ti}_{1-x}\text{O}_{3-\sigma}$  solid solution powders in reduced and oxidized chemical state. It was demonstrated that the Fe(Ti)-O bond length depends on the oxidation state of the transition metal cation. Building on these observations, we used the EXAFS beamline A1 at HASYLAB to measure  $\text{SrFe}_x\text{Ti}_{1-x}\text{O}_{3-\sigma}$  thin films deposited via pulsed laser deposition (PLD) and Fe-doped  $\text{SrTiO}_3$  single crystals supplied by the Jülich group. The thin films were deposited on Ti-free substrates ( $\text{NdGaO}_3$ ) for Fe and Ti-K edge EXAFS and on a conducting, Nb-doped  $\text{SrTiO}_3$  substrate to do Fe-K edge EXAFS on a thin film resistive switching device. The single crystals were subjected to an electroforming treatment prior to the experiments at HASYLAB, resulting in optically colored regions. Analysis of the data is still in progress, however, preliminary results are very promising.

Fe-K edge EXAFS of an electroformed single crystal shows a clear correlation between the sample color and the oxidation state of Fe (figure). Preliminary analysis in Jülich shows that the optically absorbing part of the sample contained  $\text{Fe}^{4+}$  in perfect octahedral oxygen coordination with a Fe-O bond length of 1.94 Å, whereas the optically transparent part of the sample contained  $\text{Fe}^{3+}$  with a Fe-O bond length of 1.97 Å. The  $\text{Fe}^{4+}$ -O bond length is slightly shorter than the nominal  $\text{Ti}^{4+}$ -O bond length in bulk  $\text{SrTiO}_3$ , which can be explained by the smaller ionic radius of  $\text{Fe}^{4+}$ . The increased bond length of  $\text{Fe}^{3+}$ -O indicates a structural change in the local first coordination shell of Fe. As the reference compound  $\text{LaFeO}_3$  exhibits a bond length of 2.01 Å for  $\text{Fe}^{3+}$  in octahedral coordination, the results indicate the presence of an oxygen vacancy in the first coordination shell, confirming earlier results.

Thin films deposited on  $\text{NdGaO}_3$  with a film thickness of 500 nm were selectively subjected to chemical reduction ex-situ and compared to appropriate standards measured in the same beamline ( $\text{SrFe}_{0.1}\text{Ti}_{0.9}\text{O}_{3-\sigma}$  powder in oxidized and reduced state). Fe-K edge EXAFS shows clearly that the films are in a reduced state after deposition and contain mainly  $\text{Fe}^{3+}$ -ions substituted on the B-site.

It was demonstrated that EXAFS spectroscopy at the Fe-K edge is possible on thin films as thin as 100 nm and containing as little as 1% iron (figure, right). This fact becomes very important for further experiments on thin film structures for resistive switching, since it enables us to investigate thin metal-insulator-metal (MIM) structures. For these investigations, a micro-focused beam is necessary to reduce the beam size to the dimensions of the active electrode area of the MIM structure, which will improve the amount of signal detected from electrically active areas over that detected from non-active regions of the sample.

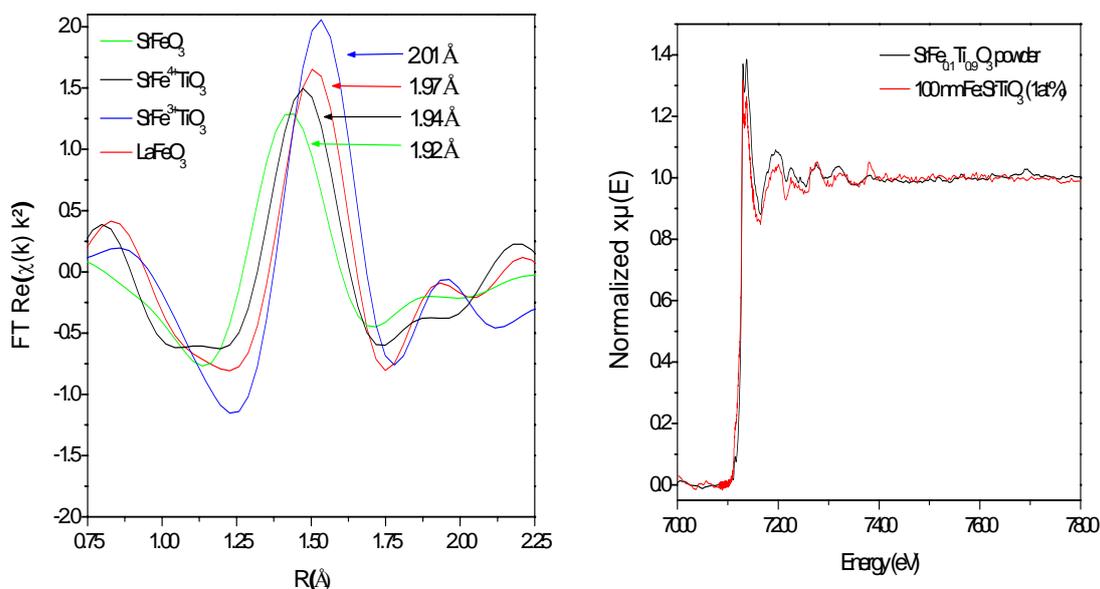


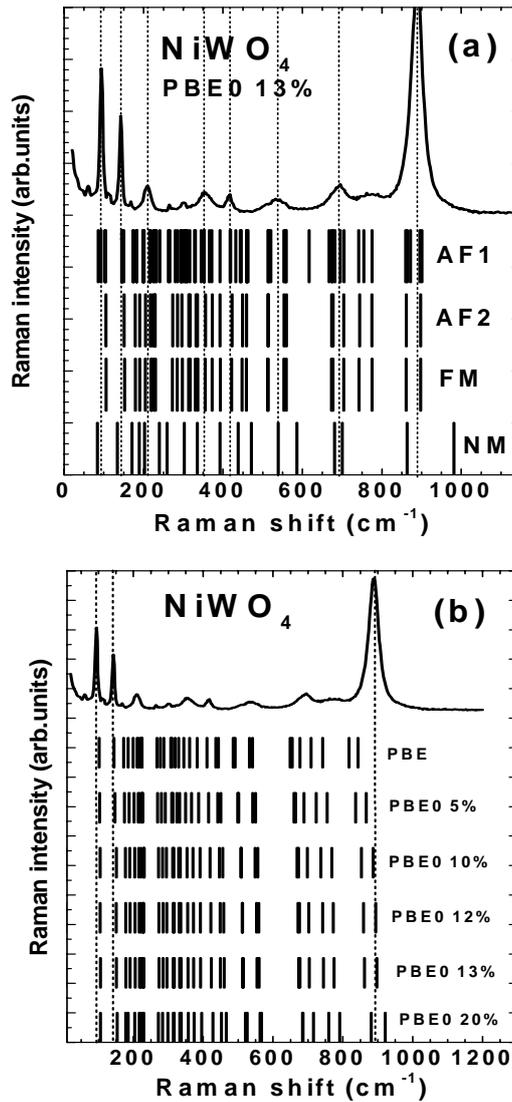
Figure 1: Left: The real part of the Fourier Transform of Fe-K edge EXAFS spectra taken on powder references ( $SrFeO_3$ ,  $LaFeO_3$ ) and on an electroformed  $SrTiO_3$  single crystal containing 0.13 at% Fe. The shift in the curves demonstrates nicely the behaviour of the Fe-O bond length. Right: Fe-K edge EXAFS spectra of a Fe-doped thin film containing 1 at% Fe - 100 nm thick - deposited on Nb: $SrTiO_3$  (red). For comparison, the EXAFS of a powder reference  $SrFe_{0.1}Ti_{0.9}O_3$  taken at BM 29, ESRF. Both spectra were recorded on fluorescence mode and demonstrate the possibility to do XAS on thin film with dopant

### FIRST-PRINCIPLES LCAO STUDY OF PHONONS IN $NiWO_4$

A.Kuzmin, A.Kalinko, R.A.Evarestov\*

*\*Department of Quantum Chemistry, St.Petersburg State University,  
Stary Peterhof, Russia*

The electronic, structural and phonon properties of antiferromagnetic wolframite-type  $NiWO_4$  have been studied using first-principles spin-polarized LCAO calculations based on the hybrid Hartree-Fock (HF)/density functional (DFT) scheme. The influence of different percentages of HF contribution, i.e. different correlation strength, on the structure and phonon frequencies has been investigated and compared with the available experimental data.



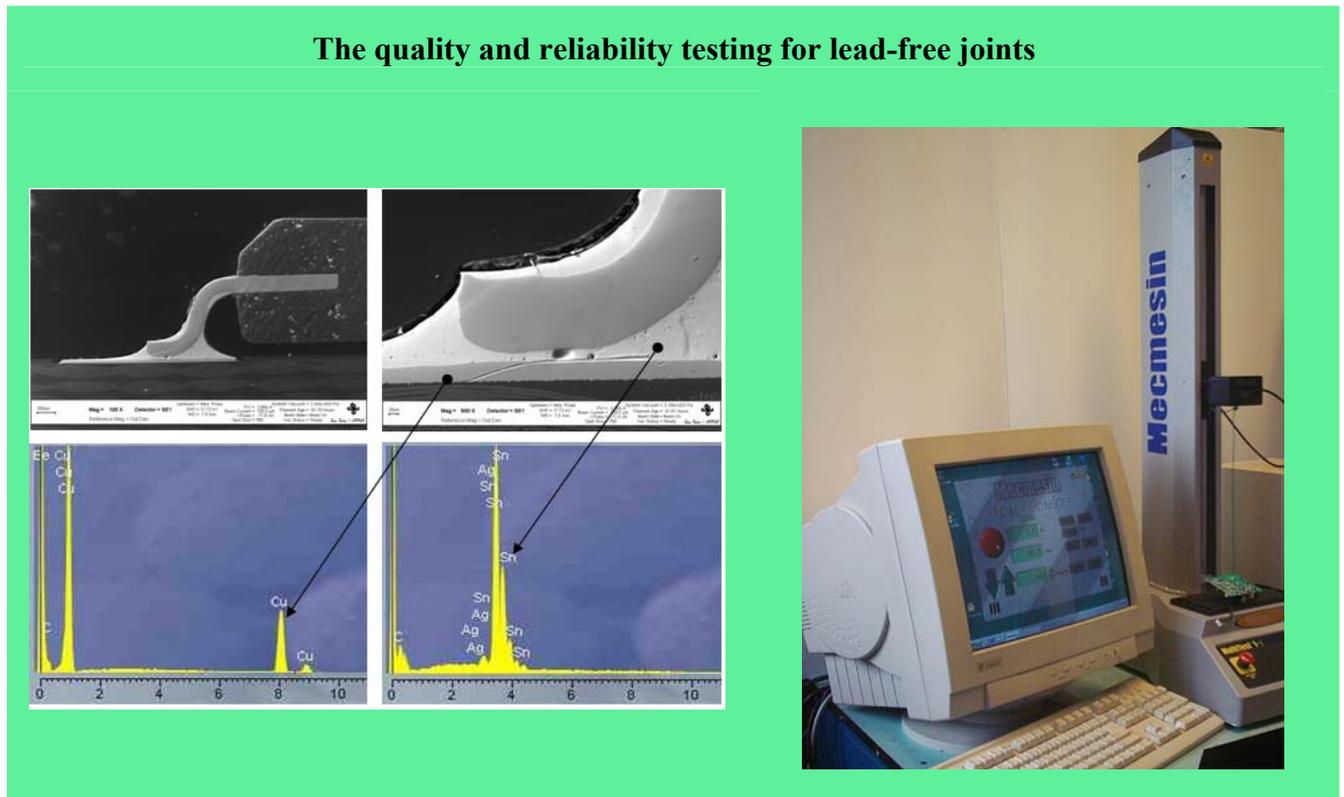
(a) Comparison of the room-temperature experimental Raman spectrum for NiWO<sub>4</sub> with mode frequencies (vertical lines), calculated by the first-principles LCAO method using hybrid PBE0 13% HF Hamiltonian for AF1, AF2, FM, and NM states. (b) LCAO results for hybrid PBE0-type Hamiltonian with different percentages (0÷20%) of HF contribution in the AF2 state.

The first-principles spin-polarized LCAO calculations have been performed for antiferromagnetic wolframite-type NiWO<sub>4</sub>. The indirect band gap of  $E_g=3.7$  eV was calculated in good agreement with experiment. The variation of the HF/DFT mixing allowed us to determine the best HF admixture to be ~13%: it results in a good reproduction of the crystal structure (including local octahedra distortions), band gap and phonon frequencies.

## ACTIVITIES FOR IMPLEMENTATION OF THE “GreenRoSE” PROJECT ON LEAD-FREE SOLDERING ACCORDING EC “RoHS” DIRECTIVE

Ē. Pentjušs, G. Bajārs, A. Vītiņš, A. Lūsis

**Lead-free soldering quality and reliability laboratory.** According tasks of EC FP6 project “GreenRoSE” in ISSP have been set up soldering quality laboratory to help the local small and medium enterprises to change the technologies to lead-free and solve associated problems. There are developed methods and techniques for quality and reliability testing for lead-free joints of PCB. Available services for quality and reliability testing:



The guidelines (in Latvian) and handbook for SMEs about RoHS are published on internet:

[http://www.em.gov.lv/em/images/modules/items/item\\_file\\_13148\\_1.doc](http://www.em.gov.lv/em/images/modules/items/item_file_13148_1.doc)

[http://www.letera.lv/pic/rohs\\_direktiva.doc](http://www.letera.lv/pic/rohs_direktiva.doc)

## RESEARCH AND DEVELOPMENT OF MATERIALS AND DEVICES FOR HYDROGEN ENERGY TECHNOLOGIES

J. Kleperis, L. Grīnberga, G. Vaivars, G. Chikvaidze, G. Bajārs, J. Hodakovska, M. Vanags, V. Nemcevs, L. Kulikova<sup>1</sup>, V. Serga<sup>1</sup>, E. Palcevskis<sup>1</sup>, E. Rancāns<sup>2</sup>, J. Blūms<sup>2</sup>, G.Kucinskis<sup>2</sup>, I. Dirba<sup>2</sup>, J. Šmits<sup>3</sup>, I. Klepere<sup>4</sup>, A. Gruduls<sup>4</sup>, J. Dimants<sup>5</sup>, K. Jurgelis<sup>6</sup>, I.Baiža<sup>6</sup>

*Institute of Solid State Physics of University of Latvia;*

*1 – Riga Technical University, Institute of Inorganic Chemistry;*

*2 – Students from Faculty of Physics and Mathematics of University of Latvia;*

*3 - Students (12<sup>th</sup> year) from France Lyceum Riga, Latvia;*

*4 – Students from Faculty of Biology of University of Latvia;*

*5 – Student from Faculty of Economics and Management of University of Latvia*

*6- Students from Faculty of Chemistry of University of Latvia*

**Sample Activation for Hydrogen Absorption - Dependence on Grain Size.** Sustained studies demonstrate that solid materials can be utilized to solve the storage problem of large amounts of hydrogen by reversible absorption and desorption. Experimental data shows that maximal sorption capacity material can reach after pre-treatment procedures to dispose of impurity gasses and oxides. There are several ways to perform pre-treatment procedures – sequence of absorption-desorption cycles that follows after alkali treatment, heating or ball-milling. Speed in which activation takes place within hydrogen sorption materials is depending on sample grain size. If one could reduce amount of energy that is needed to activate sample, then we could greatly cut down sample costs. Determining grain size that is optimal for sample activation, can give a basic idea whether best way is to reduce grain size by mechanical means or by hydrogen sorption - desorption process.

**Hydrogen Sorption in Modified Silica Glass Grains.** An efficient storage media for hydrogen is desirable for the common applications of fuel cells and the adoption of hydrogen as an energy source. Nanostructuring of materials and enhancement of surface absorption capability are two main factors to increase the amount of sorbed hydrogen. One way to combine the effectiveness of hydrogen absorption in metal hydrides and the desirable weight/volume proportion is to make composite material from alloy forming hydride and appropriate support material. In a regular circumstances SiO<sub>2</sub> glass are not absorbing notable amount of hydrogen, however doping small quantities of palladium in these materials can provide a capturing of significant amount of this gas. We studied hydrogen sorption properties in composites made of palladium nano-particles coated on the surface of porous nano-powder of SiO<sub>2</sub> by using extractive-pyrolytic method. To investigate an interaction of hydrogen with Pd/oxide composites the volumetric method was used. Phase composition of materials was determined by XRD method.

**Determination the Conditions for Minimal Reaction Energy for Electrolysis.** Initial process of electrolysis is investigated using platinum and tungsten wires as hydrogen electrodes and inductive kickback voltage (IKV) peak based power unit. Microelectrodes from Unisense (Denmark) are used to determine concentrations of dissolved hydrogen and pH close to wire electrodes. It is observed that concentration of dissolved hydrogen increases faster on tungsten electrode as on platinum. Authors explain this fact with differences of hydrogen evolution reaction (HER) on both materials – IKV peak power unit is supplying very short voltage pulses with limited energy what is enough only for hydrogen adsorption on platinum electrode, but is sufficient for full HER reaction on tungsten electrode.

**SPEEK and PANI Based Proton and Electron Conducting Membranes for Fuel Cells.** Fuel cells are made of several parts, thus raising a problem of good contact between them. Now carbon cloth is used as a catalyst holding layer and electron conducting media. If it could be replaced with another material based on polymer like as the membrane material, it could improve contact. In this case the new material is needed, both with proton and electron conductive. One of the possible solutions is discussed in our work. Complex polymer is made from sulfonated PEEK and PANI. Obtained materials are analyzed with FTIR absorption method.

**SPEKK Membranes for Hydrogen Separation from Gas Mixtures.** Hydrogen has a relatively small molecular size compared to other gases and exhibits high selectivity ratios in glassy polymers. The ideal membrane possesses a high flux as well as a high selectivity. The degree of separation is highly dependent on both membrane selectivity and permeability. Additionally, the membrane must be stable at the operating conditions of the process. Both polyimide and polysulfone membranes are commercialized for hydrogen separation purposes. The lifetime of the polyimide membrane is in the range of seven to ten years. Lower cost polysulfone membranes typically could not provide comparable longevity. In this work, More stable variety of polysulfone as potential polyimide replacement is synthesized and investigated.

**Electro-Conductive Ion Liquids and they Potential Application in Hydrogen Energy Devices.** Room temperature ionic liquids are air stable salts, composed of an organic cation and either an organic or an inorganic anion. They are available in high variety. They have a high electro-conductivity, a low viscosity, a non-measurable vapour pressure and other properties non-typical for polar solvents. In this work, the formiats with different cations have been synthesized. The electro-conductivity and its activation energy have been measured by impedance spectroscopy. The temperature stability of the chemical composition studied with thermal analysis. The impact of the cation size on properties was estimated.

**Formation of Hydrogen Gas Oversaturated Liquid in Bioreactor with Hydrogen Producing Bacteria *E.Coli*.** Biological hydrogen production is an alternative way to produce hydrogen from renewable resources for storage and usage in Hydrogen Economy. Bacteria are producing hydrogen in the liquid phase and when thermodynamic equilibrium is reached hydrogen is diffusing from liquid to gaseous phase. Different methods are used to collect hydrogen from the gaseous phase. For hydrogen concentration determination in gaseous phase it is necessary to study properly the hydrogen production kinetics in liquid phase during the fermentation process. In our experiments the hydrogen microsensor from Unisense Ltd. (Denmark) was used and hydrogen oversaturation in the liquid phase observed. The presence of hydrogen in gaseous phase was measured using massspectrometer but registered concentrations were comparatively small. To decrease the hydrogen partial pressure in liquid phase reactor with a system for continuous bubbling with inert gas was developed. Contradictory results were obtained therefore alternative methods for hydrogen collection directly from the liquid using specific adsorption membranes are considered to be implemented.

**Black Platinum Electrode for Measurement the Concentration of Dissolved Hydrogen in Liquids.** Alternative energy production and usage methods have to be developed to reduce current developing climate changing risks. Hydrogen as an energy carrier is used in all most promising ecological energy forms. To ensure hydrogen production from renewable resources optimization of biological systems and a comprehensive research is required. One of the hydrogen productivity determination methods in biological systems is hydrogen concentration measurement in liquid phase.

Dissolved hydrogen concentration in liquid can be measured by using commercial sensors although they have some disadvantages: large size, small durability, ability to only make measurements in a certain point of the sample and they are expensive in price. In this work we test the platinum electrode as potential sensor of dissolved hydrogen. Platinum wire was coated with black platinum using electrochemical plating method. In such a way it is possible to develop sensor systems for measurements of hydrogen concentrations in different places of liquid simultaneously and it would ensure data about gradients of hydrogen concentrations.

**Photocatalysis for Hydrogen Production.** At the moment almost 100% of hydrogen production directly or indirectly is provided from fossil fuels that emits large amount of greenhouse gases. To provide a clean and renewable life cycle of hydrogen it is necessary to produce it from clean and renewable energy sources as well. Photocatalytic water splitting using solar energy could be one of solutions of environmentally friendly and clean ways of hydrogen production. The basic material for the production of 'solar hydrogen' is water that is a renewable resource and on the earth it is enough and easy to access. However, there are many problems that must be solved before this technology become economically feasible. One of tasks is the development of efficient photocatalyst that works in the visible light and hydrogen storage. The other task is to increase the efficiency of solar energy utilization. The basic principles of photocatalytical hydrogen production and possible solutions of incensement of process efficiency is investigated on the base of titanium oxide materials.

**Investigation of Driving Distance of Electric - Hydrogen Cars.** Hydrogen economy is a new energy distribution system based on hydrogen gas as the energy carrier also in transport sector. Hydrogen is not available on Earth as gas, only in different compounds, therefore infrastructure for hydrogen production, storage and transport is necessary. Development of such hydrogen infrastructures needs a lot investments and time to develop appropriate technologies. One possibility to increase an application of hydrogen in economics could be the development of portable hydrogen generators. Currently, the hydrogen-on-demand systems that are being developed for the automotive industry either use electrolysis or a chemical reaction in order to generate hydrogen as needed for a car equipped with either an internal combustion engine or a fuel cell. The hydrogen-on-demand systems that use electrolysis or some other metal catalyst such as aluminum, magnesium, or sodium borohydride, or another hydrogen-rich chemical compound, needs energy supply to force a reaction that releases the hydrogen as needed. In our work the possibility to construct small and efficient hydrogen on demand system is discussed. Pulse powered electrolysis unit is used to recycle water from car's fuel cells into hydrogen and oxygen and to extend the maximal driving distance.

**Success Examples of Hydrogen Economy in the World and what can Latvia Learn from them.** For energy and transport sectors the research of hydrogen as an energy carrier and fuel is becoming important more and more. An important contributor to a future with a sustainable energy economy and a gradual reduction in dependency from fossil fuels will be the hydrogen and fuel cell technologies; - it is recognized by many countries in the world. A global development has begun towards a widespread use of hydrogen – the so called Hydrogen Economy. Iceland announced that will be the first country in World with Hydrogen Economy. In 2003 the first three hydrogen buses began routes on the streets of Reykjavic; the World's first commercial hydrogen station was open in 2003; by 2006, the first demonstration project for a fuel cell-powered ocean vessel was completed. In the World different hydrogen projects are implemented which could be good examples for Latvia. Evaluating hydrogen as energy carrier usage possibilities in economics it seems that hydrogen production in small quantities would

be efficient only when alternative, renewable energies are used to produce it. What can Latvia learn from them? The implementation of hydrogen in energy sector and as fuel in transport sector will give political and economical freedom to Latvia. Do we need it?

## **THIN FILMS OF LITHIUM IRON PHOSPHATE FOR THIN FILM BATTERIES AND EFFICIENCY OF SOLAR PANELS**

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**Investigation of Structure and Impedance of Lithium Iron Phosphate.** Recently increased attention has been dedicated to  $\text{LiFePO}_4$  as a perspective material in Li-ion batteries for use in consumer electronics and electric vehicles. In comparison with the more widely used  $\text{LiMn}_2\text{O}_4$  and  $\text{LiCoO}_2$  batteries,  $\text{LiFePO}_4$  batteries are less exposed to risks of ignition/explosion, are more cyclable, more environmentally benign and cheaper to produce. In our work  $\text{LiFePO}_4$  was synthesized from  $\text{Li}_2\text{CO}_3$ ,  $\text{FeC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  and  $\text{NH}_4\text{H}_2\text{PO}_4$  with different carbon content at different conditions. Thermogravimetric analysis was performed on each of the reactants as well as a stoichiometric mixture of the four. Raman spectra and XRD analysis were performed on the obtained compounds. To establish the conductivity of the obtained material we performed impedance measurements for a compressed tablet of  $\text{LiFePO}_4$  in a two electrode cell with frequencies ranging from 0.01 Hz to 65 000 Hz. Results show the correlation between electronic conductivity and carbon content in  $\text{LiFePO}_4$ . An equivalent circuit was found that describes the electrochemical processes on the  $\text{LiFePO}_4/\text{Pt}$  boundary.

**$\text{LiFePO}_4$  Thin Film Coatings as Cathode Materials for Thin Film Lithium Power Sources.**  $\text{LiFePO}_4$  is a perspective cathode material for use in Li-ion batteries due to its high charge capacity, low manufacturing costs, environmental friendliness, safety and high cyclability. One of the main problems preventing a wider use of  $\text{LiFePO}_4$  cathodes in consumer electronics and hybrid/electric vehicles is its low electronic conductivity. One way to solve this problem is the increase of surface area by the use of thin films. In our research we created thin films of  $\text{LiFePO}_4$  on silicon, glass, tungsten and ITO (on polyester) in different sputtering conditions (sputtering time between 10-20 minutes, coil power ranging from 250-500 W) with targets prepared by different methods. Profilometric and element analysis were performed on the films. Results show that thin films between 200 nm and 500 nm were obtained with elements matching those of  $\text{LiFePO}_4$ . To investigate the electrochemical properties of the thin film a two electrode electrochemical cell ( $\text{LiFePO}_4$  on ITO/1M  $\text{LiClO}_4$  – PC/graphite) was prepared and used to obtain voltammograms and open circuit potential changes during charge/discharge. These showed that our  $\text{LiFePO}_4$  thin film could be used in Li-ion batteries.

**Temperature Influence on the Power Efficiency of Commercial Photovoltage Batteries.** From May 2009 there are installed 4 Solar panels KS-160 (KoraxSolar, Hungary) with total area 4,5 m<sup>2</sup> on the roof of Institute of Solid State Physics. Analysis of results collected during 6 months showed that on similar sunny days with different ambient temperatures there are quite different amounts of collected energy. The output (product of electricity and voltage) of a solar cell is temperature dependent. Higher cell temperatures lead to lower output, and hence to lower efficiency. The level of efficiency indicates how much of the radiated quantity of light is converted into useable electrical energy. Regarding information from producer, the output of Solar panel KS-160 reduces by 0,4- 0,6% increasing temperature by 1 degree. We experimentally tested panel KS-160 in closed thermal camera equipped with 4 halogen lamps (300W) as light source. An output of Solar panel decrease 2.6 times increasing temperature from 20 to 61 oC.

Physical aspects of deterioration of the output power and the conversion efficiency of solar cell and PV module with increasing temperature are discussed in our work. In order to diminish these effects, it is useful to decrease the module temperature by removing the heat produced by non-active absorption of photons, which do not generate pairs, by recombination of electron-hole pairs, by photocurrent (Joule's heat generated during the current flow in the series resistance of the p-n junction) and parasitic currents.

## APPLICATION TECHNOLOGIES OF AN GAS SENSORS AND SENSOR ARRAYS FOR AIR QUALITY CONTROL

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**Search for Rapid Diagnostic Methods to Detect Wheat Diseases.** Dwarf bunt is a winter wheat disease that is caused by the fungus *Tilletia controversa*. During last years dwarf bunt is widely observed in Latvia and reduces crops by 30% or in some cases 95%. The kernels of diseased plants are replaced by bunt balls, which contain masses of black spores with a foul odour (like rotten fish). The bunt balls rupture at harvest, contaminating the grain. Rapid diagnostic method is necessary to reveal infected crops. We used spectroscopic methods and electronic nose to separate diseased wheat grains containing specific gas –trimethylamine, from healthy ones. The control of diseases in crops is still largely dominated by the use of fungicides, but with the increasing incidence of fungicide resistance, plus mounting concern for the environment resulting from excessive agrochemical use. Therefore the search for alternative, reliable methods of disease control is gaining momentum. The direct germicide action of Ozone is well-known against all type of microorganisms, as much fungi as bacteria and virus. Ozone is also effective against the spores of those microorganisms which are able to propagate and reproduce by this route. The resistance of *Tilletia controversa* against the treatment with ozone is tested.

## TRITIUM RELEASE FROM NEUTRON-IRRADIATED BERYLLIUM PEBBLES UNDER ACTION OF TEMPERATURE

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Beryllium pebbles are foreseen as a neutron multiplier to ensure sufficient tritium breeding in a ceramic breeder in a blanket of a future fusion power reactor. Helium and tritium are produced in beryllium as a result of neutron-induced transmutations. One of tasks of blanket designs is to reduce tritium inventory in the beryllium pebbles.

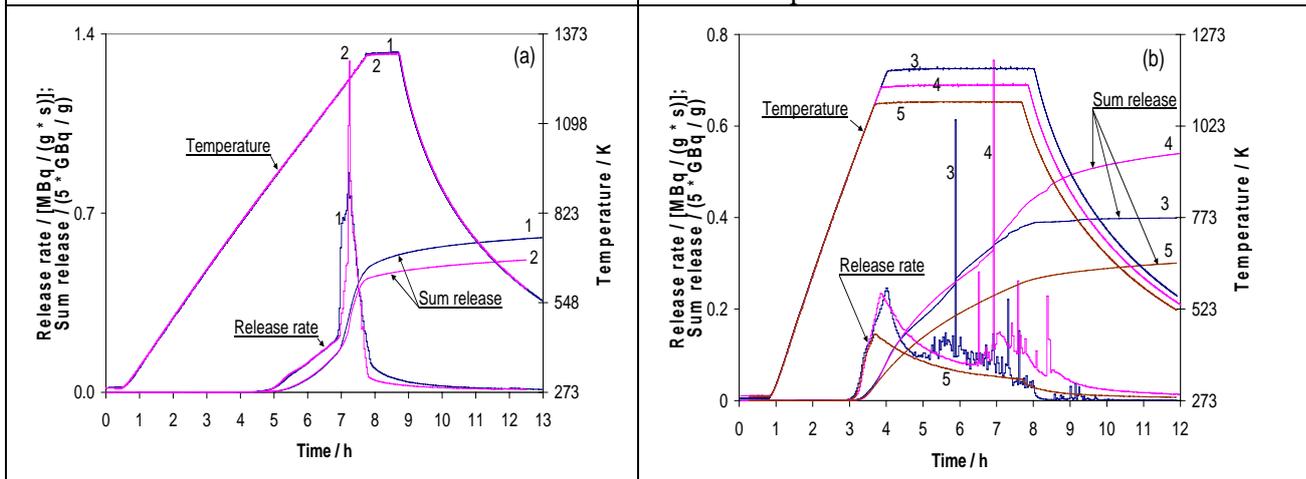
In this study, we present results on tritium release from the beryllium pebbles ( $\varnothing \approx 1$  mm) irradiated for 294 full power days from 17 April 2003 to November 2004 to the neutron fluence of  $3-4 \times 10^{25} \text{ m}^{-2}$  ( $E > 0.1$  MeV) at temperature 523-773 K in the pebble-bed assemblies (PBA) experiment in the high flux reactor at Petten, the Netherlands [1,2].

This study is a report on post irradiation tritium release experiments under action of both temperature ramps of  $\beta = 2.3-4.8$  K/min from room temperature to 1310-1520 K and anneals at a constant temperature of 1000-1180 K for 4-23 h on the beryllium pebbles in the flow of the purge gas He + 0.1% H<sub>2</sub> of 14-15 L/h. One PBA Be pebble was investigated in each tritium release experiment. Disassembled view of the setup for the tritium release experiments is shown in Fig. 1.

Histograms of the tritium release rate and curves of the tritium sum release from two PBA beryllium pebbles at the given temperature program consisting of a ramp at 2.3 K/min to 1308 K and anneal at 1308-1317 K for 1 h are given in Fig. 2a. A significant tritium release started at 830 K. The PBA Be pebbles of 1.12 and 0.98 mg had the histogram with a shoulder at 920-1192 K and a maximum at 1230-1238 K. The shoulder and the maximum may be related to the stages of



**Fig. 1 (on the left side).** Disassembled view of the setup for the tritium release experiments: 1 and 2 – compartments of the quartz tube for the sample and for a bed of granulated zinc respectively; 3 – a porcelain boat for the sample under study; 4 – a white cylindrical ceramic holder for the cold junction of a type S thermocouple of 300 mm in length; 5 – a type K thermocouple to measure the temperature of the cold junction of the type S thermocouple; 6 – a “Nabertherm” RT 50-250/13 tube furnace; 7 – a P 320 controller for the “Nabertherm” tube furnace; 8 – a tube furnace for heating the zinc bed; 9 and 10 – measuring and driving type K thermocouples for the zinc bed respectively; 11 – an ice bath for the cold junctions of type K thermocouples 5 and 9.



**Fig. 2 (on the top).** Tritium release rate and tritium sum release from the PBA beryllium pebbles heated at the given temperature: curves 1 and 2 – a linear ramp of 2.3 K/min to an anneal temperature of 1308-1317 K; curves 3-5 – a linear ramp of 4.5 K/min to an anneal temperature of 1173-1183 K (curve 3), 1129-1135 K (curve 4) and 1083-1090 K (curve 5). The PBA Be pebbles had the following masses (mg), final values of the tritium sum release for 1 g of the sample (GBq/g) and final values of the tritium fractional sum release (%): 1 – 1.12, 3.02, 100%; 2 – 0.98, 2.58, 100%; 3 – 1.13, 2.00, 91.7%; 4 – 0.90, 2.71, 84.5%; 5 – 1.05, 1.50, 56.8%.

gradual and burst release of tritium respectively. Under the temperature program given in Fig. 2a, four other PBA Be pebbles of 0.96-1.24 mg had tritium release patterns of the final sum release of 2.6-3.0 GBq/g that were qualitatively similar to curves 1 and 2 of Fig. 2a. At the temperature ramps to 1308-1525 K, the main maximum of the tritium release rate of the PBA Be pebbles was found to be in the stage of burst release, in the temperature ranges of 1178-1309 K ( $\beta=2.4$  K/min) and 1178-1350 K ( $\beta=4.8$  K/min).

Curves of the tritium release for the lower final anneal temperatures of 1083-1183 K are shown in Fig. 2b. In curves 3 and 4, a transition from the gradual to burst release of tritium at the final anneal temperatures of 1129-1183 K is evident. The time

lag of release burst can be determined for curves 3 and 4: about 1 h at 1178 K (curve 3) and about 2.5 h at 1132 K (curve 4). The stages of gradual and burst release may be related to the tritium release by atomic diffusion and bubble venting respectively. The total tritium inventory in the PBA Be pebbles was found to be 2-4 GBq/g.

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11. M.Vanags, G.Bajars, J.Kleperis, A.Lusis (2010) Peculiarities of short pulse water electrolysis: Ion transport and discharge at electrodes. 9th International Symposium on Systems with Fast Ionic Transport. Book of Abstracts, Riga, p.133.
12. M.Vanags, J.Kleperis, G.Bajars, A.Lusis (2010) Peculiarities of water electrolysis with high voltage short pulses. 61<sup>st</sup> Annual Meeting of ISE, Nice, France, ise102638.
13. G.Bajars, G.Kucinskis, J.Smits, J.Kleperis, M.Vanags (2010) Kinetic behavior of  $\text{LiFePO}_4/\text{C}$  thin film cathode material for lithium-ion batteries. 61<sup>st</sup> Annual Meeting of ISE, Nice, France, ise102700.
14. G.Bajars, E.Pentyush, A.Lusis, J.Gabrusenoks (2010) Simulation of voltammetric characteristics of electrochemical electrodes by variable RC chain at a potential sweep condition. 61<sup>st</sup> Annual Meeting of ISE, Nice, France, ise102875.
15. G.Bajars, J.Kleperis, L.Grinberga, M.Vanags (2010) Study course „Sources of energy and their environmental impacts” at the University of Latvia. Proceedings of the 4<sup>th</sup> International Conference “Environmental Science and Education in Latvia and Europe: Education and science for climate change mitigation”, Riga, pp.66-67.
16. G.Bajars, M.Vanags, J.Kleperis (2010) Efficiency improvement of water electrolysis for hydrogen production. 6<sup>th</sup> Russian conference on Physical problems of hydrogen energetics. Book of Abstracts, p.20.
17. G.Kucinskis, J.Smits, L.Grinberga, G.Bajars, J.Kleperis (2010) Physical and electrochemical characteristics of  $\text{LiFePO}_4/\text{C}$  thin film cathode material for lithium-ion batteries. 6<sup>th</sup> Russian conference on Physical problems of hydrogen energetics. Book of Abstracts, pp.167-168.

18. J.Smits, L.Grinberga, G.Kucinskis, G.Bajars, J.Kleperis (2010) Preparation of LiFePO<sub>4</sub>/C target for thin film electrodes in lithium microbatteries. 6<sup>th</sup> Russian conference on Physical problems of hydrogen energetics. Book of Abstracts, pp.172-173.
19. J.Kleperis, G.Bajars, B.Sloka, J.Dimants (2010) Integration the renewable energy and hydrogen technology topics in Latvian higher education establishments. 6<sup>th</sup> Russian conference on Physical problems of hydrogen energetics. Book of Abstracts, pp.203-204.
20. I.Klepere, I. Muižnieks, J. Kleperis. Formation of hydrogen gas oversaturated liquid in bioreactor with hydrogen producing bacteria E.Coli. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 56.
21. G.Vaivars, I.Baiža, E.Gžibovska. Electro-conductive ion liquids and they potential application in hydrogen energy devices. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 57.
22. G.Vaivars, K.Jurģelis, A.Krjučkovska. Polyether ether ketone membranes for hydrogen separation from gas mixtures. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p.58.
23. L. Grīnberga, Photocatalysis for hydrogen production. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 59.
24. I.Dirba, Critical analysis of possibilities to use geomagnetic energy. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 60.
25. Z.Lapiņa, V.Ogorodņiks, J.Kleperis, Search for rapid diagnostic methods to detect wheat diseases. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 65.
26. V.Kuzmovs, J.Kleperis, Available driving distance of electric - hydrogen cars and possibilities to make it larger. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 66.
27. J. Dimants, B. Sloka, J. Kleperis, Success examples of hydrogen economy in the world and what can Latvia learn from them. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 73.
28. Gruduls, I. Klepere, G. Bajārs, J. Kleperis, Black platinum electrode for measurement the concentration of dissolved hydrogen in liquids. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 74.
29. J. Hodakovska, G. Čikvaidze, J. Kleperis, Proton and electron conducting membranes for fuel cells. Abstracts of Annual 26th Conference of Institute of

- Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 75.
30. M. Vanags, G. Bajārs, J. Kleperis, Conditions of minimal reaction energy for electrolysis and possibilities to reduce it. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 76.
  31. E. Rancāns, L. Grīnberga, J. Kleperis, Sample activation rate dependence on grain size. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p.77.
  32. L. Grīnberga, L. Kuļikova, V. Serga, J. Kleperis, Hydrogen sorption of modified SiO<sub>2</sub> glass. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p.78.
  33. J. Blūms, M. Vanags, J. Kleperis, Temperature influence on the power efficiency of commercial photovoltage batteries. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p. 79.
  34. J. Šmits, G. Kučinskis, G. Bajārs, J. Kleperis, J. Balodis, LiFePO<sub>4</sub> thin film coatings as cathode materials for thin film lithium power sources. Abstracts of Annual 26th Conference of Institute of Solid State Physics of University of Latvia, February 17-19, 2010, Riga, Latvia, p.81.
  35. G.Bajars, J.Smits, G.Kucinskis, J.Kleperis. Study of Structure and Electrochemical Characteristics of LiFePO<sub>4</sub>/C as Cathode Material for Lithium Batteries. Abstracts of International Conference „Functional Materials and Nanotechnologies” FM&NT 2010, March 16-19, 2010, Riga (Latvia), p. 81.
  36. J.Kleperis, M.Vanags, J.Hodakovska, J.Klavins. Oriented Nanostructures for Solar-Hydrogen Technologies. Abstracts of International Conference „Functional Materials and Nanotechnologies” FM&NT 2010, March 16-19, 2010, Riga (Latvia), p. 82.
  37. J.Hodakovska, J.Kleperis. SPEEK and PANI based membranes for fuel cells. Abstracts of International Conference „Functional Materials and Nanotechnologies” FM&NT 2010, March 16-19, 2010, Riga (Latvia), p. 127.
  38. L.Grinberga, Nanosized Perovskites for Photocatalytical Water Decomposition. Abstracts of International Conference „Functional Materials and Nanotechnologies” FM&NT 2010, March 16-19, 2010, Riga (Latvia), p. 126.
  39. H.Luo, G.Vaivars, S.Nonjola, M.Rohwer, M.Mathe. Anion Exchange Membrane Based on Alkali Doped Poly(2,5-benzimidazole) for Alkaline Membranes Fuel Cell. Abstracts of International Conference „Functional Materials and Nanotechnologies” FM&NT 2010, March 16-19, 2010, Riga (Latvia), p. 128.
  40. J. Hodakovska, G. Chikvaidze, J. Kleperis. Electron and proton conductive polymer membranes for fuel cells. 7th International Conference Of Young Scientists On Energy Issues Cyseni 2010; May 26-27, 2011, Lithuanian Energy Institute, Kaunas, Lithuania. Abstract 1 page.

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42. P. Shipkovs, A. Snegirjovs, M. Vanags, K. Lebedeva, J. Shipkovs, L. Vasilevska, M. Pankars. Comparison of solar collectors operation methods. 7th International Conference Of Young Scientists On Energy Issues Cyseni 2010; May 26-27, 2011, Lithuanian Energy Institute, Kaunas, Lithuania. Abstract 1 page.
43. J. Blums, M. Vanags, J. Kleperis. Effect of ambient temperature on commercial photovoltaic solar cells. 7th International Conference Of Young Scientists On Energy Issues Cyseni 2010; May 26-27, 2011, Lithuanian Energy Institute, Kaunas, Lithuania. Abstract 1 page.
44. Julija Hodakovska, G. Chikvaidze, J. Kleperis, Multiple-layered proton-electron conductive polymer membrane for fuel cells. Abstracts of 18th World Hydrogen Energy Conference WHEC 2010, May 16–21, 2010, Messe Essen (Germany), 1 page.
45. J. Kleperis, L. Grinberga, A. Lūsis Energy storage solutions using hydrogen insertion compounds. Abstracts of 9th International Symposium on Systems with Fast Ionic Transport (9th ISSFIT), June 1 – 5, 2010, Riga, University of Latvia (Latvia), p. 131.
46. L. Grinberga, E. Rancans, J. Kleperis An impact of grain size on the rate of hydrogen sorption in LaNi<sub>5</sub>. Abstracts of 9th International Symposium on Systems with Fast Ionic Transport (9th ISSFIT), June 1 – 5, 2010, Riga, University of Latvia (Latvia), p. 132.
47. Klepere I., Gruduls A., Nikolajeva V., Kleperis J., Muiznieks I. Bio-hydrogen production from industrial food waste by anaerobic microorganism associations. The 9th International Hydrogenase Conference, June 27 – July 2, 2010, Uppsala, Sweden, p. 107.
48. J. Dimants, B. Sloka, J. Kleperis, I. Klepere. Hydrogen as innovative technology for a sustainable energy supply. Abstracts of the 11th Bi-Annual Conference on European Association for Comparative Economic Studies: Comparing Responses to Global Instability. August 26-28, 2010, Tartu, 1 page.
49. G. Vaivars, K. Jurgelis, I. Klepere. Hydrogen diffusion in modified poly(ether ether ketone) membranes. Abstracts of XII International Symposium on Polymer Electrolytes ISPE-12; 29 August - 3 September 2010, Padova, Italy, 1 page.
50. J. Dimants, B. Sloka, J. Kleperis, I. Klepere. Course on Alternative energy as a Road map for a Sustainable Public Education. Abstracts of International Conference „Employability & Entrepreneurship”- 2nd Edition, September 27-28, 2010; Porto, Portugal, 1 page.
51. Martins Vanags, Janis Kleperis, Gunars Bajars, Andrejs Lūsis. Peculiarities of water electrolysis with high voltage short pulses. Abstracts of 61st Annual Meeting of the International Society of Electrochemistry „Electrochemistry from Biology to Physics”, September 26 - October 1, 2010, Nice (France). Format CD, 1 page.

52. Janis Kleperis, Biruta Sloka, Justs Dimants, Ilze Klepere. Interdisciplinary Courses on Renewable Energies in Latvian Higher Education Establishments and Hydrogen Technologies. Abstracts of The 4th International Conference "Environmental Science and Education in Latvia and Europe: From Green projects to Green society", 22 October, 2010, Latvia University of Agriculture, Jelgava (Latvia), 2 pages.
53. Justs Dimants, Ilze Klepere. Teaching Renewables for Master Program Students at the School for Renewable Energy Science in Iceland: Sharing Study Experience. Abstracts of The 4th International Conference "Environmental Science and Education in Latvia and Europe: From Green projects to Green society", 22 October, 2010, Latvia University of Agriculture, Jelgava (Latvia), 2 pages.
54. G. Bajars, M. Vanags and J. Kleperis. Efficiency Improvement of Water Electrolysis for Hydrogen Production. VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages..
55. L. Grinberga, J. Kleperis, L. Kulikova, V. Serga. Hydrogen Sorption of Modified Oxides. VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages.
56. I. Klepere, A. Gruduls, V. Nikolajeva, I. Muižnieks and J. Kleperis. Bio-Hydrogen Application Possibilities in Latvia: Substrates and Microorganism Research Using Micro-Electrodes And Test-System Fermentation Reactor. VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages.
57. I. Dirba, M. Vanags, J. Kleperis. Upgrading the Wind Power Generator for Direct Hydrogen Production. VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages.
58. G. Kucinskis, J. Smits, L. Grinberga, G. Bajars, J. Kleperis. Physical and Electrochemical Characteristics of LiFePO<sub>4</sub>/C Thin Film Cathode Material for Lithium-Ion Batteries. VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages.
59. J. Hodakovska, V. Nemcevs, G. Cikvaidze, J. Kleperis. SPEEK and PANI Based Membranes for Fuel Cells. VI Российская Конференция "Физические

проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages.

60. J. Smits, L. Grinberga, G. Kucinskis, G. Bajars and J.Kleperis. Preparation of LiFePO<sub>4</sub>/C Target for Thin Film Electrodes in Lithium Microbatteries. VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия. 6th Russian Conference „Physical Problems of Hydrogen Energetics”, November 22-24, Saint Petersburg (Russia). Abstract 2 pages.
61. M. Haļitovs, G. Ķizāne, A. Vītiņš, E. Pajuste, A. Kirillova, J. Gabrusenoks. Tritium accumulation in the tiles of the JET divertor. – In the book: Institute of Solid State Physics. University of Latvia. Abstracts of the 26<sup>th</sup> Scientific Conference. / Ed. by A. Krūmiņš. – Riga, February 17-19, 2010. – P. 69.
62. V. Zubkovs, G. Ķizāne, A. Vītiņš, E. Pajuste, J. Jansons. Tritium thermo diffusion from the ITER relevant beryllium pebbles. – In the book: Institute of Solid State Physics. University of Latvia. Abstracts of the 26<sup>th</sup> Scientific Conference. / Ed. by A. Krūmiņš. – Riga, February 17-19, 2010. – P. 70.
63. A. Vitins, V. Zubkovs, G. Kizane, E. Pajuste, G. Ivanov. Tritium release properties of beryllium products for fusion devices. – In the book: International conference “Functional Materials and Nanotechnologies 2010” (FM&NT-2010). Conference program. Book of abstracts. Riga, March 16-19, 2010. – Institute of Solid State Physics, University of Latvia, Riga, 2010. – P. 132.
64. A. Vitins, V. Zubkovs, G. Kizane, E. Pajuste, V. Kinerte. Tritium release characteristics of neutron-irradiated reference beryllium pebbles for the helium cooled pebble bed (HCPB) blanket. – In the book: 9th International Conference on Tritium Science and Technology “Tritium 2010”, Nara, Japan, October 24-29, 2010. Abstracts. – National Institute for Fusion Science, Japan, 2010. – P. 93. – Available online at the website: <http://tritium2010.nifs.ac.jp/>
65. [http://tritium2010.nifs.ac.jp/Topic3/3\\_x\\_273\\_Vitins\\_Aigars\\_Tritium\\_Release\\_Characteristics\\_of\\_Neutr.pdf](http://tritium2010.nifs.ac.jp/Topic3/3_x_273_Vitins_Aigars_Tritium_Release_Characteristics_of_Neutr.pdf)

### Participation in Conferences

#### **Annual 25<sup>th</sup> Conference of Institute of Solid State Physics of University of Latvia, February 11-13, 2009, Riga, Latvia:**

1. J.Gabrusenoks Phase stability of ordered Pb<sub>2</sub>ScTaO<sub>6</sub> crystal lattice, LU cietvielu fizikas institūta 26. Zinātniskā konference, tēzes, 2010g. 17.-19.febr., lpp. 35.
2. G.Vaivars, I.Baiža, E.Gžibovska. Electro-conductive ion liquids and they potential application in hydrogen energy devices.
3. L. Grīnberga, Photocatalysis for hydrogen production.
4. G. Kučinskis, J. Šmits, G. Bajārs, J. Kleperis, G. Čikvaidze, Investigation of structure and impedance of lithium iron phosphate.
5. J. Šmits, G. Kučinskis, G. Bajārs, J. Kleperis, J. Balodis, LiFePO<sub>4</sub> thin film coatings as cathode materials for thin film lithium power sources.
6. G.Vaivars, K.Jurģelis, A.Krjučkovska. Polyether ether ketone membranes for hydrogen separation from gas mixtures.

7. L. Grīnberga, L. Kuļikova, V. Serga, J. Kleperis, Hydrogen sorption of modified SiO<sub>2</sub> glass.
8. J. Blūms, M. Vanags, J. Kleperis, Temperature influence on the power efficiency of commercial photovoltage batteries.
9. I. Dirba, Critical analysis of possibilities to use geomagnetic energy.
10. Z. Lapiņa, V. Ogorodņiks, J. Kleperis, Search for rapid diagnostic methods to detect wheat diseases.
11. V. Kuzmovs, J. Kleperis, Available driving distance of electric - hydrogen cars and possibilities to make it larger.
12. J. Dimants, B. Sloka, J. Kleperis, Success examples of hydrogen economy in the world and what can Latvia learn from them.
13. Gruduls, I. Klepere, G. Bajārs, J. Kleperis, Black platinum electrode for measurement the concentration of dissolved hydrogen in liquids.
14. J. Hodakovska, G. Čikvaidze, J. Kleperis, Proton and electron conducting membranes for fuel cells.
15. M. Vanags, G. Bajārs, J. Kleperis, Conditions of minimal reaction energy for electrolysis and possibilities to reduce it.
16. Klepere, I. Muižnieks, J. Kleperis. Formation of hydrogen gas oversaturated liquid in bioreactor with hydrogen producing bacteria *E. Coli*.
17. E. Rancāns, L. Grīnberga, J. Kleperis, Sample activation rate dependence on grain size.
18. M. Haļitovs, G. Ķizāne, A. Vītiņš, E. Pajuste, A. Kirillova, J. Gabrusenoks. Tritium accumulation in the tiles of the JET divertor. (Oral presentation by M. Haļitovs.)
19. V. Zubkovs, G. Ķizāne, A. Vītiņš, E. Pajuste, J. Jansons. Tritium thermo diffusion from the ITER relevant beryllium pebbles. (Oral presentation by V. Zubkovs.)

**International Conference "Functional Materials and Nanotechnologies" (FM&NT-2010), Riga, Latvia (16-19.03.2010):**

1. J. Gabrusenoks Lattice dynamics and phase transitions of AlF<sub>3</sub>, Abstracts, Int.conf. FMNT 2010, Riga, March 16-19 2010, p.190.
2. G. Bajars, J. Smits, G. Kucinskis, J. Kleperis. Study of Structure and Electrochemical Characteristics of LiFePO<sub>4</sub>/C as Cathode Material for Lithium Batteries.
3. J. Kleperis, M. Vanags, J. Hodakovska, J. Klavins. Oriented Nanostructures for Solar-Hydrogen Technologies.
4. J. Hodakovska, J. Kleperis. SPEEK and PANI based membranes for fuel cells.
5. M. Vanags, J. Kleperis, G. Bajars. Short Duration Voltage and Current Transients on Water Electrolysis Cell.
6. L. Grinberga, Nanosized Perovskites for Photocatalytical Water Decomposition.
7. H. Luo, G. Vaivars, S. Nonjola, M. Rohwer, M. Mathe. Anion Exchange Membrane Based on Alkali Doped Poly(2,5-benzimidazole) for Alkaline Membranes Fuel Cell.
8. A. Vitins, V. Zubkovs, G. Kizane, E. Pajuste, G. Ivanov. Tritium release properties of beryllium products for fusion devices. (Poster presentation by A. Vītiņš.)

**7th International Conference Of Young Scientists On Energy Issues Cyseni 2010; May 26-27, 2011, Lithuanian Energy Institute, Kaunas, Lithuania**

1. J. Hodakovska, G. Chikvaidze, J. Kleperis. Electron and proton conductive polymer membranes for fuel cells.

2. M. Vanags, J. Kleperis, G. Bajars. Water electrolyses powered with inductive spikes.
3. P. Shipkovs, A. Snegirjovs, M. Vanags, K. Lebedeva, J. Shipkovs, L. Vasilevska, M. Pankars. Comparison of solar collectors operation methods.
4. J. Blums, M. Vanags, J. Kleperis. Effect of ambient temperature on commercial photovoltaic solar cells.

**18th World Hydrogen Energy Conference WHEC 2010, May 16–21, 2010, Messe Essen (Germany):**

1. Julija Hodakovska, G. Chikvaidze, J. Kleperis, Multiple-layered proton-electron conductive polymer membrane for fuel cells.
2. LATVIA: The Latvian competition focused on the topic “Fuel Cell and Hydrogen Technology usage in transport”. Armands Ikaunieks, Lauris Ozolins, Martins Melkis and teacher Ieva Rodzina (Ziemeļvalstu Ģimnazija, Rīga, Latvia), Consulting J.Kleperis

**9<sup>th</sup> International Symposium on Systems with Fast Ionic Transport (9<sup>th</sup> ISSFIT), June 1 – 5, 2010, Riga, University of Latvia (Latvia):**

1. G. Bajars, J. Kleperis, G. Kucinskis, J. Smits, G. Chikvaidze Physical and electrochemical properties of LiFePO<sub>4</sub>/C thin films deposited by DC and RF magnetron sputtering.
2. G. Kucinskis, G. Bajars, J. Kleperis, A. Lūsis, J. Smits Kinetic characteristics of LiFePO<sub>4</sub>/C thin films.
3. J. Kleperis, L. Grinberga, A. Lūsis Energy storage solutions using hydrogen insertion compounds.
4. L. Grinberga, E. Rancans, J. Kleperis An impact of grain size on the rate of hydrogen sorption in LaNi<sub>5</sub>.
5. M. Vanags, G. Bajars, J. Kleperis, A. Lūsis Peculiarities of short pulse water electrolysis: Ion transport and discharge at electrodes.

**9th International Hydrogenase Conference (H<sub>2</sub>ase), June 27 – July 2, 2010, Uppsala (Sweden):**

1. Klepere I., Gruduls A., Nikolajeva V., Kleperis J., Muiznieks I. Bio-hydrogen production from industrial food waste by anaerobic microorganism associations.

**EACES 2010; 11th Bi-Annual Conference on European Association for Comparative Economic Studies: Comparing Responses to Global Instability. August 26-28, 2010, Tartu, Estonia:**

1. J. Dimants, B. Sloka, J. Kleperis, I. Klepere. Hydrogen as innovative technology for a sustainable energy supply.

**XII International Symposium on Polymer Electrolytes ISPE-12; 29 August - 3 September 2010, Padova, Italy:**

1. G. Vaivars, K. Jurgelis, I. Klepere. Hydrogen diffusion in modified poly(ether ether ketone) membranes.

**International Conference „Employability & Entrepreneurship”- 2nd Edition, September 27-28, 2010; Porto, Portugal:**

1. J. Dimants, B. Sloka, J. Kleperis, I. Klepere. Course on Alternative energy as a Road map for a Sustainable Public Education.

**61<sup>st</sup> Annual Meeting of the International Society of Electrochemistry „Electrochemistry from Biology to Physics”, September 26 - October 1, 2010, Nice (France):**

1. Gunars Bajars, Gints Kucinskis, Janis Smits, Janis Kleperis, Martins Vanags. Kinetic Behavior of LiFePO<sub>4</sub>/C Thin Film Cathode Material for Lithium-Ion Batteries. Abstracts of 61<sup>st</sup> Annual Meeting of the International Society of Electrochemistry „Electrochemistry from Biology to Physics”, September 26 - October 1, 2010, Nice (France). Format CD, 1 page.
2. Martins Vanags, Janis Kleperis, Gunars Bajars, Andrejs Lasis. Peculiarities of water electrolysis with high voltage short pulses. Abstracts of 61<sup>st</sup> Annual Meeting of the International Society of Electrochemistry „Electrochemistry from Biology to Physics”, September 26 - October 1, 2010, Nice (France). Format CD, 1 page.

**The 4th International Conference “Environmental Science and Education in Latvia and Europe: From Green projects to Green society”, 22 October, 2010, Latvia University of Agriculture, Jelgava (Latvia):**

1. Janis Kleperis, Biruta Sloka, Justs Dimants, Ilze Klepere. Interdisciplinary Courses on Renewable Energies in Latvian Higher Education Establishments and Hydrogen Technologies.
2. Justs Dimants, Ilze Klepere. Teaching Renewables for Master Program Students at the School for Renewable Energy Science in Iceland: Sharing Study Experience.
3. Gunars Bajars, Janis Kleperis, Liga Grinberga, Martins Vanags. Study Course „Sources Of Energy And Their Environmental Impacts” At The University Of Latvia; Studiju Kurss „Enerģijas Avoti Un To Ietekme Uz Vidi” Latvijas Universitātē.

**VI Российская Конференция "Физические проблемы водородной энергетики" 22–24 ноября 2010 года; Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия**

1. G. Bajars, M. Vanags and J. Kleperis. Efficiency Improvement of Water Electrolysis for Hydrogen Production.
2. J. Kleperis, G. Bajars, B. Sloka, J. Dimants. Integration the Renewable Energy and Hydrogen Technology Topics in Latvian Higher Education Establishments.
3. L. Grinberga, J. Kleperis, L. Kulikova, V. Serga. Hydrogen Sorption of Modified Oxides.
4. I. Klepere, A. Gruduls, V. Nikolajeva, I. Muižnieks and J. Kleperis. Bio-Hydrogen Application Possibilities in Latvia: Substrates and Microorganism Research Using Micro-Electrodes And Test-System Fermentation Reactor.
5. I. Dirba, M. Vanags, J. Kleperis. Upgrading the Wind Power Generator for Direct Hydrogen Production.
6. G. Kucinskis, J. Smits, L. Grinberga, G. Bajars, J. Kleperis. Physical and Electrochemical Characteristics of LiFePO<sub>4</sub>/C Thin Film Cathode Material for Lithium-Ion Batteries.
7. J. Hodakovska, V. Nemcevs, G. Cikvaidze, J. Kleperis. SPEEK and PANI Based Membranes for Fuel Cells.
8. J. Smits, L. Grinberga, G. Kucinskis, G. Bajars and J. Kleperis. Preparation of LiFePO<sub>4</sub>/C Target for Thin Film Electrodes in Lithium Microbatteries.

**The 9<sup>th</sup> International Conference on Tritium Science and Technology “Tritium 2010”, Nara, Japan, October 24-29, 2010:**

A. Vitins, V. Zubkovs, G. Kizane, E. Pajuste, V. Kinerte. Tritium release characteristics of neutron-irradiated reference beryllium pebbles for the helium cooled pebble bed (HCPB) blanket. (Poster presentation by A. Vītiņš.)

# LABORATORY OF THEORETICAL PHYSICS AND COMPUTER MODELLING

**Head of Laboratory 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).

## **Scientific staff**

1. Dr. hab. E. Kotomin
2. Dr. hab. V. Kuzovkov
3. Dr. O. Dumbrajs
4. Dr. R. Eglitis
5. Dr. D. Gryaznov
6. Dr. V. Kashcheyevs
7. Dr. Yu. Mastrikov
8. Dr. S. Piskunov
9. Dr. A. Popov
10. Dr. Yu. Zhukovskii
11. Dr. G. Zvejnieks

## **PhD students**

12. D. Bocharov
13. A. Gopejenko

## **MsC students**

14. J. Shirmane

## **Scientific visits abroad**

1. Dr. hab. E. Kotomin, Max Planck Institute for Solid State Research, Stuttgart, Germany (8 months), The Eurasian University, Astana, Kazakhstan (2 weeks).
2. Dr. hab. V. Kuzovkov; Northwestern University, Evanston, USA (3.5 months).
3. Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (1 month), University of Maryland, USA (1 month), University of Fukui, Japan (3 months), Karlsruhe Institute of Technology, Germany (1 month).
4. Dr. D. Gryaznov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (7 months), Imperial College London, UK (2 months)
5. Dr. Yu. Mastrikov, University of Maryland, USA (10 months).
6. Dr. S. Piskunov, University of Duisburg-Essen (1 month).
7. Dr. A. Popov, Max Planck Institute for Solid State Research, Stuttgart, Germany (2 months), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (10 weeks)

8. Dr. Yu. Zhukovskii, Institute for Materials Research-I, Karlsruhe, Germany (1 month), St. Petersburg State University, Russia (1 week), Technical University of Braunschweig, Germany (3 weeks)
9. D. Bocharov, EC Institute of Transuranum Elements, Karlsruhe, Germany (1 week).
10. A.Gopejenko, Forschungszentrum Karlsruhe, Institut für Materialforschung I, Karlsruhe, Germany (2 months).

### **International Cooperation**

<b>France</b>	1. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober)
	2. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)
	3. Physikalisch-Technische Bundesanstalt, Braunschweig (Dr. Bernd Kästner).
	4. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm)
	5. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov)
<b>Germany</b>	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)
	9. Institut für Materialforschung I (KIT), Karlsruhe (Dr. A. Möslang)
<b>Greece</b>	10. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. K. Avramides)
<b>Israel</b>	11. Ben Gurion University, Beer Sheeva (Prof. A. Aharony, Prof. D. Fuks)
<b>Italy</b>	12. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
<b>Japan</b>	13. FIR Center, University of Fukui (Prof. T. Idehara)
<b>Lithuania</b>	14. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
<b>Poland</b>	15. Warwaw University, Dept of Chemistry (Dr A. Huczko)
<b>Romania</b>	16. University of Craiova (Dr. D. Constantinescu)
<b>Russia</b>	17. St. Petersburg University (Prof. R.A. Evarestov)
<b>UK</b>	18. Imperial College London (Prof. M.Finnis)
	19. University College London (Prof. A.L. Shluger)
<b>Ukraine</b>	20. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)
	21. Idaho National Laboratory (Dr. S.N. Rashkeev)
<b>USA</b>	22. Northwestern University, Evanston, Illinois (Prof. M.Olvera de la Cruz, Prof. D.E. Ellis)
	23. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

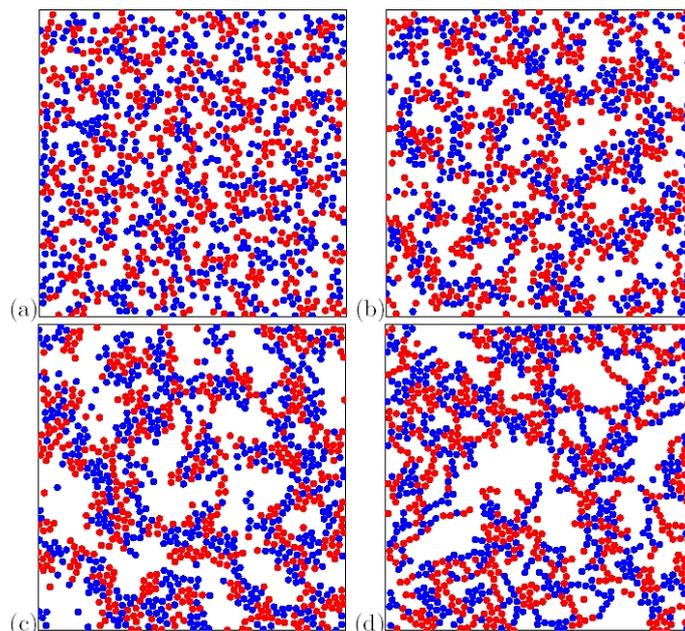
### **Main Results**

#### **THE MICROSCOPIC APPROACH TO KINETICS OF PATTERN FORMATION OF CHARGED MOLECULES ON SURFACES/INTERFACES**

V.N. Kuzovkov, G. Zvejnieks, E.A. Kotomin,  
M. Olvera de la Cruz (*Northwestern University, Evanston, USA*)

Patterning of surfaces is of paramount importance in biophysics, chemistry, technology. In particular, charged patterns generated by the adsorption of cationic and anionic

molecules on surfaces and on membranes is of great importance in electrochemistry and biosciences.



**Fig.1.** Fragments of the characteristic snapshots obtained using the reverse Monte Carlo for the correlation functions

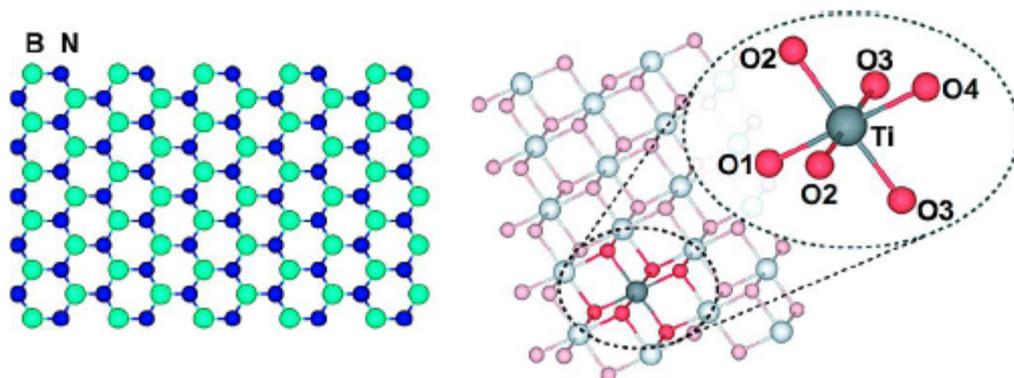
*In collaboration with Northwestern University, Evanston, USA, a microscopic formalism based on computing many-particle densities was applied to the analysis of the diffusion-controlled kinetics of pattern formation of oppositely-charged molecules on surfaces or adsorbed at interfaces with competing long-range Coulomb and short-range Lennard-Jones interactions. Particular attention was paid to the proper molecular treatment of energetic interactions driving pattern formation in inhomogeneous systems. The reverse Monte Carlo method is used to visualize the spatial molecular distribution based on the calculated radial distribution functions (joint correlation functions). We have shown the formation of charge domains for certain combinations of temperature and dynamical interaction parameters. The charge segregation evolves into quasi-crystalline clusters of charges, due to the competing long- and short-range interactions.*

## **FIRST-PRINCIPLES CALCULATIONS ON SINGLE-WALLED BN AND TiO<sub>2</sub> NANOTUBES AND THEIR SYMMETRY ANALYSIS**

Yu. Zhukovskii, S. Piskunov,

R.A. Evarestov, A.V. Bandura (*Department of Quantum Chemistry, St. Petersburg University, Russia*)

Use of the line group formalism allows us the construction of nanotubes of different crystalline morphology. The exploitation of the rotohelical symmetry for NTs permits drastic reductions of the computation time. A new approach to the generation of the line group irreducible representations developed *in collaboration with Prof. R.A. Evarestov and Dr. A.V. Bandura (St. Petersburg University, Russia)* is based on the isomorphism between line and plane groups. The application of the approach has been used for thorough theoretical description of BN and TiO<sub>2</sub> single-wall (SW) nanotubes (NTs) of both hexagonal and centered rectangular morphologies.



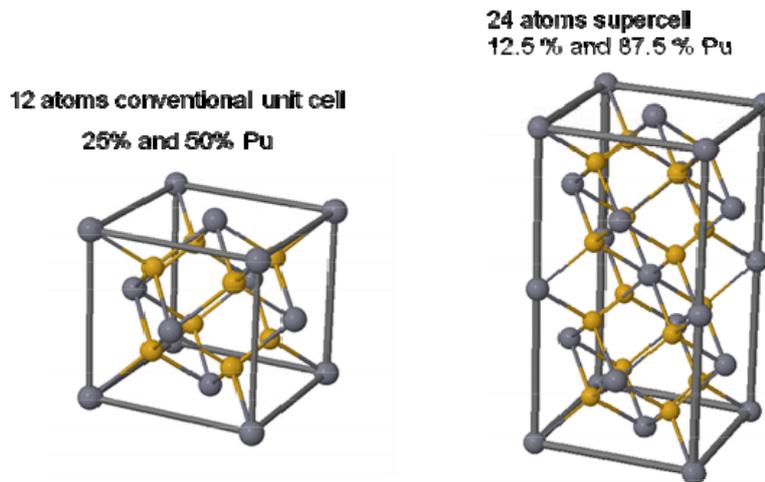
**Fig. 2.** Stoichiometric hexagonal sheets of BN(0001) and TiO<sub>2</sub>(111) scrolling to SW NTs

Large scale *ab initio* LCAO calculations have been performed for the analysis of the atomic and electronic structure of BN and TiO<sub>2</sub> 2D sheets and 1D nanotubes produced from the former by rolling up. For this aim, there was applied the hybrid Hartree-Fock/Kohn-Sham exchange-correlation functional *PBE0* with the total geometry relaxation as implemented in the *CRYSTAL* code. To optimize the atomic basis sets, necessary for the proper calculations there was applied the original program package *OPTBAS* interfaced with *CRYSTAL* code. The strain energies of SW BN and TiO<sub>2</sub> nanotubes of different chiralities have been found to be reduced with increasing NT diameter approaching to minimum energy limit beginning with nanotube diameter > 2 nm while their energy band gaps approach to those for the corresponding 2D slabs. To gain a deeper theoretical insight into the technologically important BN and TiO<sub>2</sub> nanomaterials, the next step is outlined to be simulations on the double-wall boron nitride and titania nanotubes.

## POINT DEFECT MODELLING IN NUCLEAR FUELS

D. Gryaznov, Yu. Mastrikov, Yu. Zhukovskii, E. Kotomin,  
P. Van Uffelen (*EC Institute for Transuranium Elements, Karlsruhe, Germany*)  
S.N. Rashkeev (*Idaho National Laboratory, USA*)  
E. Heifets (*Max Planck Institute, Stuttgart, Germany*)

UO<sub>2</sub> and (U,Pu)O<sub>2</sub> solid solutions (the so-called MOX) nowadays are used as commercial nuclear fuels. One of the safety issues during the storage of these fuels is related to their self-irradiation that produces and accumulates point defects and helium therein. *In close collaboration with Dr S. Rashkeev (Idaho National Laboratory) and Dr Van Uffelen (EC Institute for Transuranium Elements, Karlsruhe, Germany)* we have performed DFT calculations on UO<sub>2</sub>, PuO<sub>2</sub> and MOX crystalline solids containing He atoms in octahedral interstitial positions.



**Fig.3.** Two models of Pu atom substitutes for U in MOX solid solutions.

In particular, we have calculated the basic MOX properties and He incorporation energies as functions of Pu concentration within the spin-polarized, generalized gradient approximation (GGA) DFT calculations. We have also included the on-site electron correlation corrections using the Hubbard model (in the framework of the so-called DFT + U approach). We have found that PuO<sub>2</sub> remains semiconducting with helium impurity atom in the octahedral position while UO<sub>2</sub> requires a specific lattice distortion. Both materials reveal a positive energy for He atom incorporation, which, therefore, is an exothermic process. He incorporation energy increases with the Pu concentration in the MOX fuel.

### COMPUTER MODELLING OF IMPURITY CLUSTERS IN ODS STEELS

A. Gopejenko, Yu. Zhukovskii, E. Kotomin,  
P.V. Vladimirov, A. Möslang (*Institut für Materialforschung I, Karlsruhe, Germany*)  
V.A. Borodin (*Research Center Kurchatov Institute, Moscow, Russia*)

Development of the oxide dispersion strengthened (ODS) steels for fission and fusion reactors requires a deep understanding of the mechanism and kinetics of Y<sub>2</sub>O<sub>3</sub> nanoparticle precipitation in the steel matrix. Therefore, it is necessary to perform a large-scale theoretical modeling of the Y<sub>2</sub>O<sub>3</sub> formation. A series of first principles calculations were performed in *collaboration with Dr. A. Möslang and Dr. P.V. Vladimirov (Institut für Materialforschung I, Karlsruhe, Germany)* on different nanoclusters consisting of pair and triple solute atoms and containing: (i) the Y-Fe-vacancy pairs, (ii) the two Y atoms substituted for Fe lattice atoms and (iii) the O impurity atoms dissolved in *fcc*-Fe matrix. The latter is represented by a face-centered cubic  $\gamma$ -Fe single crystal. This structure is relevant because a phase transition  $\alpha \rightarrow \gamma$  occurs in low Cr ferritic-martensitic steels at typically hot isostatic pressing temperatures. The results clearly demonstrate a certain attraction between the Y substitute and Fe vacancy whereas no binding has been found between the two Y substitute atoms. Results of calculations on different Y-O-Y cluster configurations in lattice show that not only a presence of oxygen atom favors a certain binding between the impurity atoms inside the  $\gamma$ -Fe lattice but also the increased concentration of Fe vacancies is required for the growth of the Y<sub>2</sub>O<sub>3</sub> precipitates within the iron crystalline matrix

## FIRST-PRINCIPLES CALCULATIONS OF COMPLEX PEROVSKITES FOR FUEL CELLS AND PERMEATION MEMBRANE APPLICATIONS

E. A. Kotomin, D. Gryaznov,  
J. Maier, R. Merkle, V. Alexandrov, E. Heifets  
(*Max Planck Institute, Stuttgart, Germany*)  
Yu. Mastrikov, M.M. Kuklja (*Maryland University, USA*)  
M. Finnis (*Imperial College London, UK*)

Mixed conducting ABO<sub>3</sub>-type perovskites have been used as cathode materials in solid oxide fuel cells (SOFC) since early 1980s, and La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3±δ</sub> (LSM) was the first material which found wide application. Currently, Ba<sub>0.5</sub>Sr<sub>0.5</sub>Co<sub>0.75</sub>Fe<sub>0.25</sub>O<sub>3-δ</sub> (BSCF) shows the best oxygen exchange performance, despite several drawbacks. As it is well understood now, *both* high oxygen vacancy concentration at the SOFC cathode surface and high vacancy mobility are two key factors controlling high BSCF material performance.

While vacancy concentrations and mobilities in the materials bulk are available from experiments, the respective quantities for the surface layer - which are decisive for the surface reaction - are almost impossible to be measured. Thus, *in collaboration with the Max Planck Institute, Stuttgart, Germany, and Maryland University, USA*; we performed an extensive set of large-scale first principles DFT calculations. We have analyzed the atomic and electronic structure of oxygen vacancies, their formation and migration energies in the bulk and in the surface layer and how these properties depend on the chemical composition of the host perovskite. We have shown that optimal BSCF chemical composition is 50-50-80-20 percent.

*In collaboration with Prof. M. Finnis (Imperial College London)* a detailed study of the electron correlation effects was performed for the pure and defective LaCoO<sub>3</sub> and (La,Sr)(Co,Fe)O<sub>3</sub>. In particular, the results of the electronic and magnetic structure obtained using the GGA+U and hybrid exchange-correlation functionals were compared, the oxygen vacancy formation energy estimated as a function of the temperature.

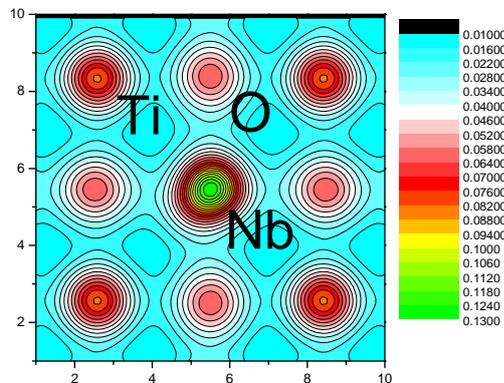
## FIRST-PRINCIPLES CALCULATIONS OF PURE AND DEFECTIVE PEROVSKITE AND FLUORITE SURFACES

R. Eglitis, E.A. Kotomin,  
M. Rohlfing (*Universität Osnabrück, Germany*)  
H. Shi, X. He (*School of Science, Beijing Institute of Technology, China*)  
R. Jia (*Bergische Universität Wuppertal, Germany*)  
A. Vassilyeva, A. Dauletbekova (*L. Gumilyov National University, Astana, Kazakhstan*)

*In collaboration with University of Osnabruck, Germany*, we performed calculations of the surface relaxations, rumplings, energetics, optical band gaps, and charge distribution for the SrZrO<sub>3</sub> and PbZrO<sub>3</sub> (001) and (011) surfaces using the *ab initio* code CRYSTAL and a hybrid exchange-correlation functionals. Both SrO(PbO) and ZrO<sub>2</sub> terminations of the (001) surface and Sr(Pb), ZrO, and O terminations of the polar SrZrO<sub>3</sub> and PbZrO<sub>3</sub> (011) surfaces were studied. We predict a considerable increase in the Zr-O chemical bond covalency near the SrZrO<sub>3</sub> and PbZrO<sub>3</sub> (011) polar surfaces as compared to both the bulk and to the (001) surface.

We have calculated also properties of Nb impurities substituting for Ti ions in SrTiO<sub>3</sub> perovskite using supercells containing 135 atoms. The local structure optimisation, the electronic charge redistribution, chemical bond covalence and the band-structure changes induced by the defects were analyzed. According to the results of our

calculations, Nb is a shallow donor; six nearest O atoms are slightly displaced outwards from the Nb ion. The calculated bond population between nearest Ti and O ions (64 me) is much larger than that between Nb and O ions (8 me), since Nb impurity is more ionic than the host Ti.



**Fig.4.** Charge density map of Nb doped SrTiO<sub>3</sub> bulk from (001) side view

Similar calculations were also performed *in collaboration with L.Gumilyov University, Kazakhstan* for optical materials-- MgF<sub>2</sub> (001) and (011) surfaces. These neutral and polar surfaces show very small relaxation and negligible increase of covalent contribution to the chemical bonding thus remaining considerably ionic. The calculated bulk optical band gap is in a good agreement with the experimental value, whereas optical band gap for the polar (011) surface is reduced by 0.6 eV compared with the calculated bulk value, in contrast to the (001) surface gap which remains very close to the bulk.

The ground state of interstitial F ions (*H*-centres) was calculated in SrF<sub>2</sub> for two different arrangements, which are oriented along either [100] or [111] axes. The local atomic relaxation and charge redistribution are discussed. Lastly, we studied also two different configurations of the *H* center at the BaF<sub>2</sub> (111) surface which considerably differ in the electron density, lattice relaxation and spin distributions.

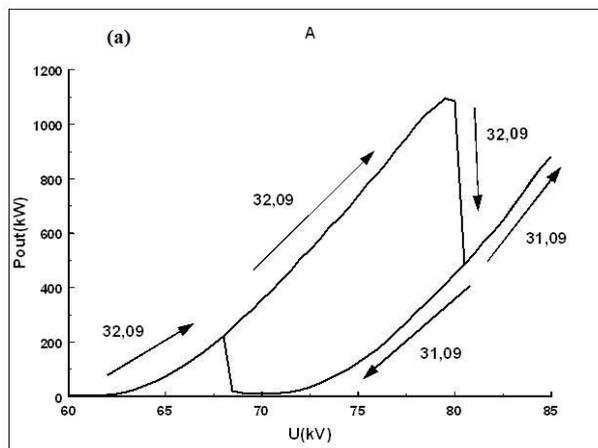
## ON THE THEORY OF HIGH-POWER GYROTRONS WITH UPTAPERED RESONATORS

O. Dumbrajs

G.S. Nusinovich (*Institute for Research in Electronics and  
Applied Physics, University of Maryland, USA*)

In high-power gyrotrons it is desirable to combine an optimal resonator length with the optimal value of the resonator quality factor. In resonators with the constant radius of the central part, the possibilities of this combination are limited because the quality factor of the resonator sharply increases with its length. Therefore, the attempts to increase the length for maximizing the efficiency leads to such increase of the quality factor which makes the optimal current too small. Resonators with slightly uptapered profiles offer more flexibility in this regard. In such resonators, one can separate optimization of the interaction length from optimization of the quality factor, because the quality factor determined by diffractive losses can be reduced by increasing the angle of uptapering.

These issues were analyzed *in collaboration with Maryland University*, by studying a typical high-power 170GHz gyrotron which is currently under development in Europe for ITER (<http://en.wikipedia.org/wiki/ITER>). The effect of a slight uptapering of the resonator wall on the efficiency enhancement and the purity of the radiation spectrum in the process of the gyrotron start-up and power modulation are studied. Results show that optimal modification of the shape of a slightly uptapered resonator may result in increasing the gyrotron power from 1052kW to 1360kW .



**Fig. 5.** Output power as a function of voltage in a gyrotron with the cavity *A*. Calculations were carried out from 60kV to 85kV and from 85kV to 60kV . The parasitic  $TE_{31,09}$  parasitic is excited at 80.5kV . Due to the hysteresis, this mode survives when the voltage decreases until 64.5kV where the operating  $TE_{32,09}$  mode reappears. A clear hysteresis loop can be observed.

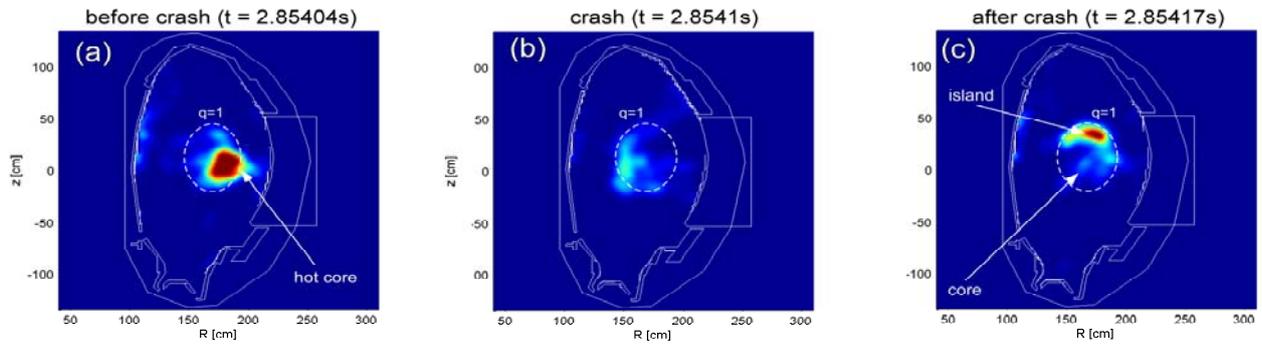
## STRUCTURE AND DYNAMICS OF SAWTEETH CRASHES IN ASDEX UPGRADE

O. Dumbrajs

V. Igochine, S. Günter, H. Zohm, K. Lackner, G. Pereverzev  
( *MPI für Plasmaphysik, Garching, Germany* )

J. Boom, I. Classen (*FOM-Instituut voor Plasmafysica Rijnhuizen, Nieuwegein,  
The Netherlands*)

The crash phase of the sawteeth in ASDEX Upgrade tokamak was investigated in detail by means of soft X-ray (SXR) and electron cyclotron emission (ECE) diagnostics. Analysis of pre-cursor and post-cursor (1,1) modes shows that the crash does not affect the position of the resonant surface  $q=1$ . Our experimental results suggest that sawtooth crash models should contain two ingredients to be consistent with experimental observations: (1) the (1,1) mode structure should survive the crash; (2) the flux changes should be small to preserve the position of the  $q=1$  surface close to its original location. Detailed structure of the reconnection point was investigated with ECE imaging diagnostic. It is shown that reconnection starts locally. The expelled core is hot which is consistent with SXR tomography results. The observed results can be explained in the framework of a stochastic model.



**Fig.6.** Soft X-ray tomography of the sawtooth crash (#25854,  $t=2.85$ s). Three different time frames are shown: (a) hot core rotates in clockwise direction before the crash; (b) crash phase; (c) hot island rotates in clockwise direction after the crash.  $q=1$  position is marked by the dashed line. (Each figure has its own color scheme to increase the contrast.)

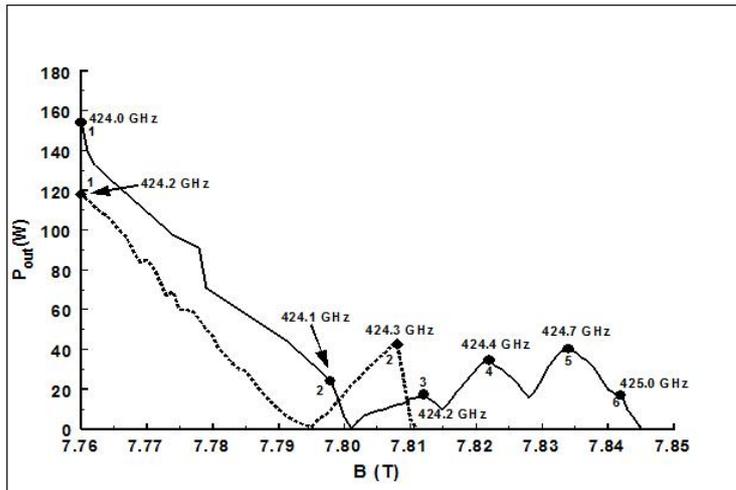
It should be noted that electrons with different azimuthal coordinates of guiding centers exhibit different dynamics in the process of mode switching. This can be considered as a specific feature of the electron interaction with the fields of more than one mode. In the case of single-mode operation, electrons with different azimuthal coordinates of guiding centers exhibit the same behavior in the phase space. However, in the process of mode switching, where two modes are present, electron dynamics depends on the azimuthal coordinate of the guiding center. This can be explained by the fact that the phase difference of these modes is azimuthally dependent. This conclusion can be illustrated by the right figure in the second row in Fig. 2 showing electron distribution at the exit for  $t=72$

## DESIGN OF AN OPTIMIZED RESONANT CAVITY FOR A COMPACT SUB-TERAHERTZ GYROTRON)

O. Dumbrajs

T. Idehara, S. Sabchevski (*Research Center for Development of Far-Infrared Region, University of Fukui, Japan*)

Coherent sources of radiation in the sub-terahertz and the terahertz frequency range are in great demand for various spectroscopic studies (e.g. electron spin resonance spectroscopy, DNP/NMR spectroscopy *etc.*). The required levels of the output power as well as the needed specific spectral characteristics make the gyrotrons the most promising and high-performance devices for such applications. Recently, an initial design of a versatile second harmonic gyrotron utilizing a compact cryo-free 8T superconducting magnet has been accomplished. *In collaboration with the University of Fukui, Japan*, we presented an optimized resonator for this gyrotron. Instead of a regular (cylindrical) part as in the conventional cavities it contains an uptapered section. Such configuration offers a significant increase of the efficiency and improves the overall performance of the tube.



**Fig. 7.** Output power and frequency as a function of the magnetic field in the cylindrical cavity (dashed) and in the uptapered cavity (solid). Positions of the axial wave numbers  $q$  are marked by diamonds and dots respectively. The output power forms a fingerlike shape. In the mode transition region, the output power is small but nonzero and the oscillation frequency can be smoothly tuned.

## BASIC PROPERTIES OF THE F-TYPE CENTERS IN HALIDES, OXIDES AND PEROVSKITES

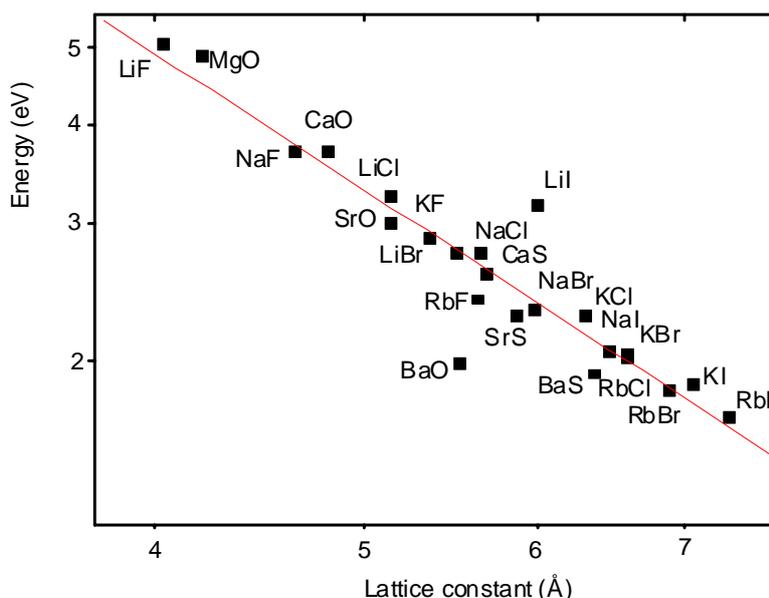
A.I. Popov , E.A. Kotomin

J. Maier (*Max Planck Institute for Solid State Research, Stuttgart, Germany*)

Recently, *in collaboration with Prof. J. Maier from Max Planck Institute for Solid State Research, Germany* we presented (Nucl. Instr. Meth. B, 2010, 268, p. 3084-3089) a short survey of the optical properties of primary radiation-induced point defects in alkali halides, simple oxides and some  $ABO_3$  perovskites. We have discussed in details the optical properties of the single-electron  $F$  and  $F^+$  centers in rock-salt (f.c.c.) alkali halides and oxides and show that the Mollwo-Ivey law well-known for the  $F$ -type centers in alkali halides may be extended for other rock-salt structure insulators (Fig.8).

We discussed in details the major differences in point defect production mechanisms in halides and oxides. It was known for a long time that in alkali halides with NaCl (f.c.c.) structure absorbed energy to produce the  $F-H$  pair varied inversely with the space available to accept an interstitial ion. It can be characterised by  $S/D$ , the ratio of the separation between halogen ions in the [110] direction and the diameter of the halogen ion  $D$ .

We have shown how the Rabin-Klick diagram may be generalized for a whole family of alkali halides (NaCl (f.c.c.) CsCl (b.c.c.) structures. The  $F$ -type center migration and aggregation into metal colloids in alkali halides and oxides was also discussed.



**Fig.8.** The generalized plot of Mollwo-Ivey relation for the  $F$  band in alkali halides and  $F^+$  oxides and sulfides with f.c.c. structure.

### SURFACTANT-ASSISTED SYNTHESIS OF $Cd_{1-x}Co_xS$ NANOCLUSTER ALLOYS AND THEIR STRUCTURAL, OPTICAL AND MAGNETIC PROPERTIES

A.I. Popov

R. Sathyamoorthy, P. Sudhagar (*R & D Department of Physics, Kongunadu Arts & Science College, Coimbatore, Tamilnadu, India*);

A. Balerna, S. Bellucci (*INFN-Laboratori Nazionali di Frascati, Frascati, Italy*);

C. Balasubramanian (*Facilitation Centre for Industrial Plasma Technologies, Institute for Plasma Research, Bhat, Gandhinagar 382428, India*);

K. Asokan (*Inter University Accelerator Centre, New Delhi, India*);

The synthesis of Co-doped CdS nanoclusters ( $Cd_{1-x}Co_xS$ ) was performed for different doping concentrations ( $x = 0.10, 0.20$  and  $0.30$ ) and characterization of their structural, optical, and magnetic properties. The structural properties studied by X-ray diffraction revealed hexagonal-greenockite structure and a decrease of the lattice parameters ( $a$  and  $c$ ) with doping, showing incorporation of Co in the lattice. The morphology of the nanoclusters was studied by scanning electron microscopy. The optical absorption studies, using diffused reflectance spectroscopy, revealed that Co doping modifies the absorption band edge. Ferromagnetic phase was observed in the magnetization measurements at room-temperature due to high carrier concentration. X-ray absorption near edge fine structure measurements at the sulfur (S) K-edge of the Co-doped samples revealed that the valence remains divalent and that there are some changes with Co doping in the spectral intensity

## Scientific publications

### SCI

1. Yu.A. Mastrikov, M.M. Kuklja, E.A. Kotomin, and J. Maier, First-principles modelling of complex perovskite  $(\text{Ba}_{1-x}\text{Sr}_x)(\text{Co}_{1-y}\text{Fe}_y)\text{O}_{3-d}$  for solid oxide fuel cell and gas separation membrane applications. - *Energy Environ. Sci.*, 2010, 3, p. 1544–1550.
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#### **Presentations at scientific conferences, congresses, meetings, schools and workshops**

##### **I. 26<sup>th</sup> ISSP Conference (Riga, Latvia, February, 2010)**

1. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin and A. Möslang, "Y, O and Fe- vacancy defect complex modeling in fcc Fe lattice". Abstracts: p. 30.
2. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii and E.A. Kotomin, "Surface and subsurface vacancies in uranium nitride: first principles calculations". Abstracts: p. 31.
3. P. Merzlakovs and G. Zvejnieks, "Modeling of cluster scaling behavior with kinetic Monte-Carlo and cellular automata methods". Abstracts: p. 32.
4. O. Dumbrajs, V. Igochine, A. Gude, M. Maraschek, H. Zohm and ASDEX Upgrade Team, "Temporal evolution of neoclassical tearing modes in the frequently interrupted regime". Abstracts: p. 55.

##### **II. International conference "Functional materials and nanotechnologies" FM&NT-2010 (Riga, Latvia, March, 2010)**

5. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin and S. Bellucci, "Growth mechanism for CNT bundle upon both flat and nanostructured Ni catalyst: ab initio simulations". Abstracts: p. 16.
6. R.A. Evarestov and Yu.F. Zhukovskii, "Symmetry and models of BN and TiO<sub>2</sub> nanotubes". Abstracts: p. 21.

7. E.A. Kotomin, Yu.A. Mastrikov, R. Merkle and J. Maier, "Oxygen incorporation reaction into mixed conducting  $ABO_3$  - type perovskites for fuel cell applications". Abstracts: p. 22.
8. Yu.N. Shunin, Yu.F. Zhukovskii, S. Bellucci and N. Burlutskaya, "Resistance simulations for junctions of SW and MW carbon nanotubes with various metal substrates". Abstracts: p. 33.
9. G. Zvejnieks and E.E. Tornau, "Modeling of Au-Ni surface alloy instability". Abstracts: p. 35.
10. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii and E.A. Kotomin, "First principles calculations on oxygen impurities incorporated in the vacancies of UN(001) substrate". Abstracts: p. 37.
11. S. Piskunov, E.A. Kotomin, Yu.F. Zhukovskii and V. Alexandrov, "First-principles modeling of oxygen interaction with  $ABO_3$  type perovskite surfaces". Abstracts: p. 38.
12. D. Gryaznov, R.A. Evarestov, E.A. Kotomin and J. Maier, "Electronic, phonon and magnetic structure of pure and Sr-doped  $LaCoO_3$ ". Abstracts:p. 39.
13. R.I. Eglitis, "Ab initio calculations of  $SrTiO_3$ ,  $BaTiO_3$ ,  $PbTiO_3$ , and  $CaTiO_3(001)$  and (011) surfaces". Abstracts: p. 40.
14. E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, and D. Engers, "Temperature development of chemically ordered nanoregions in relaxor ferroelectric  $Pb(Mg_{1/3}Nb_{2/3})O_3$  (PMN)". Abstracts: p. 41.
15. A. Huczko, A. Dabrowska, V. Davchyn, I. Karbovnyk, V. Pankratov, and A.I. Popov, "Silicon carbide nanowires: synthesis and luminescence properties". Abstracts: p. 176.
16. R. Sathyamoorthy, P. Sudhagar, A. Balerna, C. Balasubramanian, S. Bellucci, A.I. Popov, and K. Asokan, "Surfactant-assisted synthesis of  $Cd_{1-x}Co_xS$  nanocluster alloys and their structural, optical and magnetic properties". Abstracts: p. 177.
17. A. Voloshynovskii, P. Savchyn, I. Karbovnyk, S. Myagkota, M. Cestelli Guidi, M. Piccinini, and A.I. Popov, "CsPbCl<sub>3</sub> nanocrystals dispersed in the  $Rb_{0,8}Cs_{0,2}Cl$  matrix studied by farinfrared spectroscopy". Abstracts: p. 178.
18. A.I. Popov, V. Pankratov, A. Kotlov, I. Aulika, A.G. Dejneka, D. Engers, E. Klotins, K. Kundzins, V.A. Trepakov, V. Zauls, and E.A. Kotomin, "Luminescence of  $SrTiO_3$  single crystals excited under synchrotron radiation". Abstracts: p. 179.
19. L. Shirmane, A. Kotlov, A.I. Popov, W. Lojkowski, T. Chudoba, P. Gluhowski, D. Hreniak, W. Strek, and V. Pankratov, "Luminescence properties of YAG:Ce<sup>3+</sup> nanocrystals in vacuum ultraviolet spectral range". Abstracts: p. 180.
20. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Ab initio calculations of yttrium and vacancy point defects for ODS steels modeling". Abstracts: p. 182.
21. A. Kalinko, A. Kotlov, A. Kuzmin, V. Pankratov, A.I. Popov, and L. Shirmane, "Electronic excitations in  $ZnWO_4$  and  $ZnWO_4:Ni$  using VUV synchrotron radiation". Abstracts: p. 184.
22. P. Merzlakovs, G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, K.D. Li, and L.M. Wang, "Analysis of void superlattice formation in  $CaF_2$ ". Abstracts: p. 185.
23. R.I. Eglitis, and E.A. Kotomin, "Ab initio calculations of Nb-doped  $SrTiO_3$ ". Abstracts: p. 186.
24. R.I. Eglitis, A.F. Vassilyeva, E.A. Kotomin, and A.K. Dauletbekova, "Ab initio calculations of  $MgF_2$  (001) and (011) surfaces". Abstracts: p. 187.

### III. The 8<sup>th</sup> International Conference "Information Technologies and Management", IT&M'2010 (Riga, Latvia, April, 2010)

25. Yu.F. Zhukovskii, "Theoretical modeling of 0D and 1D inorganic nanostructures". Abstracts: p. 17-18.

26. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Simulation of yttrium oxide particle formation in iron in support of ODS steel development". Abstracts: p. 20-21.
27. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, "Ab initio calculations on pure and oxygen-occupied vacancies upon the UN(001) surface". Abstracts: p. 38-39.
28. Yu.N. Shunin, Yu.F. Zhukovskii, S. Bellucci and N. Burlutskaya, "Nano-sized systems modeling: carbon-based electronic structure calculations and CNT interfaces simulations". Abstracts: p. 52-53.

#### **IV. GENNESYS International Congress on Nanotechnology and Research Infrastructures (Barcelona, Spain, May 2010)**

29. Yu.N. Shunin, Yu.F. Zhukovskii, S. Bellucci, and N. Burlutskaya, "Nano-sized systems modeling: CNT electronic structure calculations and CNT-metal interconnect simulations".

#### **V. 9<sup>th</sup> International Symposium on Systems with Fast Ionic Transport, ISSFIT-9 (Riga, Latvia, June, 2010)**

30. E.A. Kotomin, Yu.A. Mastrikov, M.M. Kuklja, R. Merkle, and J. Maier, "First principles calculations of oxygen vacancy formation and migration in mixed conducting ABO<sub>3</sub>-type perovskites for solid oxide fuel cell applications". Abstracts: p. 18.
31. R.I. Eglitis, "Ab initio calculations of SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, PbTiO<sub>3</sub> and CaTiO<sub>3</sub> (001) and (011) surfaces and F centers therein". Abstracts: p. 74.
32. B. Andriyevsky, I. Bolesta, O. Bovgyra, W. Ciepluch-Trojanek, I. Karbovnyk, I.V. Kityk, A.I. Popov, and S. Velgosh, "First principles calculations of the electronic structure for Ag<sub>2</sub>CdI<sub>4</sub> superionic". Abstracts: p. 75.

#### **VI. 16<sup>th</sup> International Seminar on Physics and Chemistry of Solids (Lviv, Ukraine, June, 2010)**

33. I. Bolesta, S. Velgosh, I. Karbovnyk, I. Rovetsky, V. Pankratov, and A.I. Popov, "Luminescent properties of metal-activated cadmium iodide crystals". Abstracts: p. 101.

#### **VII. Spring European Materials Research Society (E-MRS) Meeting (Strasbourg, France, June, 2010)**

34. R.I. Eglitis and E.A. Kotomin, „Ab initio calculations of Nb-doped SrTiO<sub>3</sub>”. Abstracts: EP1-9.
35. R.I. Eglitis, „Ab initio calculations of SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, PbTiO<sub>3</sub> and CaTiO<sub>3</sub> (001) and (011) surface structures”. Abstracts: EP2-3.
36. V. Pankratov, A.I. Popov, A. Kotlov, C. Feldmann, „Peculiarities of luminescence of LaPO<sub>4</sub>: Ce, Tb nanocrystals”. Abstracts: K12-2.
37. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, „Pair and triple point defect complex modeling in fcc Fe lattice”. Abstracts: NPVI-13.
38. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, „Ab initio modeling of oxygen impurities incorporated within UN (001) surface and subsurface vacancies”. Abstracts: NPVI-23.
39. R.A. Evarestov, Yu.F. Zhukovskii, S. Piskunov, M.V. Losev, A.V. Bandura, and E. Spohr, „Symmetry and models of single- and double-walled titania nanotubes: comparative analysis using ab initio calculations”. Abstracts: PP8-6.

40. S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, „Atomic carbon adsorption on nano-structured Ni catalyst and further CNT growth: Predictions from first principles calculations”. Abstracts: PP8-50.

**VIII. CECAM Conference on Actinides: Correlated Electrons and Nuclear Materials (Manchester, UK, June 2010)**

41. E.A. Kotomin, and D. Gryaznov, "DFT+U calculations of the electronic structure of perfect and defective PuO<sub>2</sub>". Abstracts: p. 7.

**IX. Annual Monitory Meeting of European Fusion Development Agreement, EFDA - 2010 (San-Sebastian, Spain, July, 2010)**

42. Yu.F. Zhukovskii, A. Gopejenko, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "First-principles simulations on Y<sub>2</sub>O<sub>3</sub> cluster formation in fcc iron".

**X. 11<sup>th</sup> Europhysical Conference on Defects in Insulating Materials, EURODIM-2010 (Pecs, Hungary, July, 2010)**

43. R.I. Eglitis, and E.A. Kotomin, "Ab initio calculations of Nb impurity in SrTiO<sub>3</sub>". Abstracts: 4.2.
44. A. Voloshinovskii, P. Savchyn, I. Karbovnyk, S. Myagkota, M. Cestelli Guidi, M. Piccinini, and A.I. Popov. "MIR spectra of CsPbCl<sub>3</sub> nanocrystals embedded in the Rb<sub>0,8</sub>Cs<sub>0,2</sub>Cl matrix". Abstracts: A122.
45. R.I. Eglitis, A.F. Vassilyeva, E.A. Kotomin, and A.K. Dauletbekova, "Ab initio calculations of MgF<sub>2</sub> (001) and (011) surfaces as well as bulk and surface F centers". Abstracts: B45.
46. R.I. Eglitis, "First-principles calculations of SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, PbTiO<sub>3</sub> and CaTiO<sub>3</sub> (001) and (011) surfaces". Abstracts: B46.
47. V. Pankratov, L. Shirmane, A.I. Popov, A. Kotlov, W. Lojkowski, and W. Strek, "VUV luminescence spectroscopy of cerium doped Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> Nanocrystals". Abstracts: B72.

**XI. International Workshop on Nanocarbon Photonics and Optoelectronics, NPO-2010 (Koli, Finland, August, 2010)**

48. Yu.N. Shunin, Yu.F. Zhukovskii, S. Bellucci, and N. Burlutskaya, "CNT-metal interconnect electronic structure calculations and resistivity simulations".

**XII. 35<sup>th</sup> International Conference on Infrared, Millimeter, and Terahertz Waves, IRMMW-THz 2010 (Roma, Italy, September, 2010)**

49. O. Dumbrajs and G.S. Nusinovich, „To the theory of high-power gyrotrons with up tapered resonators”.
50. O. Dumbrajs, “Influence of Possible Reflections on the Operation of European ITER Gyrotrons”.
51. S. Kern, K.A. Avramidis, O. Dumbrajs, G. Gantenbein, S. Illy, A. Samartsev, A. Schlaich, M. Thumm, and A.R. Choudhury “Simulation and experimental investigations on dynamic after cavity interaction (ACI)”.
52. K.A. Avramides, O. Dumbrajs, J.L. Vomvoridis, and S. Kern “Gyrotron interaction simulations with tapered magnetostatic field”.

**XIII. The First International Conference of Luminescence in Lanthanides (ICLL-1) (Odessa, Ukraina, September, 2010)**

53. V. Pankratov, A.I. Popov, A. Kotlov, and C. Feldmann, "Comparison of the time-resolved characteristics of Ce<sup>3+</sup> and Tb<sup>3+</sup> luminescence in LaPO<sub>4</sub> host upon excitation in UV-VUV range". Abstracts: p. 57.

**XIV. 7<sup>th</sup> International Conference on Inorganic Materials (Biarritz, France, September, 2010)**

54. R.I. Eglitis, "Ab initio calculations of SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, PbTiO<sub>3</sub> and CaTiO<sub>3</sub> (001) and (011)". Abstracts: P1.84.
55. R.I. Eglitis, and E.A. Kotomin, "Ab initio calculations of Nb-doped SrTiO<sub>3</sub> bulk and surfaces". Abstracts: P1.85.

**XV. Psi-k Meeting on Ab initio (from the electronic structure) Calculations of Processes in Materials (Berlin, Germany, September, 2010)**

56. E. Blokhin, D. Gryaznov, E.A. Kotomin, R.A. Evarestov, and J. Maier, "Comparative ab initio hyper-GGA DFT study of phonons in several phases of SrTiO<sub>3</sub>". Abstracts: S11-P183.

**XVI. Workshop on Nanoscience and Nanotechnology, n&n-2010 (Frascati, Italy, September, 2010)**

57. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopejenko, N. Burlutskaya, and S. Bellucci, "Ab initio simulations on electric properties for junctions between carbon nanotubes and metal electrodes". Abstracts: p. 78.

**XVII. F-BRIDGE School on Ceramic Nuclear Fuel and Cladding Materials (Karlsruhe, Germany, September-October, 2010).**

58. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, "First principles calculations of surface and subsurface vacancies as well as oxygen impurity atoms on UN (001) substrate".

**XIX. International Conference on Nuclear Materials, NuMat-2010 (Karlsruhe, Germany, October, 2010)**

59. D. Gryaznov, S. Rashkeev, and E.A. Kotomin, "Density functional theory calculations on point defects and helium behavior in (U,Pu)O<sub>2</sub>".

**XX. 4<sup>th</sup> International Conference on Innovative Information Technologies, IIT-2010 (Vilnius, Lithuania, November, 2010)**

60. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burluckaya, T.D. Lobanova, and S. Bellucci, "Novel nanoelectronic devices based on carbon nanotubes and graphene". Abstracts: p. 6-7.

**XXI. Fall Meeting of Materials Research Society (Boston, USA, December, 2010)**

61. E. Heifets, and D. Gryaznov, "Density Functional Theory Calculations on Magnetic Properties of Actinide Compounds". Abstracts: Q 14.6.
62. E. Heifets, Yu.A. Mastrikov, R. Merkle, E.A. Kotomin, and J. Maier, "A DFT-Based Analysis of Pathways for Oxygen Incorporation and Diffusion in Mixed Conducting Perovskites". Abstracts: GG 12.7.

**XXII. 3rd International Workshop "Ab initio Phonon Calculations" (Cracow, Poland, December, 2010).**

63. E. Blokhin, D. Gryaznov, E.A. Kotomin, R.A. Evarestov, and J. Maier, "Phonon calculations in cubic and tetragonal phases of SrTiO<sub>3</sub>: a comparative LCAO and plane wave study".

**XXIII. International Workshop "Towards Reality in Nanoscale Materials'10" (Levi, Finland, December, 2010)**

64. A. Sorokin, S. Piskunov, D. Bocharov, and V. Kashcheyevs, „Electronic charge redistribution in LaAlO<sub>3</sub>(001) thin films deposited at SrTiO<sub>3</sub>(001) substrate: predictions from first principles". Abstracts: p. 44-45.

**XXIV. International Workshop on Carbon Based Interconnects: Current Achievements and Future Perspectives (Rome, Italy, December, 2010)**

65. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin, and S. Bellucci, "Mechanism of CNT growth upon nano-structured Ni catalyst: Predictions from first principles calculations".
66. V. Kashcheyevs, A. Tamburrano, and M.S. Sarto, "Modeling on electron transport and signal propagation for MW CNT interconnects".
67. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, A. Tamburrano, and M.S. Sarto, "Modeling on electric properties for junctions between carbon nanotubes and metal electrodes".

## LABORATORY OF OPTICAL RECORDING

Head of Laboratory Dr. J.Teteris

### Research Area and Main Problems

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

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### Main Results

#### SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

M.Reinfelde, J.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  $0.15 \mu\text{m} - 1 \mu\text{m}$  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  $\Lambda = \lambda_0 / 2n \sin\theta$ , where  $\lambda_0$  is the wavelength of laser light in vacuum,  $n$  is refractive index of the resist and  $\theta$  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  $\theta$ . 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

J.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 discussed. 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  $\text{As}_2\text{S}_3$  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, M.Reinfelde

The recording of the surface-relief and refractive index modulated gratings with a period of  $0.15 - 1.0 \mu\text{m}$  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  $\Lambda = \lambda_0 / 2n \sin\theta$ , where  $\lambda_0$  is the wavelength of laser light in vacuum,  $n$  is refractive index of the prism and  $\theta$  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  $0.488 \mu\text{m}$  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  $90^\circ$ , a grating with a period of  $0.345 \mu\text{m}$  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  $0.197 \mu\text{m}$  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<sub>2</sub>S<sub>3</sub> 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, 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<sup>0</sup>C. 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, 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<sup>0</sup>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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3. A.Gerbreders, J.Teteris, Formation of direct surface relief in photochrome-chalcogenide composites, *Latvian Journ. Phys.Techn. Sciences*, Vol.47 (Nr.2) (2010) 49-59.
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2. J.Aleksejeva and J.Teteris, Ultraviolet holographic recording in photopolymers, *4th Intern.Conf. on Optical, Optoelectronic and Photonic Materials and Applications ICOOPMA 2010*, 15-20 August, 2010, Budapest, Hungary, A-0120.
3. J.Teteris, Photoinduced mass transfer in disordered materials, *17th Intern.Symposium on Non-Oxide and New Optical Glasses (XVII ISNOG 2010)*, Ningbo, China, June 13-18, 2010.
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5. A.Gerbrederts, J.Teteris, Optisko kompozītu virsmas reljefu veidošanas īpatnības (Features of surface relief formation in optical composites), *LU CFI 26. zinātniskā konference, Rīga, 2010.gada 17.-19.februāris, 26<sup>th</sup> Scientific Conference of the*

*Institute of Solid State Physics, University of Latvia, February 17-19, 2010, Book of Abstracts, p.23*

6. A.Bulanovs, G.Kirilovs, V.Gerbreders and J.Teteris, Investigations of As-S-Se thin films for use as inorganic photoresist for digital image-matrix holography, *International Conference on Functional materials and Nanotechnologies FM&NT 2010*, March 16 – March 19, 2010, Riga, Latvia, Abstracts, p.154.

## LABORATORY OF VISUAL PERCEPTION

Head of Division Dr.hab.phys., Prof. I.Lācis

### Research Areas and Main Problems

Laboratory is trying to find synergies between material science (physics), vision research (perception) and everyday optometry (profession). 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 brain, and as a result in some provocative cases it is very hard for us to accept the final outcome.

Research in laboratory is focused on following problems:

- investigation of advanced optical materials and designs of vision appliances – tinted, high refractive glasses, antireflective coatings, multifocal and progressive, and contact lenses;
- quality of stereovision;
- visual evoked potentials related to visual perception;
- changes of eye parameters after laser refractive surgery;
- aberrations of the eye and their effect on retinal image quality
- evaluation of colour vision and spectral analysis of colour deficiency tests;
- eye kinematics studies
- variability of fixation disparity, its origin and role in vergence models; vergence problems;- effect of intraocular straylight on vision
- retroreflective materials and road safety
- changes in vision with aging

### Scientific Staff

Prof. I. Lācis

Prof. M. Ozoliņš

Dr.phys. G. Krūmiņa

Dr.phys. G. Ikaunieks

### PhD Students

M.Sc. A. Švede

M.Sc. S. Fomins

M.Sc. V. Karitāns

M.Sc. K. Lūse

### Master Student

B.Sc. A. Paušus

### Educational

Every year up to 35 bachelor and 20 master students of Department of Optometry and Vision science are graduated from University of Latvia. Lot of them performs their diploma experimental works tied with research topics of Laboratory of Visual perception.

### Partners abroad

#### Estonia

Tallinn Health Care College, department of Optometry (Vootele Tamme)

## **Italy**

Florence University, Italy, (Prof. S. Villani)  
Universita` di Roma "Tor Vergata" (Prof. I. Davoli)

## **Spain**

Laboratorio de Optica, Universidad de Murcia, Spain (Prof. P. Artal)  
Universidad Complutense Madrid, Spain (Prof. Miguel Ángel Muñoz)

## **France**

Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand (Dr. M.Colomb).

## **Great Britain**

Cardiff University Eye Clinic (Prof. Tim Wess, Dr. Paul Murphy)

## **Germany**

Institut für Arbeitsphysiologie an der Universität Dortmund  
(Dr. Wolfgang Jaschinski)

## **Russia**

Pavlov Institute of Physiology of Russian Academy of Sciences, Laboratory of motion physiology. (Dr. V.A.Lyakhovetskii)

## **Main results**

### **HOWARD-DOLMAN STEREOVISION TEST AT DIFFERENT OPPONENT COLOUR STIMULI**

Maris Ozolinsh<sup>1</sup>, Isabel Martín<sup>2</sup>, Didzis Lauva<sup>3</sup> and Varis Karitans<sup>3</sup>

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The purpose of this study was to investigate visual depth perception of real physical colour stimuli with red-green and blue-yellow opponency. We modified Howard-Dolman stereotest where subjects should determine the closer of two bars emitting the light of definite colour placed in front of a CRT monitor served as colour background. Two-alternative forced-choice paradigm was used to determine depth perception threshold values. Thresholds close to 5-10 arcsec for luminance and colour contrast stimuli were revealed both for red-green and blue-yellow stimuli. A term stereosensitivity - a reciprocal magnitude of the stereothreshold was introduced to analyze separately luminance and colour contrast contributions in total depth perception. Comparing stereo sensitivity values for different colour stimuli, stereo sensitivity in case of red-green still is better comparing to blue-yellow colour contrast. The colour and luminance contrast in CIE L\*a\*b\* units (at least in restricted dynamic range) could be applicable as psychophysical metric to characterize stereo sensitivity. We suppose the colour and luminance contrast guided stereo mechanisms as two additive contributions in total stereo sense. Stereosense thresholds are more sensitive to luminance contrast changes as compared to colour contrast changes (in L\*a\*b\* metric).

## MESOPIC VISION CHARACTERISTICS AT DECREASED CONTRAST IN FOG

M. Ozolinsh<sup>1,2</sup>, M.Colomb<sup>3</sup>, D. Lauva<sup>1</sup> and S. Fomins<sup>1</sup>

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Perception of different color contrast stimuli was studied in the presence of light scattering in a fog chamber in Clermont-Ferrand and in laboratory conditions where light scattering of similar levels was obtained. Blue (shortest wavelength) light is scattered in fog to the greatest extent, causing deterioration of vision quality especially for the monochromatic blue stimuli. We have done spectral measurements of the light source in different density fog conditions and no spectral changes were found produced by the fog. Psychophysical measurements of the acuity in fog were done for two subjects with optotypes analyzed for red and blue stimuli.

## SIMULATING RETINAL VASCULAR DISORDERS BY IMPOSING DIFFERENT TYPES OF HIGHER-ORDER ABERRATIONS ON RETINAL IMAGES

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Each aberration distorts the image of a point according to its point spread function. We impose different higher-order aberrations on retinal images so distorting appearance of retinal blood vessels and trying to simulate different retinal vascular disorders.

Each type of higher-order aberrations (HOAs) has a certain point spread function (PSF) and thus it distorts an image in its own way. By distorting appearance of retinal blood vessels HOAs give rise to possibility that some vascular pathology may be falsely diagnosed. We simulate the effect of several types of HOAs on appearance of retinal blood vessels and try to find similarity between the simulated images and certain retinal vascular disorders. As basis for convolving point spread function with an image Matlab code found at John Loomis's homepage [1] is used.

We guess that two retinal vascular pathologies most likely to be wrongly diagnosed due to HOAs are retinal microaneurysms and abnormal tortuosity of blood vessels.

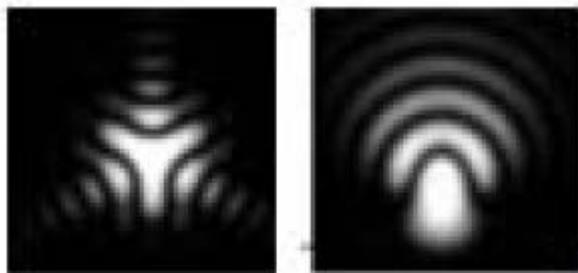


Fig 1. Point spread functions for trefoil (left) and coma.

Microaneurysms look like red spots and may appear in fundus images due to trefoil aberration whereas exaggerated tortuosity may result from coma. Corresponding point spread functions are shown (see Fig 1).

Secondary maxima in PSF may be intense enough to be visible. Before making final diagnosis of retinal vascular disorders it is recommended to take into account both the HOAs of the patient and those of the ophthalmologist. Otherwise, these disorders may be over- or under-estimated.

Reference

[1] Internet [http://www.johnloomis.org/eop601/notes/matlab/psf/fft\\_psf.html](http://www.johnloomis.org/eop601/notes/matlab/psf/fft_psf.html)

## **COLLINEAR SUPPRESSION IN TEXTURE SEGMENTATION FOR TEMPORALLY MODULATED STIMULI**

L. Zarina and S. Fomins

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Collinear stimuli facilitate the neural signal in the case of Gabor's stimuli when a low-contrast stimulus inside the receptive field is flanked by higher contrast collinear elements located in surrounding regions of the visual space. Our previous studies pointed to the contextual modulation in the case of the textured stimuli. Collinear suppression was observed in 63% of the responses. In the current research we used Gabor's primitives for building the circular texture objects of vertical and diagonal orientation to be recognized on the horizontally-oriented background in the presence of collinear and orthogonal peripheral stimuli. The two-alternative forced choice (2AFC) psychophysical method with constant stimuli was used to gather the responses of the subjects which choose between left or right position of diagonally-oriented stimuli. The experimental stimuli consisted of two circularly shaped objects presented in visual angle of 2.76 degrees. The expositions of the stimuli varied from 13.3 to 93.3 ms arbitrarily. Visual stimuli were presented with a CRS Visage stimulus generator and shown on a CRT monitor of 75 Hz refresh rate. Our new findings support the concept of suppressing the target stimuli of the same orientation in the presence of a peripheral collinear stimulation.

## **STRENGTH JUDGMENT OF FILLING-IN COLOR ILLUSION**

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The strength of chromatic after-effect was studied using the filling-in after-effect image illusion (Van Lier et al.). In our experiments, two stimuli, each consisting of round and sharp-edged overlapping chromatic shapes, were presented to the subjects for 1.2 s on both sides of the fixation point. After that the empty shapes of the stimuli appeared for 0.6 s, and in the next 0.6 s changed the orientation on both sides of the fixation point thus changing the after-effect color from side to side. The subjects made judgments about the strength of the perceived after-effect on a ten-grade scale for different color pairs. The color of one stimulus was kept constant, while the color of the other was changed; as a result of color changes of both stimuli 192 color pairs in total were formed. Some of them were found to arouse a powerful sensation of the after-effect with a color not directly arranged on the opposite axis of chromaticity diagram. Blue and yellow colors were valued as creating the most pronounced after-effect.

## PROBLEMS OF CODING STEREO IMAGES IN HUMAN MEMORY

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The objectives of this study were human memorization and recognition processes in respect of 2-D and 3-D objects sequences. In each trial we used six sequential slides, each of them containing a 2-D or 3-D bar located on the chessboard. This bar was positioned in one of 8×8 (for 2-D) or 8×4×2 (for 3-D) locations. At the recognition stage there were the target and three distracters on each slide, the subject to recognize the target. It was shown that performance as well as memorization time and recognition time for the 3-D stimuli were significantly lower than for the 2-D ones. For the 3-D trial, the error distribution depended on whether the target and the chosen distracter had same or different binocular disparities.

The data obtained were simulated by creating a model developed on the basis of bidirectional associative memory network. The model successfully reproduced the error distribution for the 2-D sequences, but not for the 3-D ones if the target and the chosen distracter had different disparities. Thus, we conclude that the internal representation of 3-D objects fundamentally differs from that of 2-D objects.

Keywords: spatial memory, stereovision, bidirectional associative memory network.

## LATENCIES OF VISUAL EVOKED POTENTIALS BY STIMULATING CENTRAL AND PERIPHERAL RETINA

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Pilot study goal was to evaluate the visual evoked potential by stimulating central and peripheral area of retina. The experiment was done using four monitors. One was placed for stimulation the central part of retina and three for stimulation the periphery. The stimulation of retina was done in three ways: central part, peripheral part and full field retina (central together with periphery). Peripheral visual stimuli were placed in binocular field area. The stimuli size was 4, 8 and 16 degree and temporal frequency was 1 Hz (two reversals per second). Visual evoked potentials were recorded monocularly and binocularly.

First findings showed the amplitudes of peripheral retinal parts were less than measured from central retina. However latencies values of first negative peak from stimulating peripheral retinal parts were smaller (up to 47-52 msec) as from stimulating central or full field retina (up to 74-79 msec). The same is for first positive peak. The latencies value from stimulating peripheral retinal parts were up to 68-72 msec.

The findings of peripheral and central retinal parts could be characterisation of margo- and parvo-pathway information flow speed. The next study steps will be to find the latencies values by normal peripheral visual field and by damaged periphery.

## INTRAOCULAR PRESSURE MEASUREMENTS WITH THREE TONOMETRY METHODS

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**Purpose:** To evaluate diurnal changes in intraocular pressure measured with three different tonometry methods.

**Methods:** Thirteen healthy subjects were included in this study. Intraocular pressure was measured with three different tonometry methods – applanation (Goldmann), impression (Schiotz), non-contact („Keeler” PulsAir) – three times in one day for each subject.

**Results:** Impression method showed higher intraocular pressure than applanation method, but applanation method showed higher intraocular pressure than non-contact method. There is a statistically significant difference between the morning and lunchtime measurements of intraocular pressure with impression and non-contact method as well as difference between morning and evening measurements with impression method. Intraocular pressure mainly decreased till 2 mmHg in the morning-lunchtime period with all three tonometry methods. In general, intraocular pressure decreased in the morning-evening period, but increased in the lunchtime-evening period.

**Conclusion:** It is important to notice the daytime when intraocular pressure measurements are taken with impression (Schiotz) method because there was a significant difference between morning, lunchtime and evening measurements. It is also important to notice the daytime measurements are taken with non-contact („Keeler” PulsAir) method. Applanation (Goldmann) method did not show significant fluctuations between the measurements during the day.

**Keywords:** intraocular pressure, applanation method, impression method, non-contact method.

## EFFECT OF YELLOW TINTED SPECTACLE LENSES ON INTRAOCULAR STRAYLIGHT

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There is a lot of discussion about the effect of yellow spectacle lenses on vision. One of the main questions is: can we improve visual functions with yellow lenses? It has been suggested that removal of blue light with yellow lenses may reduce light scattering and this could increase visual performance. We wanted to test this suggestion.

Intraocular straylight with and without yellow lenses in front of the eye was measured with the direct compensation method [van den Berg, 1986, *Doc. Ophthalmol.* 61(3-4), 327–333]. Additional to these measurements, the effect of yellow lenses on contrast sensitivity was assessed using Pelli-Robson contrast sensitivity chart and special computer program.

Results showed that the straylight was stronger in the measurements with yellow lenses than in normal conditions. Contrast sensitivity measurements didn't show statistically significant improvement with yellow lenses; however, most of the subjects feel more comfortably with yellow lenses, especially in mesopic light conditions. Our results agree with those of previous studies [Rabin and Wiley, 1996, *Ophthalmic Physiol. Opt.* 16(1), 68-72] which showed that improvement of vision looking through yellow lenses is related more with neural factors than optical.

## EFFECT OF YELLOW FILTERS ON VISION

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In literature there is controversial information found whether the yellow filter may enhance the quality of vision. To find out what is the effect of yellow filters on the quality of vision, 27 individuals were examined for contrast sensitivity, by using Pelli-Robson chart, under normal (photopic) and reduced (mesopic) illumination. Measurements were carried out without and with yellow filter (light transmission 67%). More measurements were taken by using grey filter with similar transmission as the yellow lense (73%). The results did not show statistically significant enhancement, looking through yellow filters. However, 56% of individuals claimed that under reduced illumination they found it more agreeable to look through yellow filters. 2 individuals were extra examined by low contrast visual acuity measurements with a computerized test and by objective measurements with the electrophysiologic method VEP. Also these measurements did not show statistically significant enhancement, looking through yellow filters.

Our measurements do not confirm the data found in literature about the improvement of the visual contrast sensitivity, looking through yellow filters. However the obtained improvement of the subjective sensation, looking through yellow filter, under mesopic conditions shows that under very low illumination yellow filter may give a slight increment of visual quality.

Key words: yellow filter, contrast sensitivity, visual acuity, VEP.

## FACTORS EXPLAINING FIXATION DISPARITY, MEASURED WITH DICHOPTICALLY PRESENTED NONIUS LINES

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Fixation disparity refers to the steady-state error in vergence angle between the visual axes. The neural network model of Patel et al (2001) explains fixation disparity as a result of the asymmetry between convergent and divergent dynamic responses to disparity step stimuli. This concept extends previous feedback control theory based models that refer to one direction of dynamic vergence responses. Further research showed that fixation disparity reflects a bias towards resting vergence. We combined these approaches in order to predict the inter-individual variability in fixation disparity measured subjectively with dichoptic nonius lines for a stationary fusion stimulus. Multiple regression analyses showed the following percentages of variance explained by three independent variables in a sample of 20 subjects. 54% was due to the objectively measured asymmetry in vergence dynamics (calculated from convergent and divergent velocities) and objectively measured heterophoria (as a result of tonic, accommodative, and proximal vergence components). Additional 22% of variance was due to the nonius bias, ie the physical nonius offset required for perceived alignment of binocularly (non-dichoptically) presented nonius lines. Together, these components were able to explain 76% of the inter-individual differences in subjectively measured fixation disparity, showing the influence of oculomotor and perceptual factors.

## LABORATORY OF WIDE BAND GAP MATERIALS

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

### Research Area and Main Problems

The research interests of the Laboratory of Wide Band Gap Materials are focused on spectral characterization of compounds formed from the III-V group elements (AlN, h-BN) and some related materials such as Al<sub>2</sub>O<sub>3</sub>. Recently it was shown that some optical properties of nitride compounds are prospective for its application as new UV light and visible light emitters (Watanabe, Taniguchi), besides, features of AlN could rate it among materials available for UV light dosimetry (our results). Presently different forms of these materials are synthesized including a bulk material and its nanostructured forms and it is also known that their optical properties could be different. The interests of our research are largely focussed on revealing of the difference between the optical properties of the bulk material and its nanostructured forms. The spectral investigations performed in our laboratory are based on luminescence studies (photoluminescence (PL) and its excitation (PLE) spectra within a wide temperature range between 8 K and 300 K), optically stimulated luminescence (OSL) and thermo-luminescence (TL)) including also optical absorption. This complex can give essential information about the defects and optical properties of the material, containing revealing of light-induced processes, luminescence mechanisms, energy accumulation and its release mechanisms. These problems could be prevalently related to the fundamental physics. In the field of innovations the interests are focussed on application of AlN and related-materials for the UV light dosimetry and h-BN – as light emitter; AlN and Al<sub>2</sub>O<sub>3</sub> seems to be prospective for elaboration of new luminescent materials for energy saving compact luminescent lamps. Part of investigations was performed together with the collaboration partners from abroad.

### Scientific Staff

1. Dr. Hab.Phys, Assoc. Prof. B.Berzina
2. Dr. L.Trinkler (senior researcher)
3. V.Korsaks (Ph.D. student, researcher)

### Students - Technicians

1. D.Jakimovica (assistant)
2. Jana Grigorjeva (technician)
3. Zanna Jevsjutina (technician)

### Collaborations

#### Latvia

Institute of Inorganic Chemistry, Riga TU (Dr. E.Palcevskis, Prof. J.Grabis)  
Institute of Solid State Physics, University of Latvia, Lab. of Nonlinear Processes Theory, (Prof. Y.Zhukovskii, Dr. S.Piskunov)

#### USA

Wake Forest University, Department of Physics, Winston-Salem (Prof. R.T. Williams, Dr. U.Burak)

#### Belarus

Institute of Solid State Physics and Semiconductors, Belarus Academy of Sciences, Minsk (Dr.E.Shishonok).

#### Taiwan

Center of Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan (Prof. Li-Chyong Chen)

#### Lithuania

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

## **Main results**

### **LUMINESCENCE PROPERTIES OF $\text{Al}_2\text{O}_3$ BULK AND NANOSIZE POWDERS**

L.Trinkler, B.Berzina, D.Jakimovica, Z.Jevsjutina

Photoluminescence has been studied in the aluminum oxide ( $\text{Al}_2\text{O}_3$ ) bulk and nanosize powders in the 300-8 K temperature range. In both samples luminescence spectrum is characterized by presence of broad blue and red bands caused mainly by emission from the uncontrolled titanium impurity. It was found that at low temperatures luminescence intensity increases by several times and the red band obtains fine structure. Explanation of the fine structure was proposed suggesting manifestation of splitting of the  $\text{Ti}^{3+}$  emitting level due to Jahn-Teller effect or overlapping of  $\text{Ti}^{3+}$  emission band with narrow lines from other emitting ions. The observed differences in low-temperature spectral features of nanopowder compared to its bulk counterpart were explained by lattice structure of nanopowder, which belongs to transition phase of  $\text{Al}_2\text{O}_3$ . These investigations are in progress. Materials used for investigation are synthesized in Institute of Inorganic Chemistry RTU (Dr J. Grabis).

### **SPECTRAL CHARACTERIZATION OF BULK h-BN AND MULTIWALL NANOTUBES**

B. Berzina, L.Trinkler, V.Korsak

Photoluminescence (PL) spectra of h-BN powder and multi-wall BN nanotubes were investigated within a wide spectral region from 8 K up to 300 K. A similarity of complex luminescence spectra was found for both the BN nanotubes and bulk h-BN powder. Three main spectral groups can be distributed from the complex luminescence spectra demonstrating a well resolved phonon substructure. It was established that the first group around 300 nm could be related to the intrinsic luminescence of carbon impurity characterizing the bulk material. According to our previous results and literature data the second luminescence wide band around 400 nm could be related to the some sorts of defects probably containing the oxygen substituting the nitrogen located near the material surface. The third part from the luminescence spectra forms a wide band around 500 nm and its intensity and maximum location highly depend on previous treatment of material: ageing, previous irradiation with UV light, heating etc. It allows conclusion that this luminescence is caused by surface defects. All these spectral groups are common for both the bulk h-BN powder and nanomaterial, nevertheless, a ratio of luminescence intensities characterizing these spectral groups is different for various materials.

Investigation of influence of different gasses such as  $\text{Ar}_2$ ,  $\text{N}_2$ ,  $\text{O}_2$  on BN luminescence is in progress.

### **LOW TEMPERATURE LUMINESCENCE OF $\text{AlN}$**

L.Trinkler, B. Berzina, J.Grigorjeva

Photoluminescence of  $\text{AlN}$  ceramics were investigated within a wide spectral range from 8 K up to 300 K in order to reveal the luminescence mechanisms and luminescence centers useful for elaboration of new white light sources. These studies were performed within a support of European project ERAF 2010/0253/2DP / 2.1.1.1.0/10/APIA/VIAA/079.

## Scientific Publications

1. L. Trinkler, B. Berzina, D. Jakimovica, J. Grabis, I. Steins. „*UV-light induced luminescence processes in Al<sub>2</sub>O<sub>3</sub> bulk and nanosize powders*”. Optical materials, 32 (2010) 789-795.
2. L. Trinkler, B. Berzina, D. Jakimovica, J. Grabis, I. Steins. “*Peculiarities of photoluminescence of Al<sub>2</sub>O<sub>3</sub> bulk and nanosize powders at low temperatures*”. Optical Materials, 33 (2011) 817-822. doi:10.1016/j.optmat.2010.12.020
3. V. Korsaks, B. Berzina, L. Trinklere. “*Low twmperature 450 nm luminescence of hexagonal boron nitride*”. Submitted and accepted to Latvian Journal of Physics and Technical Sciences.

## Lectures on Conferences

### **26<sup>th</sup> LU Scientific Conference of Institute of Solid State Physics, University of Latvia, February 17 - 19, 2010, Riga, Latvia**

1. V.Korsaks, B.Berzina, L.Trinklere. “*Luminescence of hexagonal boron nitride at low temperatures*”. Book of Abstracts, 2010 p.9.
2. D.Jakimovica, L.Trinklere, B.Berzina, Korsaks. “*Luminescence of Al<sub>2</sub>O<sub>3</sub> powder at low temperatures*”. Book of Abstracts, 2010 p. 47.

### **International Conference FM&NT; Functional materials and nanotechnologies 2010; Institute of Solid State Physics University of Latvia March 16 – 19, Riga**

- 3.V.Korsaks, B.Berzina, L.Trinkler. “*Luminescence of hexagonal boron nitride powder and nanotubes at different temperatures*”. (Oral report) Book of Abstracts, p.173.
- 4.D.Jakimoviča, L.Trinkler, B.Berzina, J. Grabis, I.Steins. „*Photoluminescence of Al<sub>2</sub>O<sub>3</sub> bulk and nanosize powders at low temperature*”. (Oral report). Book of Abstracts, p. 174.

### **International Conference EXCON'10 on Excitonic and Photonic Processes in Condensed and Nano Materials, 11 – 16 July, 2010, Brisbane, Australia.**

- 5.B.Berzina, V Korsaks, L,Trinkler, R.Williams, B.Ucers. „*Excitonic processes and defect luminiscence in bulk h-BN and multiwalled nanotubes*”. (Oral report). Book of Abstracts.

### **EURODIM 2010 11<sup>th</sup> Europhysical Conference on Defects in Insulating Materials, 12 -16 July, Pecs, Hungary**

- 6.B.Berzina, L.Trinklere, V.Korsaks. „*Luminescence of hexagonal boron nitride powder and nanotubes at different temperatures and pretreatments*”.(Oral report). Book of Abstracts 1.3.

## **LABORATORY OF SURFACE PHYSICS**

**Head of Laboratory Dr.phys. F.Muktepavela**

### **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 2010**

- Obtaining of nanostructured functional coatings by mechanoactivated oxidation and investigating their mechanical and optical properties;
- Studies of the structure and micromechanical properties of thin film systems, grain boundaries and interfaces in heterogeneous structures;
- Surface modification by irradiation with swift heavy ions.

### **Scientific Staff**

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

### **Technical Staff**

A.Petersons

### **PhD Students**

Mg.Phys.G.Bakradze  
Mg.Phys. R.Zabels

### **Students**

1. B.sc.R.Grants

### **Scientific visits abroad**

1. Dr.F.Muktepavela, Chernogolovka, ISSP, Moscow (1 week)
2. R.Zabels, Warsaw, Poland (1 week)

### **Visitors from Abroad**

1. Dr.M.Tomut, GSI, Darmstadt, Germany (1 week).

## **Cooperation**

### **Latvia**

Daugavpils University (Dr. E.Tamanis).  
Institute of Physics, University of Latvia (Dr.A.Shishko).

### **Germany**

GSI, Darmstadt (Prof. K.Schwartz, Dr.M.Tomut).

## Israel

Technion, Haifa (Dr.S.Stolyarova).

## Russia

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

## Main Results

### NANOINDENTATION AND RAMAN SPECTROSCOPY STUDY OF GRAPHITE IRRADIATED WITH SWIFT $^{238}\text{U}$ IONS

I.Manika<sup>1</sup>, J.Maniks<sup>1</sup>, R.Zabels<sup>1</sup>, J.Gabrusenoks<sup>1</sup>, M.Tomut<sup>2</sup>

<sup>1</sup>*Institute of Solid State Physics, University of Latvia*

<sup>2</sup>*GSI, Darmstadt, Germany*

The isotropic fine-grained graphite is a promising material for future high-energy ion beam facilities [1]. Modifications of the structure and mechanical properties of R6650 graphite irradiated with 2.6 GeV  $^{238}\text{U}$  ions at fluences up to  $10^{13}$  ions/cm<sup>2</sup> at room temperature were studied using nanoindentation and Raman spectroscopy. Indentation tests confirm that the material withstands high-fluence irradiation. Moreover, a strong ion-induced increase of Young's modulus and hardness is observed that points to a structural change and formation of a hard form of carbon. The maximum effects are observed on the irradiated surface where an ion-induced increase of hardness and modulus reaches up to 500% and 280%, respectively. A change of hardness and modulus under ion-induced stresses around the interface between the irradiated layer and the non-irradiated bulk material was observed. Raman measurements demonstrate ion-induced disordering and reduction of dimensions of crystallite domains. After high-fluence irradiation, the Raman spectrum becomes similar to that of the glassy carbon. A similar modification of structure occurs also in HOPG crystals irradiated with swift ions. The results show that despite of sp<sup>2</sup> bonding the structure of the glassy carbon ensures a high hardness and modulus.

### AGGREGATION PROCESSES AND NANOSTRUCTURING IN LiF CRYSTALS IRRADIATED WITH 150 MeV $^{84}\text{Kr}$ IONS

I. Manika, R. Zabels, R. Grants

*Institute of Solid State Physics, University of Latvia*

Beams of swift heavy ions with the MeV-GeV energy have increasingly gained an interest for their application in the structuring of materials on the micro- and nanometre scale. Generally, heavy ions (e.g. U, Pb and Au) cause more substantial modifications of the structure and properties compared to lighter projectiles. However, the irradiation with swift heavy ions is accompanied by undesirable effects of swelling and a generation of long-range stresses. The results of the present study show that the nanostructuring in LiF crystals can be ensured also under the irradiation with lighter  $^{84}\text{Kr}$  ions. With this aim, we used 150 MeV Kr ions, the energy loss of which in the surface layer exceeds the threshold for the track core damage. Irradiations were performed at the fluence  $10^{12}$  cm<sup>-2</sup> ensuring the overlapping of the halo regions of tracks, saturation and aggregation of F centers. Methods AFM, SEM and nanoindentation in the present study were used. The results show the ion-induced formation of bulk nanostructures which consist of columnar grains with nanoscale dimensions (~50-100

nm). At the end of ion pass the structure enriched with dislocation loops of interstitial and vacancy types was found to appear. The nanoindentation tests show a strong ion-induced increase of hardness that confirms a high volume concentration of strong obstacles for dislocations e.g. defect aggregates, dislocations and grain boundaries.

The study was performed in collaboration with the Eurasian National University and Institute of Nuclear Physics, accelerator DC-60, Astana, the Republic of Kazakhstan

### Scientific publications

#### SCI publications

1. R.Zabels, F.Muktepavela, L.Grigorjeva, E.Tamanis, M.MishelsPiesins, Nanoindentation and photoluminescence characterization of ZnO thin films and single crystals, *Optical Materials* 2010, vol. 32, Is. 8, pp. 818-822 (doi: 10.1016/j.optmat.2010.02.002).

#### Other publications

2. F.Muktepavela, R.Zabels. The Role of Diffusion Accommodation and Phase Boundary Wetting in the Deformation Behaviour of Ultrafine Grained Sn-Pb Eutectic. *Defect and Diffusion Forum*) 2010, vol297 – 301, pp.1002-1009.

#### Lectures on Conferences

**3rd Intern. Symp. on transparent conductive materials. TCM2010, October 17-21, 2010, Hersonissos – Crete, Greece.**

1. L. Grigorjeva, D.Millers, F.Muktepavela, R.Zabels. Luminescent and mechanical properties of Al, In and Ti doped ZnO ceramics, R316.

**E-MRS 2010 Fall Meeting, September 13-17, 2010 Warsaw, Poland.**

2. R. Zabels, F. Muktepavela, E. Tamanis. Deformation characteristics obtained by nanoindentation on ZnO films, B214.

**VI. Intern. Conf. on phase transformations and strength of crystals, Chernogolovka, November 16-19. 2010 Chernogolovka, Russia.**

3. F Muktepavela., R., Zabels, V. Sursajeva. Deformation characteristics obtained by nanoindentation on single and nanocrystalline ZnO., Abstract p. 80.

**International Conference on Functional materials and Nanotechnologies FM&NT 2010, March 16 –19, 2010, Riga, Latvia.**

4. J. Maniks, I. Manika, R. Grants, R. Zabels, K. Schwartz, M. Sorokin, R.M. Papaleo. Nanonstructuring and hardening of LiF crystals irradiated with 3 – 15 MeV Au ions, *Book of Abstracts*, p.63.
5. R. Zabels, F. Muktepavela, V.Sursajeva. Indentation induced deformation behaviour of ZnO. *Book of Abstracts* p. 60.

**3rd International conf. on radiation interaction with material and its use in technologies, September 20-23, 2010, Kaunas, Lithuania.**

6. J.Maniks, I.Manika, R.Zabels, R.Grants, K.Schwartz, M.Sorokin Modification of the structure and nano-mechanical properties of LiF crystals under irradiation with swift heavy ions, *Program and materials*, p.12.

**International Conference on Nuclear Materials, October 4-7 2010, Karlsruhe, Germany.**

7. M. Tomut, M. Krause, I. Manika, J. Maniks, R. Zabels, C. Trautmann. Stability of HOPG and fine-grained graphite exposed to MeV-GeV heavy ions

**Workshop on ion-beam physics, March 29-31, 2010, Dresden, Rosendorf, Germany.**

8. M. Tomut, M. Krause, I. Manika, J. Gabrusenoks, J. Maniks, R. Zabels, K. Schwartz, C. Trautmann. Raman and nanoindentation study of depth profile of GeV heavy ions-induced damage in graphite. Abstracts p.O30.

**26th Scientific conference of the ISSP, February 17-19, 2010, Riga, Latvia.**

9. R.Grants, I.Manika. Nanostructuring of LiF single crystals irradiated with 15 MeV Au ions, Abstracts p36.
10. R.Zabels, F.Muktepavela, V.Sursajeva. Nanoindentation processes in Zn and ZnO single – and polycrystals. Abstracts p.37.

## DEPARTMENT OF RADIATION PHYSICS

**Head of laboratory Dr. hab. J.Berzins**

### Research Area and Main Problems

The Department includes two research groups – the Laboratory of nuclear reactions and Laboratory of Transition Metals Compounds Physics. 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;
- EPR and Raman spectroscopies exchange interaction between radiation defects and transition metals ions in the dielectric crystals doped with the transition metals ions;
- retrospective biodosimetry.
- 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

### International projects:

Participation in the project „Investigation of nuclear structure via (n, $\gamma$ ), (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

- |                             |                             |
|-----------------------------|-----------------------------|
| 1. Dr.hab. J.Berzins        | 7. Dr.D.Riekstiņa           |
| 2. Dr.hab. M.Balodis        | 8. Dr. V.Skortsova          |
| 3. Dr.hab. V.Bondarenko     | 9. Dr.O.Veveris             |
| 4. Dr.hab.N.Mironova-Ulmane | 10. Dr.Ing.sc. A.Pavlenko   |
| 5. Dr.L.Simonova            | 11. Mag. Sc. M.Polakovs     |
| 6. Dr.T.Krasta              | 12. Mag.phys. J. Proskurins |

### Technical staff

S.Afanasjeva

### Students

K.Bavrins

### Scientific visits abroad

3. Dr. hab. J. Berzins, European Commission Euratom, Brussels,Belgium (10 days).
4. Dr. hab. J. Berzins, Cyclotron Workshop, Ispra, Italy 24-26 November.
5. Dr. hab. J. Berzins, Int.Conf. Nucleus 2010, St. Petersburg, 5-10 Juli 2010.
6. Mga .phys. J. Proskurins, Int.Conf. Nucleus 2010, St. Petersburg, 5-10 Juli 2010.
7. Dr. hab. J. Berzins, Int. Conf. Hazards Detection and Management, Dresden, 20-24 September.
8. Dr. D. Riekstina, Int. Conf. Hazards Detection and Management, Dresden, 20-24 September.

9. Dr. hab. J. Berzins, Insitut Laue Lagevin, Grenoble, (2x3days).
10. Dr. D. Riekstina, International Conference on Advances in Liquid Scintillation Spectrometry. LSC 2010. Paris, France, September 6-10, 2010.
11. Dr. hab. N.Mironova-Ulmane, Institute of Physics Tartu Estonia (1week +1 week+1week)
12. Dr. M.Polakovs Institute of Physics Tartu Estonia (1week)
13. Dr. hab. N.Mironova-Ulmane, Institute of Metal Physics, Urals Division of Russian Academy of Sciences, Jekaterinburg Russia (1week)
14. Dr. hab. N.Mironova-Ulmane, Kaunas, Lithuania (1 week)
15. Dr. V. Skvortsova University of Algarve, Faro, Portugal (1week) .
16. Dr. V. Skvortsova, Institute of Physics of the University of Pecs, Hungary (1week)

## **Cooperation**

### **Latvia**

1. Medical Academy of Latvia (Dr.hab., Prof. M.Eglite, Dr.hab.Prof. I.Cema, Dr.T.Zvagule).
2. Radiation Safety Center (I. Kisite)
3. Riga Technical University, Institute of Inorganic Chemistry (Dr. I.Vitina,).
4. University of Latvia, Chemical faculty (Dr. A.Viksna,)
5. Institute of Wood Chemistry ( Dr.hab. G.Dobele, Dr.hab. G. Telesheva, Dr.hab.T.Dizbit)
6. Riga Technical University, Faculty of Material Science and Applied Chemistry (Dr.Berzina-Cimdina).
7. National Diagnostic center.
8. Institute of Technical Physics, Rīga Technical University (Dr.J.Ruža).
9. Medical Academy of Latvia (Dr.hab., Prof.M.Eglite, Dr.hab.Prof. I.Cema, Dr.T.Zvagule).
10. Institute of Wood Chemistry (Dr. hab. G. Dobele Dr.hab. G. Telesheva, Dr.hab. T.Dizbit)
11. Riga Technical University, Faculty of Material Science and Applied Chemistry (Prof. J.Dehtjar).
12. Institute of Inorganic Chemistry, Riga Technical University, 2169 Salaspils, Latvia (Dr.J. Grabis, Dr. V. Serga)

### **USA**

1. Mississippi University (Prof. A.Afanasjev).
2. Brookhaven National Laboratory, Upton (Prof. R.F. Casten).

### **Germany**

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

### **France**

1. Institute Laue-Langevin, Grenoble, France ( 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).

## **Estonia**

1. Institute of Physics, Tartu (Prof.Ch.Luschik, Prof.A.Luschik, Dr.A.Sildos, Dr.T.Kärner).

## **Italy**

1. Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Frascati (M.Cestelli Guidi, A. Marcelli)
2. Dipartimento di Scienze Geologiche, Università Roma Tre, Rome ( M.Piccinini)
3. INFN and Dipartimento di Fisica, Università di Trento, Povo (Trento)( G.Mariotto)
4. INFN and Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (Cosenza) (E.Cazzanelli)

## **Ukraine**

1. R&D Institute of Materials RPA “ Carat”, Lviv ( Dr. D.Sugak, Dr. S.Ubizskii).

## **Russia**

1. Ural State University, Ekaterinburg (Prof. A. Nikiforov).
2. Ural Technical University, Ekaterinburg (Prof. B.Shulgin)
3. St.Petersburgh Nuclear Physics Institute, Gatchina (Dr.V.Bunakov, Dr.A.Sushkov)
4. Institute of Solid State Chemistry, Ural Branch of RAS, 620219 Yekaterinburg, Russia (Dr. I.F. Berger).
5. Institute of Metal Physics, Urals Division of Russian Academy of Sciences, 620219 Yekaterinburg, Russian Federation (Dr. V.Voronin,V.A. Kazantsev).

## **Denmark**

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

## **Main results**

### **POSSIBLE TRIAXIAL STRUCTURES IN ODD-ODD $^{188}\text{Re}$ NUCLEUS**

M. Balodis, T. Krasta, L. Simonova, V. Bondarenko, J. Berzins

Structure of the doubly odd  $^{188}\text{Re}$  nucleus ( $Z=75$ ,  $N=113$ ) has been studied via  $\gamma\gamma$ -coincidences, following the thermal neutron capture reaction with enriched  $^{187}\text{Re}$  target. Analysis of the obtained experimental data allowed to correct and essentially extend the earlier known low-lying level scheme of  $^{188}\text{Re}$ : 134 levels have been established up to about 1590 keV excitation energy. Comparison with the results of axially-symmetric core plus Nilsson two-quasiparticles model calculations displays good agreement with experimental rotational bands below 400 keV excitation energy. However, a number of established  $^{188}\text{Re}$  positive parity non-rotational levels with possible spins  $3^+, 4^+, 5^+$ , observed between 400 and 800 keV energy, cannot be interpreted in terms of two-quasiparticle configurations based on Nilsson orbits observed in neighboring odd nuclei. These levels can be explained, if one assumes that some two-quasiparticle states, based on neutron orbits  $1/2^- [510]$  and  $9/2^- [505]$ , have triaxial deformation, contrary to the axially-deformed  $^{188}\text{Re}$  ground state. Oblate and triaxial structures have been identified in both neighboring  $N=113$  nuclei:  $^{187}\text{W}$ , and  $^{189}\text{Os}$ . Possible coexistence of axially-deformed and triaxial shapes has been considered also in the level schemes of  $A\sim 190$  transitional region odd-odd  $^{192,194}\text{Ir}$  nuclei. Additional indications of different shape coexistence in the structure of  $^{188}\text{Re}$  nuclei are the observed characteristic cascade depopulation patterns of some states. Also, the rotational

parameters for bands, based on configurations involving neutron orbits  $1/2-[510]$  and  $9/2-[505]$ , are in the range  $A_0=18-19$  keV, comparing with the  $A_0=15.4-16.4$  keV values for the ground state band. Non-axial deformation can be a cause of the anomalous empirical Gallagher-Moszkowski splitting of the two-quasiparticle doublet  $p:9/2^+[514] \pm n:1/2-[510]$ .

## STUDY OF THE ONSET OF CHAOS IN THE $A \sim 190$ NUCLEAR DEFORMATION PHASE TRANSITION REGION

J. Proskurins, T. Krasta, K. Bavrins

Properties of nuclei with  $A \sim 190$  demonstrate deformation phase transition from prolate to oblate shape, which can be studied employing both group theoretical and geometrical methods. Continuing the theoretical research of quantum phase transitions in the frameworks of complete version of the standard interacting boson model (IBM-1), a systematic study of quantum chaos characteristics for selected transitional region nuclei has been performed, with the aim to establish a dependence of statistical and dynamical chaos criteria from  $Z$ ,  $N$ , and nuclear quadrupole deformation parameters  $(\beta, \gamma)$ . The energies and wave functions of 12 even-even isotopes of W, Os, and Pt, belonging to the mass number region  $184 \leq A \leq 194$ , were obtained via the diagonalization of IBM-1 multipole representation Hamiltonian matrices at parameter values, which ensure a best possible agreement with available experimental data. Corresponding IBM-1 parameter values were related with the nuclear shape variables  $(\beta, \gamma)$  employing the classical energy limit expression and catastrophe theory formalism control parameters  $(r_2, r_1)$ . The parameter values obtained for each nucleus were analyzed in terms of nuclear shape phase transition from the stable prolate axial deformation (with  $\gamma=0$ ) to the stable oblate axial deformation (with  $\gamma=\pi/3$ ), corresponding to the SU(3) limit of IBM-1, via the  $\gamma$ -soft ( $\gamma=\pi/6$ ) O(6) limiting case. Behavior of evaluated quantum chaos characteristics – energy spacing distribution  $P(s)$ , and wave function entropy  $W(\Psi_i)$ , in dependence from  $Z$ ,  $N$ ,  $\beta$ , boson number  $N_B$ , and level spin value  $I$  was studied, paying special attention to the region in the vicinity of the prolate-oblate shape phase transition critical line E(5)- O(6). The results of quantum chaos studies in the frameworks of algebraic IBM-1 were compared with those obtained using geometrical rigid triaxial rotator models.

## NUCLEAR LEVELS of $^{183}\text{W}$ STUDIED WITH $(n, \gamma)$ and $(d, p)$ REACTIONS

V. Bondarenko <sup>d</sup>, I. Tomandl <sup>a,b</sup>, J. Honzátko <sup>b</sup>, H.-F. Wirth <sup>c,e</sup>, T. von Egidy <sup>c</sup>

*a Research Centrum, Rěž, Czech Republic*

*b Nuclear Physics Institute, Rěž, Czech Republic*

*c Physik-Department, Technische Universität München, Garching, Germany*

*d Institute of Solid State Physics, University of Latvia, Riga, Latvia*

*e Sektion Physik, Ludwig-Maximilians-Universität München, Garching, Germany*

The level structure of  $^{183}\text{W}$  has been studied using gamma–gamma coincidences from thermal neutron capture in  $^{182}\text{W}$  accompanied with the reaction  $(_d, p)$ . From these data and those of previous studies a total of 76 levels and about 490 connecting  $\gamma$ -transitions have been established for energies below 2.4 MeV. An analysis based on the standard distorted-wave Born approximation (DWBA) provides the  $lj$ -angular momentum transfers and spectroscopic factors for 36 levels up to 2.2 MeV excitation energy. A large number of particle transitions indicate an influence of strong mixing between particle and probably hole states. The extra exchange of phonons across the Fermi

surface leads to a fine structure in the fragmentation of most single particle strengths and at the same time has the effect of breakdown of the individual properties of Nilsson states. The extracted  $l = 1$  and 2 (d, p) sum below 2 MeV has about the same magnitude as in 185,187W. It comprises a rather small fraction of the expected strengths. The observed states below 2 MeV are compared with predictions of the quasiparticle–phonon model. Of particular interest is the identification of “quasi-bands” with inverse spin sequence based on the state  $9/2^+$  at 622.8 keV; this indicates some transition aspects from rigid rotors of light W to  $\gamma$ -soft nuclei in the Os-Pt region.

## ASSESSMENT OF RADIONUCLIDE CONCENTRATION IN VARIOUS SAMPLES BY GAMMA SPECTROMETRY AND LSC METHODS

J.Berzins, D.Riekstina, O.Veveris

The monitoring of the artificial gamma radionuclides in the soil and tritium in the groundwater around the potentially most polluted regions of Latvia: the areas of the shut-down Salaspils research nuclear reactor and the radioactive waste repository “Radon”, control of the drinking water, radioactive contaminated territory and identification of uncontrolled radioactive sources in some enterprises was carried out.

The concentrations of radionuclide in different probes: soils, waters, metal scrap and various types of samples, irradiated in the research nuclear reactor, were determined using the high resolution HPGe gamma-spectrometer within the energy range of 50-2000 keV. For measuring of large radioactive waste volums in the metal barrel gamma-spectrometer with NaJ detector were used. The uncertainty of measurements was within the range of 3-10%, but the minimal detectable activity – 0.3 Bq/kg.

The measurements of tritium activities were carried out with the liquid scintillation spectrometer Packard TRI-CARB using the scintillation liquid OptiPhase “HiSafe”3. The measurement time for H-3 didn’t exceed some hours and uncertainty was less than 2%.

The quality assurance included the main requirements of standard ISO/IEC 17025:2005.

## STRUCTURAL AND MAGNETIC PROPERTIES OF NICKEL OXIDE NANOPOWDERS

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The structure and magnetic properties of nickel oxide (NiO) nanopowders has been studied by x-ray/neutron diffraction, SQUID magnetometer and micro-Raman spectroscopy.

The nanosized NiO powders have been produced by the two methods. A precipitation method, employing reacting aqueous solutions of  $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  and NaOH, was used to prepare particles around 13-23 nm, which were further annealed in air at several temperatures up to  $T_{\text{an}}=450^\circ\text{C}$ . In the second method, particles with a size of 100 and 1500 nm were prepared by evaporation of coarse grained commercially available NiO (99.9%) powder with a particle size in the range of 20-40  $\mu\text{m}$  in radio-frequency plasma. The average size of all nanoparticles was estimated from the BET specific surface area measurements.

Our diffraction data indicate that at room temperature all NiO powders are antiferromagnetically ordered and have rhombohedral (R-3m) phase as is evidenced from the NiO(422) Bragg reflex splitting located at high scattering angle of about 130°. The structural parameters, determined by the Rietveld analysis procedure, indicate an expansion of the lattice volume when particles size decreases below 30 nm, being in agreement with the results of Li et al. [1].

SQUID magnetometer measurements of nanosized NiO, performed in the temperature range of 2-300 K and the magnetic field range of 0-50 kOe, are consistent with the presence of an antiferromagnetic particle core superimposed to a net moment due to the intrinsic weak ferromagnetism attributed to the presence of Ni<sup>3+</sup> ions.

The room temperature micro-Raman spectra of nanopowders, excited by the 514.5 nm cw argon laser, are similar to that of microcrystalline NiO [3], including a number of one-phonon/two-phonon bands located below 1200 cm<sup>-1</sup> and two-magnon band at 1500 cm<sup>-1</sup>, indicating that the powders remain in antiferromagnetic phase at RT. However, a new Raman band at 500 cm<sup>-1</sup> has been observed in nanosized NiO: its temperature and size dependence suggest magnetic origin. We attribute this band to a one-phonon (~440 cm<sup>-1</sup>) plus one-magnon (~40 cm<sup>-1</sup>) excitation, induced by the strong phonon-magnon interaction at nanoparticles surface or some defects.

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## THE OPTICAL PROPERTIES OF MAGNESIUM OXIDE CONTAINING TRANSITION METAL IONS AND DEFECTS PRODUCED BY FAST NEUTRON IRRADIATION

Vera Skvortsova, Laima Trinkler

*Abstract:* - The photoluminescence (PL), its excitation (PLE) and optical absorption of MgO crystals containing transition metal ions and defects produced by fast neutron irradiation fluence up to 10<sup>20</sup>cm<sup>-2</sup> (E>0.1 MeV) are investigated. Three range of luminescence are observed: 380-460 nm, 650-850 nm and 850-1050 nm. These luminescence bands are attributed to presence of Fe<sup>3+</sup>. We assume that the 440 nm photoluminescence band belongs to the complex V<sup>-</sup><sub>OH</sub>-Fe<sup>3+</sup> center with tetragonal symmetry, while the ~730 nm PL band observed in the irradiated MgO crystals is connected with defects, generated as a result of decay of the complex V<sup>-</sup><sub>OH</sub>-Fe<sup>3+</sup> centers. The near infrared luminescence bands in MgO crystal are connected with the Fe<sup>3+</sup>-Fe<sup>3+</sup> exchange coupled pairs. Furthermore the luminescence of chromium and manganese ions of different symmetry is observed.

### Scientific Publications

1. M.Balodis, I.Tomandl, V.Bondarenko, L.Simonova, T.Krasta, J.Bērziņš. Low-lying levels of <sup>188</sup>Re nucleus from  $\gamma\gamma$ -coincidence measurements. Nucl.Phys.A.847(2010)p.121-148,.
2. Nina Mironova-Ulmane, Alexei Kuzmin, J. Grabis, I. Sildos, V.I. Voronin, I.F. Bergerand and V.A. Kazantsev. Structural and Magnetic Properties of Nickel Oxide Nanopowders. Solid State Phenomena Vols, 168-169, 2011, pp. 341-344.
3. N. Mironova-Ulmane, A. Kuzmin, I. Sildos, M. Pärs, Polarisation dependent raman study of single-crystal nickel oxide, Cent. Eur. J. Phys. (2010) [accepted ]
4. V. Skvortsova. Luminescence of iron ion impurity in irradiated magnesium oxide crystals. LU CFI 26. sci.. conf.. 2010 g. 17.-19. Febr. Abstracts, p.43

## Presentations in Conferences

1. D.Riekstiņa. Analysis of radioactivity in drinking and groundwater. 26-th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, 17-19 February, 2010.
2. M.Balodis. Development of  $^{188}\text{Re}$  level scheme using the  $(n,\gamma\gamma)$  reaction data.
3. T.Krasta. Investigation of nuclear structure effects connecting with isospin symmetry.
- 4.V. Skvortsova. Luminescence of iron ion impurity in irradiated magnesium oxide crystals. LU CFI 26. sci. conf. 2010 g. 17.-19. Febr. Abstracts, p.43.
5. J.Berzins Possible triaxial structures in the odd-odd rhenium-188 nucleus, LX International Conference on Nuclear Physics „Nucleus 2010”. Methods of Nuclear Physics for Femto- and Nanotechnologies. Saint Peterburg, Russia, July 6-9, 2010.
6. J. Proskurins, Study of the onset of chaos in the  $A\sim 190$  nuclear deformation phase transition region. LX International Conference on Nuclear Physics „Nucleus 2010”. Methods of Nuclear Physics for Femto- and Nanotechnologies. Saint Peterburg, Russia, July 6-9, 2010.
7. D. Riekstiņa, Control of tritium in drinking and groundwater in Latvia, International Conference on Advances in Liquid Scintillation Spectrometry. LSC 2010. Paris, France, September 6-10, 2010.
8. J.Berzins. Assessment of radionuclide concentration in various samples by gamma spectrometry and LSC methods. International Conference „6th Dresden Symposium. Hazards – Detection and Management.” Dresden, Germany, September 20-24, 2010.
9. N. Mironova-Ulmane. Polarisation dependent raman study of single-crystal nickel oxide. International Baltic Sea Region conference „Functional materials and nanotechnologies FM&NT-2010” 16-19 March, Riga, Latvia, p. 117.
- 10.T. Dizhbite, G. Telysheva, G. Lebedeva, N. Mironova-Ulmane, A. Andersone, and L. Belkova. Water soluble bioactive organic-inorganic Si- and Fe- containing hybrid materials based on lignosulphonate International Baltic Sea Region conference „Functional materials and nanotechnologies FM&NT-2010” 16-19 March, Riga, Latvia, p. 164.
- 11.M.Polakovs, N. Mironova- Ulmane, A. Pavlenko and S. Lebedev EPR and Mössbauer spectra of iron ions in the hemoglobin, International Baltic Sea Region conference „Functional materials and nanotechnologies FM&NT-2010” 16-19 March, Riga, Latvia, p. 165.
- 12.Nina Mironova-Ulmane, Alexei Kuzmin, J. Grabis, I. Sildos, V.I. Voronin, I.F. Bergerand and V.A. Kazantsev. Structural and Magnetic Properties of Nickel Oxide Nanopowders. The international IV Euro-Asian Symposium "Trends in Magnetism" EASTMAG-2010, June 28 -2 July, 2010, JekaterinburgRussia, p. 39
- 13.G.M. Abramova, J. Schefer, M. Boehm, G. A. Petrakovskiy, N. Mironova-Ulmane and V.V. Sokolov FeXMn1-XS single crystals with strong electron correlations . The international IV Euro-Asian Symposium "Trends in Magnetism" EASTMAG-2010 June 28 -2 July, 2010, Jekaterinburg, Russia, p.363
- 14.M. Grube, M. Gavare, R. Rutkis, U. Kalnenieks and N. Mironova-Ulmane. Use of FT-IR spectroscopy data for systems analysis of *Zymomonas mobilis* metabolism 30th European Congress on Molecular Spectroscopy EUCMOS-2010, Florence, Italy, 29 August-3 September, p.112
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- 16.Nina Mironova-Ulmane, Alexei Kuzmin, J. Grabis, V.Serga, I. Sildos and V.I. Voronin. Structural and Magnetic Properties of Nickel Oxide powders. The 17th

International Conference on Solid Compounds of Transition Elements, SCTE 2010 September 5-10, 2010, Annecy, France.p. 75

17.Maksims Polakovs, Nina Mironova-Ulmane, Andrejs Pavlenko, Tija Zvagule, Natalija Kurjane, Natalija Gabrusheva, The investigation of chernobyl clean-up workers blood by EPR technique, Proceedings of the international conference “Medical physics in the Baltic states – 2010”, Kaunas, Lithuania, 14-16, 2010 p. 137-141.

18.V. Skvortsova, L. Trinkler. Transition metal ions luminescence in neutron irradiated magnesium oxide. 11th Europhysical Conference on Defects in Insulating Materials EURODIM 2010, Pecs, Hungary, 12 – 16 July 2010, p. A78.

19.V. Skvortsova, L. Trinkler, Luminescence of impurity and radiation defects in magnesium oxide crystals irradiated by fast neutrons. Physics Procedia, 2009, v 2, p.567-570.

20.V. Skvortsova, L. Trinkler. The Optical Properties of Magnesium Oxide Containing Transition Metal Ions and Defects Produced by Fast Neutron Irradiation. Proceedings of the 3th WSEAS International Conference on materials science (MATERIALS '10), Faro, Portugal, 3-5 November 2010, p.150-154.

#### **Physics Doctor students:**

1. Jevgenijs Proskurins – Study of quantum chaos and phase transitions in nuclear models. Supervised by Dr.T.Krasta., Submistted in december 2010.

#### **Lectures at Universities, Institutes ...**

During 2010, T. Krasta was engaged in following activities related with LU study programs:

- 1) supervision of J. Proskurins physics doctor dissertation work „Theoretical study of quantum
- 2) supervision of physics masters work of LU Physics and Mathematics Faculty student K.Bavrins.

## LABORATORY OF ORGANIC MATERIALS

Head of laboratory **Dr. hab. I.Muzikante**

### Scientific Staff

Inta Muzikante Dr.habil.phys.  
Lilita Gerca Dr.chem.  
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Mārtiņš Rutkis Dr.phys.  
Oskars Vilītis Dr.phys.

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Jānis Latvels  
Andrejs Tokmakovs  
Aivars Vembris

### Students

Edgars Nitišs  
Jurģis Sīpols  
Artis Ernstsons

Maira Indrikova  
Baiba Niparte  
Martins Porozovs  
Kaspars Pudžs

### Scientific projects of the Latvian Council of Sciences

09.1548	Physical Processes in Multilayer and Multicomponential Structures (2009-2013)
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
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### ERAF projects of the activity 2.1.1.1.”Support of science and research”

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)

No. 2010/0209/2DP/2.1.1.1.0/10APIA/VIAA/028 „Development of perspective nanocomposites on the bases of secondary polymers and elaboration of manufacturing and processing technologies” (2010-2013)

### International projects

Projects of Mutual scientific co-operation fund of Republic of Lithuania and the Republic of Latvia with R.O.C. (Taiwan):	
1. ISSP LU & RTU Institute of Physics, Vilnius, Lithuania Institute of Atomic and	Structural organization and optical nonlinearities of low-dimensional molecular structures (2007-2010)

Molecular Science Taipei, Taiwan	
2. ISSP LU Kaunas Technology University Institute of Chemistry, Academia Sinica, R.O.C., Taiwan	Design, Synthesis and Studies of New Effective Materials for Organic (Opto)electronics (2008-2011)

### Main equipments:

- Equipments for preparation of thin films:
  - the vacuum deposition of organic compounds and metals (Edwards 306A);
  - the Langmuir-Blodgett technique;
  - the self-assembled techniques;
  - the casting and spin-coating techniques (Lite Single Wafer Spin Processor, Laurell technology Corporation).
- High vacuum setups for measuring of electrical and photoelectrical conductivity between 10 and 400K. The sample is provide by a digitally controlled voltage supply over range up to 5kV and the current is measured in range 1fA to 1mA.
- Computer controlled corona poling systems.
- Computer-controlled Kelvin probe setup with the temperature control up to +130°C and measuring the surface potential in a range between -9.6 and +9.6V with the accuracy ±1mV. The diameter of vibrating gold electrode was 2mm
- Scanning Kelvin Probe SKP5050
- Surface Profile Measuring System Dektak 150
- Computer-controlled SHG setup ( $\lambda=1064$  nm) allows us to measure SHG ( $\lambda=532$  nm) intensity as function of the fundamental power, incidence angle, fundamental and SH light polarization as well as sample surface mapping by SHG intensity. The detection threshold of equipment is  $1 \times 10^{-6}$  pm/V

### Cooperations

#### Latvia

- Institute of Applied Chemistry, Riga Technical University (Prof. V.Kampars, Prof. V.Kokars).
- Latvian Institute of Organic Synthesis (Dr. E.Markava).
- Institute of Chemical Physics, University of Latvia, (Dr. D.Erts).
- Institute of Physical Energetics (Dr. I.Kaulach).

#### Lithuania

- Institute of Physics (Prof. L.Valkunas, Dr. V.Gulbinas).
- Institute of Material Science and Applied Research, Vilnius University, (Prof. S.Juršenas).
- Kaunas Technology University (Prof. J.V. Grazulevicius)

#### Germany

- Lehrstuhl Physik kondensierter Materie, Universität Potsdam, Potsdam (Prof. D.Neher, Dr. B.Stiller).

#### Taiwan

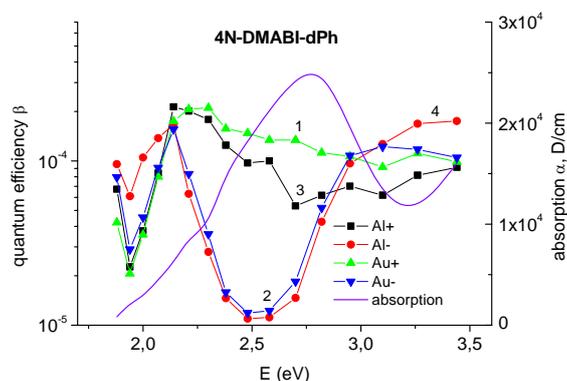
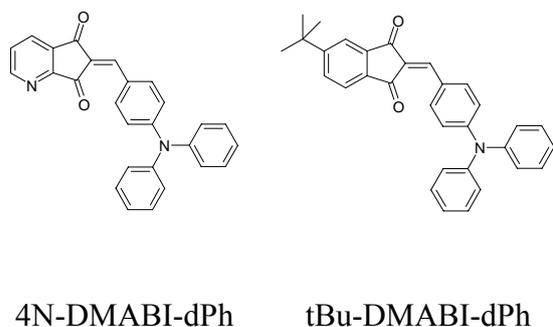
- Institute of Atomic and Molecular Science Taipei (Prof. S.H.Lin)
- Institute of Chemistry, Academia Sinica, (Prof. Chao-Ping Hsu)

## Main results

### PHOTOELECTRICAL PROPERTIES AND ENERGETICAL STRUCTURE OF THIN FILMS OF INDANDIONE DERIVATIVES

M.Indrikova, J.Latvels, I.Muzikante, B.Turovska

A sandwich type structure of two dimetilaminobenziliden-1,3-indandione (DMABI) derivatives placed between metal electrodes was made to investigate the photoelectrical properties of these derivatives. DMABI is an organic isolator with a wide energy gap and high quantum efficiency of the photogeneration, DMABI derivatives have received also considerable attention because of its large dipole moment and optical nonlinearities. Besides, since it is a photosensitive material, its use in solar systems is very promising. The energy gap of each material and combined system was observed from the spectral dependence of the quantum efficiency of the photoconductivity and results are compared with results of oxidation and reduction potential of the materials. The values showed a good correlation between experimental data of the photoconductivity and voltamperometry and calculated data of the HOMO and LUMO levels of the molecules.



*Chemical structure of DMABI derivatives under study: 4N-DMABI-dPh and tBu-DMABI-dPh*

*Spectral dependences of the photocurrent of Au/4N-DMABI/Al device. Irradiation of the sample is carried out via positive Au electrode (1), negative Au electrode (2), positive Al electrode (3) and negative Al electrode (4) at  $U=10V$ . The absorption spectrum of 4N-DMABI thin film is presented.*

The value of quantum efficiency  $\beta(h\nu)$  for the single layer thin films - 4N-DMABI-dPh is about  $1 \times 10^{-5}$  el/phot and for the tBu-DMABI-dPh films approximately  $1 \times 10^{-4}$  el/phot in the spectral range from 1.9 till 2.3eV. In comparison with DMABI thin films, the values are lower by two orders of magnitude.

The quantum efficiency of photoconductivity  $\beta(h\nu)$  of double layer devices mainly depends on the polarity of electrodes, but on the direction of irradiation. In case of positive Au electrode dominates photoelectrical properties of the 4N-DMABI-dPh layer which is deposited on Au electrode. Whereas, in case of positive Al electrode dominates properties of the tBu-DMABI-dPh layer.

The photoconductivity threshold energy for 4N-DMABI-dPh films is  $E_{th} = 1.80 \pm 0.05$  eV and for tBu-DMABI-dPh films is  $E_{th} = 1.90 \pm 0.05$  eV. The threshold values are close to the redox potential  $\Delta E_{redox}$  values of 4N-DMABI-dPh and tBu-DMABI-dPh molecules which are  $\Delta E_{redox} = 2.05$  eV and  $\Delta E_{redox} = 2.16$  eV

respectively. Besides, the difference of calculated HOMO and LOMO levels of the molecules also correlates with threshold energies

In cooperation with Riga Technical University and Latvian Institute of Organic Synthesis.

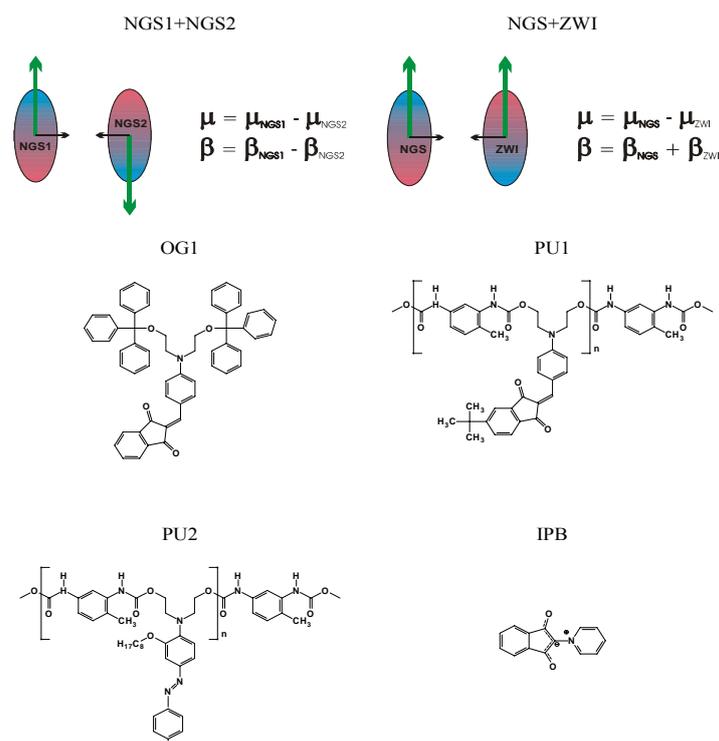
*This work is supported by Latvian National research Program in Material Science (2005-2009) and Scientific projects of the Latvian Council of Sciences No. 09.1548*

## INDANDIONE BASED BINARY CHROMOPHORE SUPRAMOLECULAR SYSTEMS AS A NLO ACTIVE POLYMER COMPOSITES

M. Rutkis, A. Tokmakovs, E. Jecs, J.Kreicberga, V. Kampars, V. Kokars

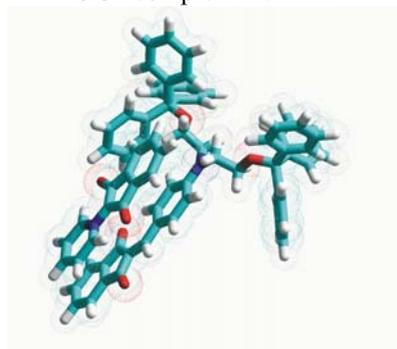
Novel route to obtain **EO** material is proposed by supramolecular assembly of neutral ground state (**NGS**) and zwitterionic (**ZWI**) **NLO** chromophores in binary chromophore organic glass (**BCOG**) host - guest system. On a basis of our Langeven Dynamics (**LD**) molecular modeling combined with quantum chemical calculations, we have shown that anticipated enhancement **NLO** efficiency of **BCOG** material is possible via electrostatic supramolecular assembly of **NGS** with **ZWI** chromophore in anti- parallel manner. Binding energy of such complex could be more dependent on molecular compatibility of components and local (atomic) charge distribution, then overall molecular dipole moments. According to our **LD** simulations these supramolecular bind structures of **NGS** and **ZWI** chromophores can sustain thermally assisted electrical field poling. For the one of experimentally investigated systems, build from dimethylaminobenzylidene 1, 3 - indandione containing host and zwitterionic indandione-1,3 pyridinium betaine as a guest, almost twofold enhancement of **NLO** efficiency was observed.

*Schematic presentation of electrostatic supramolecular assembly of bichromophores and their hyperpolarizability in cases of two NGS and NGS with ZWI chromophores and molecular structures of investigated NGS chromophores containing hosts and ZWI guest compound:*

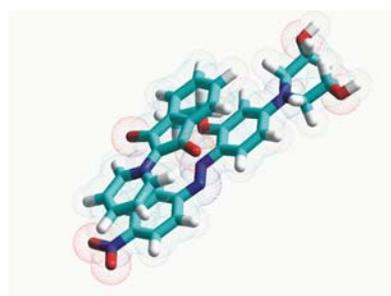


*Supramolecular bichromophore structures obtained by LD molecular modeling:*

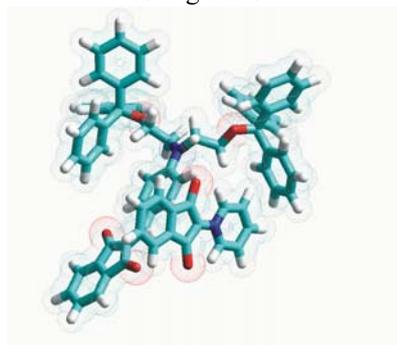
OG1 complex with IPB



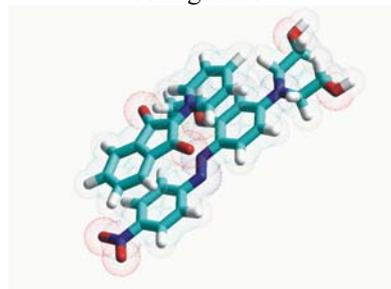
AZO with IPB



OG1 with IPB at E field break a part configuration

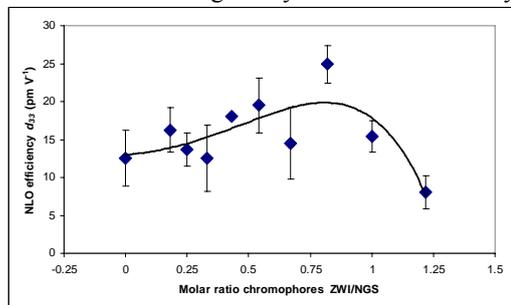


AZO with IPB at E field break a part configuration

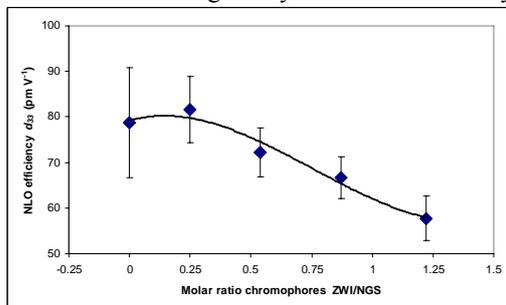


*Effect of ZWI/NGS chromophore ratio on corona poled films of prepared BCOG:*

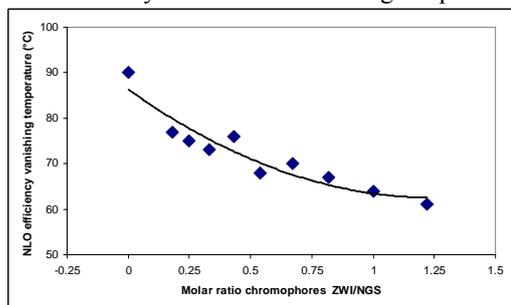
OG1 & IPB host – guest system NLO efficiency



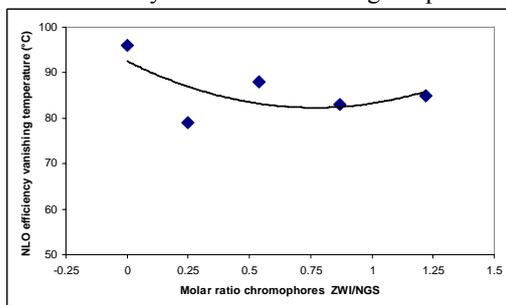
PU2 & IPB host – guest system NLO efficiency



OG1 & IPB system – NLO vanishing temperature



PU2 & IPB system NLO vanishing temperature



In cooperation with Riga Technical University

*This work is supported by scientific project of the Latvian Council of Sciences No. 10.0032.14 and*

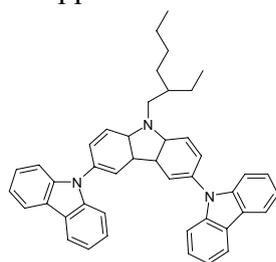
*Taiwan—Lithuanian—Latvian collaboration project*

## DESIGN, SYNTHESIS AND STUDIES OF NEW EFFECTIVE MATERIALS FOR ORGANIC (OPTO)ELECTRONICS

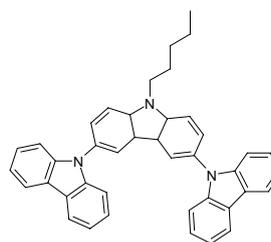
K.Pudzis, A.Vembris, J.Latvels, I.Muzikante, E.Fonavs

Study of charge carrier transport in organic electroluminescent (EL) devices, organic photovoltaic (OPV) devices, and organic field-effect transistors is one of the most important points. Many organic materials with high charge carrier mobility both for electrons and holes are under investigation. Among them derivatives of carbazole became the subject of numerous investigations.

In this work, we have studied optical, electrical properties and energy structure of two carbazole oligomers. In design of EL devices the electroluminescent materials should be included in carbazole film. In our work the electrophosphorescent compound Ir(fppy)<sub>3</sub> was applied.



JS-97



JS-100

*Chemical structure of carbazole derivatives under study: JS-97 and JS-100*

In the experiments were used two types of samples

The non-linear current-voltage characteristics were measured for vacuum evaporated and spin-coated JS-97 and JS-100 thin films with different electrodes. The electrodes were chosen in order to have hole or electron injection. For electroluminescence devices the injection both of electrons and holes are necessary. According to literature data, the Al electrode was applied for electron injection and Au electrode – for hole injection. To be sure that our choice is correct first of all the values of the ionization potential, energy gap and local trapping states of the organic thin film and work functions of the metals must be compared. In order to investigate energy structure of the JS-97 and JS-100 thin film in the regime of space charge limited current (SCLC) only monopolar injection is acceptable. So ITO, Au and Ni electrode were chosen for the hole injection.

In the SCLC regime the activation energy dependence on applied voltage  $E_a(U)$  is of decreasing character with plateau, where the value of  $E_a$  corresponds to the energy level of the trapping states. We may conclude that estimated activation energies at low voltages do not characterizes the value of the energy gap of the thin film. At higher voltages typical character of the  $E_a(U)$  curve of SCLC regime was observed. At voltages  $U > 90V$  plateau  $E_a = E_t = 0.1 \pm 0.02$  eV was estimated. In the case of mixed film of 2 organic compounds containing JS-97 and Ir(Fppy)<sub>3</sub> additional local energy states at  $E_t = 0.40 \pm 0.02$  eV and  $E_t = 0.16 \pm 0.02$  eV were observed.

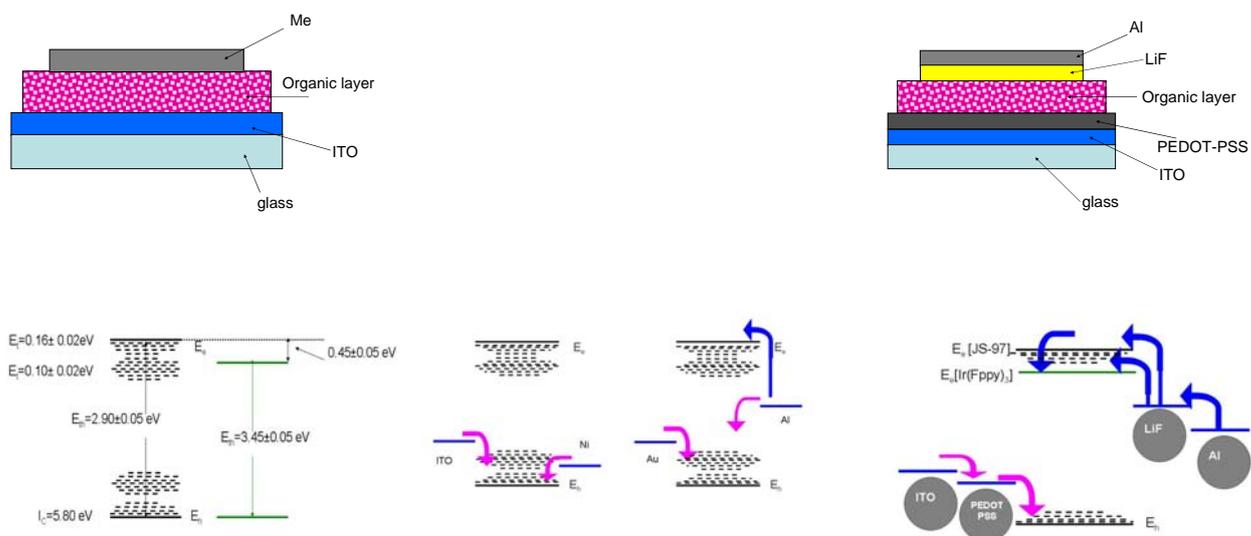
In order to obtain energy gap of the carbazole derivatives, the quantum efficiency of the photoconductivity  $\beta(h\nu)$  in spectral region from 280 nm till 730 nm was measured. The applied voltage  $U = 10$  V was chosen, where injection of charge carriers is absent. The value of the threshold energy  $E_{th} = 2.9eV \pm 0.1$  eV was estimated.

On the other hand the adiabatic energetic gap  $E_G^{Ad}$  could be estimated from the electrochemical redox potentials obtained by cyclic voltammetry (CV). The first standard reduction potential ( $E_{red}^0$ ) of the compound measured in the solution and gas phase electron affinity ( $A_C$ ) are linearly related between each other. Similarly the first

standard oxidation potentials ( $E_{ox}^0$ ) correlated linearly with the ionization potentials ( $I_c$ ). For the organic molecules with the large delocalized  $\pi$  electron systems where the gain or loss of an electron introduces small disturbances the slopes of both correlations are close to the unity. In our case the voltamperometry method to obtain oxidation  $U_{ox}$  and reduction  $U_{red}$  potential of JS-97 compounds was applied. As follows from the experimental results, the value of  $U_{redox} = 2.72$  eV, which is close to the value of the  $E_{th}$ .

The energy values of the compound  $Ir(Fppy)_3$  follows from the literature data, excluding the value of the surface potential  $U_s$ , measured by Kelvin probe method. The estimated activation energy  $E_t = 0.40 \pm 0.02$  eV is close to difference of energy gaps of the JS-97 and  $Ir(Fppy)_3$ . Consequently, this energy level corresponds to  $Ir(Fppy)_3$  molecule, while energy levels at  $E_t = 0.16 \pm 0.02$  eV and  $E_t = 0.10 \pm 0.02$  eV corresponds to structural defects in the thin films.

The energy diagrams of the devices  $EL_1/OL/EL_2$  are presented in Figure. As follows from the diagrams in the case of Al electrode injection both of electrons and holes is possible and in this case we cannot apply SCLC regime, which is valid for the monopolar charge carrier transport in the film. It may be one of the reasons to observe maxima in current-temperature dependence at 220 K. In the case of ITO and Ni electrode dominates hole transport.

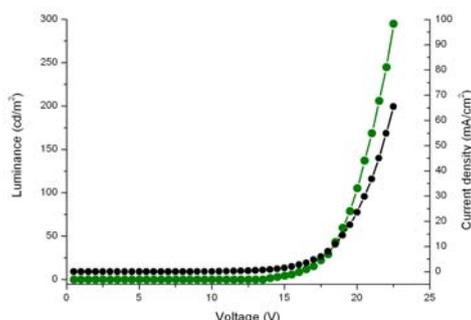


Energy diagram of the JS-97 compound and  $Ir(fppy)_3$  compound in solid state.

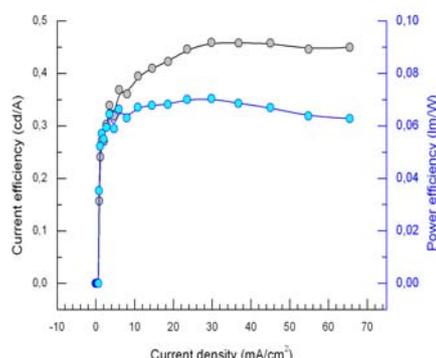
Energy diagrams of the devices ITO/JS-97/Ni and Au/Sj-97/Al. Blue arrows show injection of the electrons and red arrow – injection of holes.

The structure of OLED device was ITO/PEDOT:PSS(40nm)/JS-97+8wt% $Ir(fppy)_3$  (150nm)/LiF(1nm)/Al(100nm). Energy diagram of the device shows that injection both of the electrons and holes is possible. Besides electrons from electron conductivity level of JS-97 molecules energetically can be transported to  $Ir(Fppy)_3$  electron conductivity level. This fact is very important to observe the electroluminescence because of the increasing the density of electrons in the conducting level of electroluminescent material, namely  $Ir(Fppy)_3$ . The characteristic current density-

voltage and luminance-voltage dependences (J-L-U) were measured. In this case, when holes are injected from the positive ITO electrode and electrons are injected from the negative Al electrode, the electroluminescence process is observed. On the contrary, when the negative voltage is applied to the ITO electrode no electroluminescence process occurs.



The current density-voltage and luminance-voltage dependences (J-L-U) of the device.



The current efficiency-current density and power efficiency-current density dependences of the device

In order to characterize our device, the luminance (L) was measured, and the power and luminance efficiencies were calculated. The turn on voltage of the device was 14 V (when the luminance is  $\sim 1 \text{ cd/m}^2$ ). The luminance increases with the forward voltage, and at  $U = 22.5 \text{ V}$  it reaches  $L = 295 \text{ cd/m}^2$ . The power and luminance efficiencies at the luminance  $100 \text{ cd/m}^2$  are  $0.07 \text{ lm/W}$  and  $0.45 \text{ cd/A}$ , respectively. As is seen in Figure, the maximum efficiencies of our device are  $0.07 \text{ lm/W}$  and  $0.46 \text{ cd/A}$ . These values are slowly decreasing at higher current densities. It should be noted that the measured EL parameters are for non-optimized samples; after optimization they may be improved.

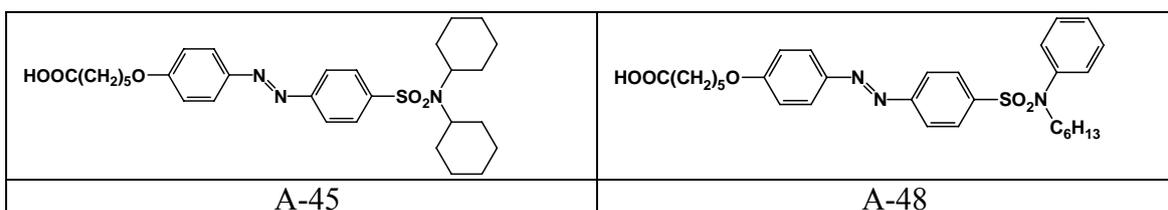
In cooperation with Kaunas University of Technology.

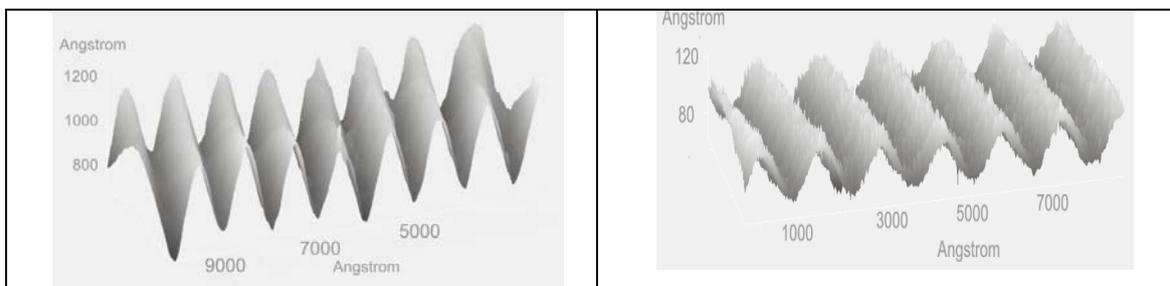
The work is supported by the Taiwan—Lithuanian—Latvian collaboration project

## OPTICALLY INDUCED SURFACE RELIEF GRATINGS IN POLYMER FILMS DOPED WITH SULPHONYL GROUP CONTAINING AZOBENZENE

E.Laizane, D.Gustina, K.Kundzins, I.Muzikante, J.Teteris

In holography, more attractive have become azobenzene compounds doped in a polymer matrix (host-guest polymer film) or chemically attached to the polymer. Azobenzene molecules exhibit reversible photoisomerization between trans- and cis-isomers which can form a surface relief grating in the films. The holographic recording and formation of surface relief gratings in a host-guest polymer film with two original azobenzene compounds are investigated. Holographic recording with 325 nm laser light was performed in host-guest polymer films with the host being polymethylmetacrylate (PMMA) and the guest 15 wt% azobenzene molecules (A-45 or A-48).





The host material was PMMA (molecule mass 440000 from Sigma – Aldrich). Solutions of PMMA and A-45 or A-48 in chloroform were prepared and ultrasonically mixed for 15 min. The amounts of compounds were chosen so as to obtain host-guest films with a concentration of azobenzene molecules of 15 wt%.

The holographic recording in host-guest polymer films with incorporated A-45 or A-48 molecules has been performed at wavelength 325 nm, which corresponds to the short-wave side of the main trans-isomer absorption band. At this wavelength a feasible explanation may be the trans-to-cis photoisomerization process. Nevertheless, simultaneously a reverse process (cis-to-trans photoisomerization) occurs, which arises due to the very diminished and broad cis-isomer band in the spectral region 300-360 nm and due to thermal influence. We may assume that the quantum efficiency of trans-to-cis photoisomerization dominates over of the reverse process. For more feasible explanation, recording of the surface relief gratings with different wavelengths is/would be advisable. For the host-guest polymer films with incorporated A-45 molecules the time of reaching the saturation of diffraction efficiency is  $\sim 1.3$  times longer, but the DE value is more than 2.5 times larger as compared to the host-guest polymer films with incorporated A-48 molecules. The depth of recorded surface relief gratings is larger for host-guest polymer films with A-45 molecules (35 to 45 nm) as compared to those with A-48 molecules (4 to 6 nm). This can be explained by different moieties in the molecules. The cyclohexane rings in an A-45 molecule are not planar, therefore a ring inversion, which involves rotation about the single bonds of cyclic conformers, takes place. At the same time, the A-48 molecule has a phenyl ring with a planar and rigid structure. Such differences of the end groups may influence the packing and reorientation of the molecules in a polymer matrix, and the mass transport of the molecules and polymer during the holographic recording.

In cooperation with Latvian Institute of Organic Synthesis.

*This work is supported by Latvian National research Program in Material Science (2005-2009)*

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2. M.Rutkis, A.Tokmakovs, E.Jecs, J.Kreicberga, V.Kampars, V.Kokars, Indandione based binary chromophore supramolecular systems as a NLO active polymer composites, *Optical Materials*, 2010, Vol. 32, 796–802, doi:10.1016/j.optmat.2010.01.006
3. B.Niparte, I.Muzikante, E.Fonavs, D.Gustina, Photoisomerization process of azobenzene compounds in thin polymer films, *Latvian Journal of Physics and Technical Sciences*, 2010, Vol. 47, No 3, pp.5-12
4. A.Vembris, M.Porozovs, I.Muzikante, J.Latvels, A.Sarakovskis, V.Kokars, E.Zarins, Novel amorphous red electroluminescence material based on pyranilidene indene-1,3-dione, *Latvian Journal of Physics and Technical Sciences*, 2010, Vol. 47, No 3, pp.23-30

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6. E.Laizane, D.Gustina, K.Kundzins, I.Muzikante, J.Teteris, Optically induced surface relief gratings in polymer films doped with sulphonyl group containing azobenzene, *Latvian Journal of Physics and Technical Sciences*, 2010, Vol. 47, No 4, pp. 51-58.

### Abstracts

#### **26<sup>th</sup> Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, Latvia, February 17-19, 2010**

1. K.Pudzis, A.Vembris, M.Porozovs, J.V.Grazulevicius, Studies of physical properties of carbazole derivative matrix for electroluminescence systems. Book of Abstracts, p.12
2. M.Indrikova, J.Latvels, K.Pudzis, P.Pastors, V.Kampars, Photoelectrical properties of double-layers films of DMABI derivatives, Book of Abstracts, p.13
3. B.Niparte, E.Laizane, D.Gustiņa, Photoinduced electrical properties of azobenzene-polymer films, Book of Abstracts, p.15
4. E.Laizane, B.Niparte, D.Gustiņa, Photoinduced optical properties of azobenzene-polymer films, Book of Abstracts, p.48
5. J.Sipols, J.Latvels, I.Muzikante, B.Turovska, Determination of energetical parameters of thin films of DMABI derivatives by Kelvin probe and electrochemical methods, Book of Abstracts, p.14
6. M.Porozovs, A.Vembris, J.Latvels, Development of green light emitting electroluminescence systems, Book of Abstracts, p.49
7. A.Tokmakovs, A.Ernstsons, M.Rutkis, Measurements of molecular hyperpolarizability of the indandione derivatives by Hyper-Rayleigh scattering, Book of Abstracts, p.16
8. E.Nitiss, M.Rutkis, Impact of Fabry–Perot cavity formed by thin film sample on EO coefficients measurement by MZI method, Book of Abstracts, p.17
9. L.Tiļuga, J.Latvels, I.Muzikante, L.Skuja, Elemental analysis and measurements of film thickness in nanometer range by X-ray fluorescence, Book of Abstracts, p.53

#### **International Conference on Functional materials and Nanotechnologies FM&NT 2010, Riga, Latvia, March 16 – 19, 2009**

1. M.Rutkis, A.Jurgis, Computer modeling of chromophore/polymer composite polarization: para-, antiferro- and ferroelectric behavior, Book of Abstracts, p 53
2. I.Muzikante, J.Teteris, J.Aleksejeva, U.Gertners, A.Tokmakov, B.Stiller, D.Gustina, Photoinduced surface relief gratings formation and properties of PMMA films with azobenzene derivative containing N, N-dicyclohexyl sulfonamide moiety, Book of Abstracts, p 141
3. A.Tokmakov, M.Rutkis, A.Ernstsons, V.Kampars, Molecular hyperpolarizabilities of indane derivatives measured by hyper Rayleigh scattering, Book of Abstracts, p 160

#### **International conference SPIE Photonics Europe, April 12-16, 2010. Brussels, Belgium, CD**

1. A.Vembris, J.Latvels, M.Porozovs, I.Muzikante, J.V.Grazulevicius, New synthesized bi-polar carbazol derivatives as host materials for electroluminescence,
2. J.Latvels, I.Muzikante, K.Pudzis, V.Kampars, New indandione based materials for organic solar cells: electrical and photoelectrical properties,

3. E.Laizane, D.Gustina, E.Markava, I.Muzikante, B.Niparte, Influence of molecular structure of azobenzene molecules on reversible photoinduced processes in polymer films

**International Student Conference “Developments in Optics and Communications DOC-5”, Riga, Latvia, April 23-25, 2010**

1. E.Nitiss, M.Rutkis, O.Vilītis, Corona discharge optimization for nonlinear optical polymer poling Book of abstracts, p. 35
2. A.Tokmakov, M.Rutkis, A.Ernstsons, V.Kampars, Indane Derivatives molekular hyperpolarizability measurment by hyper Rayleigh scattering with p-nitroaniline as external standart, Book of abstracts, p. 36
3. B.Niparte, E.Laizane, D.Gustina, Photoisomerization processes of thin – layer films of azobenzene compounds, Book of abstracts, p. 43
4. M.Indrikova, J.Latvels, K.Pudžs, P.Pastors, V.Kampars, Photoelectrical properties of thin films of indandione derivatives, Book of abstracts, p. 44
5. J.Latvels, M.Indrikova, K.Pudz, P.J.Pastors, V.Kampars, New indandione type organic materials for solar cells, Book of abstracts, p. 45
6. K.Pudz, A.Vembris, M.Porozovs, J.V.Grazulevicius, Studies of physicsl properties of carbazole derivative matrix for electroluminescence systems, Book of abstracts, p. 46
7. E.Laizane, D.Gustina, K.Kundzins, I.Muzikante, J.Teteris, Optically induced surface relief grating of PMMA films with azobenzene molecules, Book of abstracts, p. 70
8. A.Vembris, M.Porozovs, I.Muzikante, V.Kokars, E.Zarins, Novel amorphous red electroluminescence material based on indan-1,3-dione pyran, Book of abstracts, p. 71

**International coference SPIE Optics & Photonics, August 1-5, 2010. San Diego, USA, CD**

1. A.Vembris, M.Porozovs, I.Muzikante, V.Kokars, E.Zarins, Indan-1,3-dione pyran derivatives as an amorphous red electroluminescence material, CD

**9<sup>th</sup> International Conference on Global Research and Education INTER-ACADEMIA 2010, August 9-12, 2010, Riga, Latvia**

1. A.Vembris, M.Porozovs, I.Muzikante, V.Kokars, E.Zarins, Novel amorphous red electroluminescence material based on indan-1,3-dione pyran, Book of Abstracts, p.141
2. M.Indrikova, J.Latvels, I.Muzikante, J.Sipols, V.Kampars, P.J.Pastors, Investigation of energetic structure of original indandione derivatives, Book of abstracts, p. 142.

**10<sup>th</sup> Baltic Polymer Symposium, September 8-11, 2010, Palanga, Lithuania,**

1. M.Indrikova, J.Latvels, I.Muzikante, J.Sipols, Energetic structure investigation of new indandiones, Programme and Abstracts, p. 144.
2. B.Niparte, I.Muzikante, E.Fonavs, D.Gustina, Surface photoinduced potential studies in host-guest films with azobenzene derivatives, Programme and Abstracts, p. 48
3. A.Vembris, K.Pudz, I.Muzikante, J.Simokaitienė, S. Grigalevičius, J.V.Grazilevicius, Energy structure and electro-optical properties of organic layers with carbazole derivatives, Programme and Abstracts, p.3
4. A.Vembris, M.Porozovs, I.Muzikante, V.Kokars, E.Zarins, Original amorphous red electroluminescence materials, Programme and Abstracts, p.50.
5. E. Laizane, D.Gustina, E.Markava, I.Muzikante, A.Vembris, Photoisomerization processes in thin azobenzene - polymer films, Programme and Abstracts, p. 47.

6. M.Rutkis, Polymer NLO materials: history and future insights on theory based design strategy, Programme and Abstracts, p.6

**5<sup>th</sup> International meeting on molecular electronics ElecMol'10, December 6-10, 2010, Grenoble, France.**

1. I.Muzikante, M.Indrikova, J.Latvels, K.Pudzis, M.Rutkis, Determination of the energy structure of the sandwich-type organic thin films for OLED and OPV devices, Abstracts, p.250

# 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.

## Scientific Staff

1. Dr. A.Kristins
2. Dr. hab. A.Zelenkovs
3. Mg. ing. D.Gusevs
4. Mg. ing. S.Zelenkovs
5. Mg. ing. E.Garkajs

## Technical Staff

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

## Cooperation

### Latvia

1. Joint-stock company *Latvenergo*
2. *Kokarde Ltd*
3. Latvia Technology Park
4. Riga Technical University
5. *Trafik Ltd*
6. *IB Biakss*
7. *GROG Ltd*
8. *AlarmLat Ltd*
9. *Mikoniks Ltd*
10. *Energoremonts Rīga Ltd*

### Estonia

1. Tallinn University of Technology
2. Competence Centre ELIKO

The prospects of the instruments look at appendix.

## 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*
15. *Latvian Textile* Ltd;
16. *VAIDE* Ltd;
17. *Flexoplastic* Ltd  
etc.

## Lectures on Conferences

### 26<sup>th</sup> Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2010

1. I.Gvardina, A.Kristiņš, J.Melderis *Device for control and limiting of automats for delivery of dosed goods and operation algorithm of the device*. Abstracts, p.86.
2. P.Annus, E. Haldre, J Ojarand, U. Männi, A.Kristiņš. *RF Smart city: new tasks for the existing street lighting infrastrucur*. Abstracts, p.89.
3. I.Gvardina, A.Kristiņš, J.Melderis. *ISSP yard access control system*. Abstracts, p.87.
4. I.Gvardina, A.Kristiņš, J.Melderis, J.Veinbergs. *Device for Testing of Action of the Power Transformer's Step Switching Contacts „KODA-3-M”*. Abstracts, p.88.
5. I.Gvardina, A.Kristiņš, J.Melderis, G.Pikurs, J.Zvirgzds. *System for remote management and control of air compressor station*. Abstracts, p.62.
6. A.Zeļenkovs, S.Zeļenkovs. *Simulation and evaluation of noise immunity of OFDM in a Gaussian channel*. Abstracts, p.63.



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**Apparatus for Metal Determination in Liquids "AHPS-2"**

The AHPS-2 is a device for determination of metals in water and other liquids. It is based on a very sensitive electro-chemical method and allows us to determine the concentration of

**Cu, Zn, Cd, Sn, Au, Tl, Pb, Bi**

at a low levels of contents as 0,1 ppb. In special cases the sensitivity of the AHPS-2 is even higher and allows us to determine metals at concentrations below 0,1 ppb. The upper limit of the metal concentration determination by the AHPS-2 is in the ppm region.

The sample preparing procedure for analysis is very simple and can be completed within a matter of minutes. In a single analysis process more than one metal can be detected. The analysis procedure is rather fast: for ppm region measurements it lasts approximately one minute and for measurements of levels within the 0,1 ppb region it takes no more than ten minutes.

The analysis procedure is fully controlled by the computer (preferably IBM PC compatible).

The AHPS-2 can be used in environmental control as well as for analytic tasks for determination of trace elements.

The AHPS-2 is produced in cooperation with Division of Disordered Material Physics.

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**Apartment Security System**

The device is constructed for individual apartments or small offices security and alarm signalization.

The device controls different kinds of detectors (movement detectors, hermetic contacts or similar devices) on the "own – alien" base in the presence of the owner or in his absence alarming in the case of criminal non-authorized actions.

Switching on and off of system security mode is implemented with the aid of the *Dallas Semiconductor* Touch Memory™ identification code keys.

Reprogramming of the key list is operative - with the assistance of two Master keys.

The device has a sound and light indication and it provides an electrical signal for security service or alarming device in some difficult of access place.

The device works in auto testing mode and reports about all its faults or criminal actions by the light indication.

This device is very simple in using and doesn't need any special knowledge.

***Technical Specification***

Power supply:	+(10 - 15) V
Consumption:	
System in security mode:	≤ 40 mA
System in alarming mode (defined by alarming device):	< 4 A
Access time:	20 seconds
Detectors with disconnecting ability:	≤ 4 pcs.
Detectors without disconnecting ability:	≤ 3 pcs.
Possible combinations of keys:	$2,8 \cdot 10^{14}$
Maximal number of user keys:	56 (250) pcs.
Dimensions:	115x55x30 mm

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**Vehicle Alarm System and Immobilizer  
with TM Identification Code Keys**

This product is an electronic device for vehicle anti-thieves protection and can be activated and deactivated by Dallas Semiconductor firm Touch Memory™ identification keys with a brief touch of the key to the key-reader.

The electronic keys are all different, there are about  $2.81 \cdot 10^{14}$  possible combinations and it is impossible to produce 2 equal keys.

The activated protecting system takes under its control vehicles hood, trunk and doors pin switches and disconnects one or two (optionally) main electric circuits of the vehicle (ignition coil, fuel pump, starter solenoid etc.). A flashing LED on the dashboard warns potential thieves of its presence. A protecting mode is switched on by connecting of power supply.

Additional sensors - shock detectors, ultrasonic sensors etc. may be connected to this system. Also the system remind about headlight state.

This system has some operation modes and gives information to driver by LED indicator and sound signals.

***Technical Specification***

Power supply:	+(10 - 15) V
Consumption:	
System armed (including LED):	≤ 8 mA
Armed only engine deactivation:	≤ 4 mA
Consumption by driving (immobilizer relay "on"):	≤ 35 mA
Disarming delay:	10 seconds
Rearming delay:	30 seconds
"Secret" button delay:	2 minutes
Possible combinations of keys:	$2,8 \cdot 10^{14}$
Duration of alarm signal sound - 2 minutes total by 4 secs sound and 4 secs pauses.	
Alarm relay contact capacity:	20 A
Immobilizer relay contact capacity:	20 A
Dimensions:	130x100x30 mm
Automatic switching on of the immobilizing mode after ignition switching off - in 20 secs.	

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**Car parking and access control systems**

The car parking and access control systems are designed for both - ordinary and multilevel parking places. The systems can service casual as well as regular clients.

The systems consists of one PC or some personal computers, connected in network, that are connected with peripheral devices for service, control and execution (check's printers, cash machines, control devices for barriers and signal lights, readers for Dallas electronic keys, proximity cards, bar codes etc.). The system is corresponding to LR law about fiscalisation.

Software of the system allows controlling peripheral devices, to provide registration of clients and calculate service fees in accordance to client category and parking time, as well as to create necessary database.

Systems can operate with MS Windows 98, Windows NT, 2000, ME and XP.

These systems (in cooperation with "Alarm Lat" Ltd) are put into operation at multilevel parking places "Rīgas Pirmā Garāža", "Arēna Plus" and "Latvijas Gāze"

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**Device for control and limiting of automats for  
delivery of dosed goods**

The developed device allows managing the operation of automats for delivery of different dosed goods in accordance with the rights allocated to users. The device ensures storage in memory up to 56 user keys and limits of allocated rights to use the dosed goods. Operational algorithm of device allows using the keys in the individual or collective mode. Every key may be programmed for one of these quantities of dosed goods: 30, 40, 50, 60, 70, 80, 90 doses or without limit of quantity. This system can be programmed by three master keys for entering keys in memory, for deleting all keys from memory or for deleting several keys from memory accordingly. Two digit display shows the remaining amount of doses when key is touched to the reader.

This device was manufactured by Aqualogic Ltd order and it is used for dispensing refreshment in limited amounts for the staff of different institutions.



The coffee automatic device with the limited contingent of users

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**Electronic Documentation**

There is a portable system based on Dallas Semiconductor firm Touch Memory™ chips for data saving and moving without paper. The silicon chip packs in TM memory more as 8000 signs (~ 4-5 pages).

TM replaces paper documents that are difficult to attach to objects and are prone to damage or illegibility. If copying is undesirable, lock bits, add-only memory, passwords and encryption can be employed.

TM based electronic documents are very convenient and safe for persons who have contacts with confidential or strict registration papers.

Each TM chip has a unique registration number up to  $2,81 \cdot 10^{14}$  variants.

A personal computer with special interface and special software can read and write data from/to Touch Memory.

TM is housed in a durable hermetic stainless steel case ( $\varnothing$  17,4 x 5,89 mm) and is tolerant to mechanical shock, static electricity, and electromagnetic fields and to other harmful environmental factors.

TM has an ambient temperature range  $-40^{\circ}\text{C}$  to  $+85^{\circ}\text{C}$ .

Touch Memories can accommodate over one million data changes.

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**Laboratory of Electronic Engineering  
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**Digestion System**

The digestion system provides digestion of various samples in sulphuric acid, using the Kjeldahl method.

Into six deep hollows of electrical heater are placed tubes, containing samples and sulphuric acid. The temperature controller provides the thermal regime of heater. The thermal regime includes two plateaus of temperature: the first (in time) - in the temperature region of boiling water, and the second - in the temperature region of boiling acid. The temperature controller provides also three different heating rates for transition from starting temperature to the first and second plateau. The thermostation time control up to six hours is possible.

The digestion system is provided by water aspiration pump for the removal of exhaust gases, produced in digestion procedures.

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# Laboratory of Electronic Engineering Institute of Solid State Physics University of Latvia

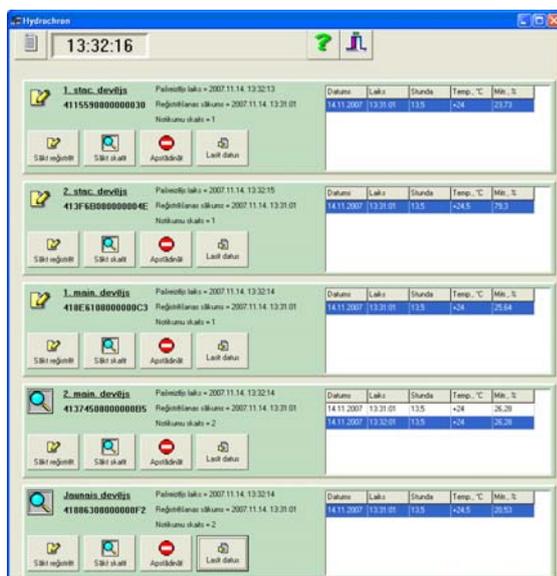
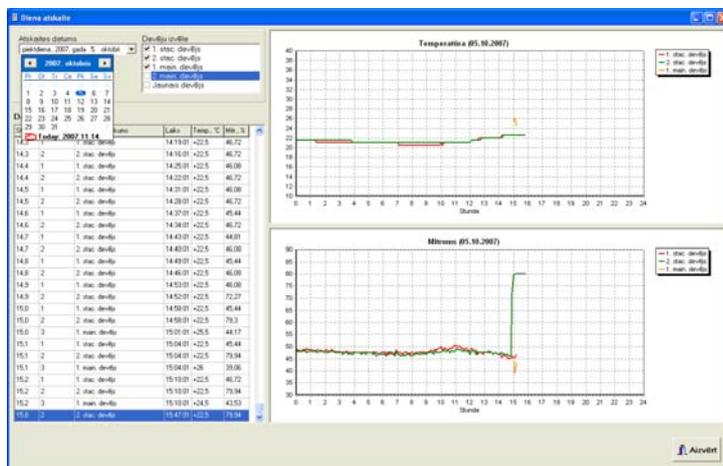
## Monitoring of the environment temperature and relative humidity

The climate monitoring system has been developed for grain warehousing and drying. It performs a temperature registration in a range from  $-20^{\circ}\text{C}$  up to  $+85^{\circ}\text{C}$  with the step of  $0.5^{\circ}\text{C}$  and a registration of relative humidity in a range 0 % up to 100 % with the step of 0.64%. This system was designed on the base of five the DS1923 Hydrochron Temperature/Humidity Logger iButtons. Such logger has no any own means of indication and control. Therefore all functions on its service and information exchange with it are carried out at contact between its case and supporting device using 1-Wire protocol. This system allows as tracing the current situation on a computer in a real time, as collecting the saved up data a posteriori. It provides controlling of the logger's parameters, storing and graphic representation of the data fixed by the loggers.

Scope of applying of such system is, first of all, monitoring sensitive to temperature and/or the humidity foods, pharmaceutical and



medical reagents and preparations, etc. at their transportation, storage and processing.



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**Device for Authorized One-Door Access System  
with TM Identification Code Keys**

The device is constructed for creation of authorized access system for apartments.

The device controls electromagnetic keys of any construction.

Accessing in the apartment is implemented with the aid of the *Dallas Semiconductor* Touch Memory™ identification code keys. In the emergency case it is possible to enter the apartment with the aid of ordinary mechanical key.

Exiting of the apartment is provided either with the button or with the TM (if the second reader is available).

Reprogramming of the TM list is operative - with the assistance of two Master keys.

The device has a sound and light indication and it provides an electrical signal for security service.

This device is cheaper than most of similar ones.

***Technical Specification***

Power supply:	+ (10 - 15) V
Consumption:	
System armed in waiting state:	≤ 8 mA
System activated in access mode (defined by el. mech. lock):	< 0,5A (typically)
Access time:	5 seconds
Sound signal on non-authorized opening of the door:	Immediately
Sound signal delay after authorized opening of the door:	5 seconds
Possible combinations of keys:	$2,8 \cdot 10^{14}$
User keys:	≤ 56 pcs.
Dimensions:	83x55x35 mm

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**Device for Authorized One-Door Access System  
with TM Identification Code Keys and Event Registering**

The device is constructed for creation of authorized access system for apartments.  
The device controls electromagnetic keys of any construction.

Accessing in the apartment is implemented with the aid of the *Dallas Semiconductor* Touch Memory™ identification code keys. In the emergency case it is possible to enter the apartment with the aid of ordinary mechanical key.

Exiting of the apartment is provided either with the button or with the TM (if the second reader is available).

Reprogramming of the TM list, setting of the time and time access zones (optionally) and also transferring of the data on the events registered from the device to PC is realized with the assistance of the special identification Master-key with 64K bits of read/write nonvolatile memory.

This device is cheaper than most of similar ones.

*Technical Specification*

Power supply:	+ (10 - 15) V
Consumption of system activated in access mode (defined by el. mech. lock):	< 0,5A (typically)
Access time (standard):	5 seconds
Sound signal on non-authorized opening of the door:	Immediately
Sound signal delay after authorized opening of the door:	5 seconds
Possible combinations of keys:	$2,8 \cdot 10^{14}$
Number of user keys (standard):	56 pcs.
Number of events registered:	500
Time of data retention in Master-key:	over 10 years

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**High-voltage Breaker Analyzer Device "OSKARS"**

The device was designed for the verification of high-voltage (110 and 330 kV) breakers. 14 timing channels and the current in the driving solenoid are simultaneously controlled and necessary time parameters calculated.

Only one minute - and you have the operating sequence and the time control results printed out on the A4 format (210 x 297 mm) paper sheet by ordinary printer without using of the computer.

The device has four modes of operation: *OPEN (O)*, *CLOSE (C)*, *OPEN-CLOSE-OPEN (O-C-O)*, *CLOSE-OPEN (C-O)*. The delay time between pulses (O-C) and (C-O) can be set on the thumbwheels ( $0 \div 0,15$  s).

The device can be used for testing of 10 types of breakers: BBIII-110; BBБ-110; BBY-110; BBH-110/6; BB-330Б; BBH-330/15; HGF-115/2B; HPL-362/B2; LTB-145D1.

The time resolution is 0,001 s.

Dimensions are 490 x 480 x 165 mm.

Weight is 20 kg.

The device specifications may be changed according to customer's requirements.

The device may be used to study reaction velocity, delay and vibrations of different kinds of the relays and for registration of different processes in other branches of science and technique.

These devices are put into operation by power engineering departments of "LATVENERGO" and "LIETUVOS ENERGIJA".

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**Operating with remote objects  
based on TCP/IP communication protocol**

Usage of this communication protocol makes possible to work without wiring of additional communication lines and allows to transmit information in far distances practically without difficulties.

In the developed remote control systems “Rabbit” controllers are used.

Different modifications of microcontrollers permit to collect information due from contact sensors (hercons, magnetic loop controllers, move detectors etc.), from data carriers based on DS19XX protocol (i-Buttons, thermometers and others) or based on Viegand protocol (Proximity cards).

It is possible to connect the system with other peripheral devices via standard RS232/485 ports.

Controllers can provide communication with main server via TCP/IP ports by using local, corporative or world wide nets.

Practical applications:

1. The system of access, control and management is worked out for LatRosTrans company. The system consists of 24 controllers (number of technological blocks on Russia-Ventspils oil pipeline), dispatcher program (in Daugavpils) and some client applications.
2. Entrance in/out system for “Latvijas Gāze” company is worked out, which consists of three in/out gates with automatic barriers, server administrator and guard programs and some other client applications.
3. The system including checkpoint, the authorized access in cabinets and the security signal system for two buildings of the Latvian Shipping Company with a unified database.

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**Security Drawers and Safes for the Cash Points**

There are some versions of safes produced by Solid State Physics Institute & Co for storage of banknotes, coins and forms. A safe has an electromechanical lock, activated by electronic system with time delay.

The safe-drawer SF-1 has the keys based on Dallas Semiconductor firm Touch Memory™ identification chips with unique registration number (up to  $2,81 \cdot 10^{14}$  numbers), but safes KT-2F may be completed both TM and mechanical key. The electronic time delay system can be activated by TM or control button, then a red LED flashes intermittently until the delay time has run out. At that moment a buzzer beeps and a green LED flashes for access time. During of that time the safe may be pulled open.

	<b>SF-1</b>	<b>KT-2FA</b>	<b>KT-2FB</b>
<b>Delay times (minutes)</b>	3, 5, 10, 15	3, 5, 10, 15	3, 5, 10, 15
<b>Access times (s)</b>	5, 10, 15, 20	5, 10, 15, 20	5, 10, 15, 20
<b>Dimensions (mm)</b>	400 x 370 x 140	300 x 300 x 300	300 x 300 x 200
<b>Weight (kg)</b>	12	14	10,5

The safe is connected to the mains (50 Hz, 220 V A.C.) by a transformer or to the 9 V 300 mA D.C. source.

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**Soft Start Devices for Electric Motors**

There are many problems with starting of high power electric devices (motors) because initial current may be some times greater as nominal current for these devices. High initial current may be dangerous for power supply devices as well as for powered devices.

In the ISSP in cooperation with “Fonons” Ltd there were worked out soft start devices for electric motors in general, but it is possible to use the soft starters also for other devices (high power heaters, for example).

The devices are based on phase drive of two thyristor pairs and are able to manage power up to 100 kVA and more.

Main features:

- digital controlled AC semiconductor soft starter
- start time from 5 to 20 seconds
- start voltage from 40 to 80%
- stop time from 1,5 to 20 seconds
- built in by-pass function.



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## Working time monitoring system

This system consists of a software package and a data reading block.

### *Software package provides the following functions:*

- adding, editing and erasing of user data (name, surname, working number, key number, telephone number);
- working time calculation by four time types (ordinary working time, reserve time, evening working time + working time on days off till ten o'clock p.m., night working time) (*these parameters could be changed*);
- event searching by surname or working number, by date and time interval;
- printing of searching results;
- function "present – absent";
- text (*or different*) password system;
- calendar for setting of days off and working days and for setting of date intervals with reserve time;
- automatic archive creating in the form of text files;
- the other functions could be added by customer wishes.

### *Data reading block with the following parameters:*

- identification device - *Dallas* identification button or *Proxy* card;
- data readers – two (entry and exit);
- real time indication / working number indication;
- user count up to 200 (*this count could be greater*);
- operational memory for 500 events (in autonomous regime) (*this count could be greater too*);
- connection with computer by RS485 port;
- powered from mains (220 V) with guarding from short voltage disappearance;
- the block is easy mounted to vertical wall.



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