Institute of Solid State Physics
University of Latvia

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INTRODUCTION

The research in solid state physics at the University of Latvia restarted after World War II. The **Institute of Solid State Physics** (ISSP) of the University of Latvia was established on the basis of Laboratory of *Semiconductor Research* and Laboratory of *Ferro- and Piezoelectric Research* in 1978. Since 1986 the ISSP has the status of an independent organization of the University and now is the main material science institute in Latvia.
Four laboratories from the Institute of Physics of the Latvian Academy of Sciences joined our Institute in 1995. Twenty scientists of the former Nuclear Research Centre joined the ISSP in 1999 and established Laboratory of Radiation Physics. In 2004 scientists from the Institute of Physical Energetics joined ISSP and established Laboratory of Organic Materials (Table 1).

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

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

In December 2000 the ISSP was awarded the **Centre of Excellence of the European Commission** (Centre of Excellence for Advanced Material Research and Technologies). This honorary recognition with the accompanying financial support of 0,7 million EUR has increased our research activities, particularly extending the list of our research partners and scientists who come to work to our Institute from the leading European research centres.

The research of the ISSP includes:

- electron and ion process in wide-gap materials with different degree of ordering;
- functional organic molecules and polymers for photonics and organic electronics;
- multifunctional and hybrid materials for energy applications: light emitting diodes, photovoltaic elements and coatings for solar baterries, storage of hydrogen for fuel cell devices;
- electrodes and plasma technologies for hydrogen production, polymer membranes with ionic conduction for fuel cells and gas separations;
- inorganic single crystals, ceramics, glasses, thin films, and nano-structured surfaces for application in optics, electronics, photonics and energetics.

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

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

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff.** At present there are 176 employees working at the Institute, 26 of 103 members of the research staff hold Dr.habil.degrees, 66 hold Dr. or PhD. At the end of 2011 there were 21 PhD students and 46 undergraduate and graduate students in physics and optometry programmes working at the ISSP.

Table 1

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2011

International Supervisory Board

Council of Institute
Dr.phys. L.Trinklere

Director
Dr.habil.phys. A. Sternberg

RESEARCH DIVISIONS AND LABORATORIES	ADMINISTRATION AND SERVICES
Department of Crystal Physics *Dr.phys* P.Kulis	**Vicedirector for Research** *Dr.habil.phys.* I.Muzikante
Department of Disordered Materials Physics *Dr.habil. phys* .D.Millers	**Vicedirector for Education** *Dr.habil.phys.* A.Krumins
Department of Ferroelectrics *Dr.habil.phys.V.Dimza*	**Finance and Accounting** A.Jozepa
Department of Semiconductor Materials *Dr.phys* A.Lusis	**Personell office** D.Popele
Department of Radiation Physics *Dr.habil.phys.* J.Berzins	**Mechanical Workshop** J.Katkevics
Lab. of Theoretical Physics and Computer Modelling *Dr.habil.phys.* J.Kotomin	**Utilities** R.Siatkovskis
Lab. of Optical Recording *Dr.phys* J.Teteris	**Energetics** J.Ruhmanis
Lab. of Wide Band Gap Materials *Dr.habil.phys.* B.Berzina	**Library** L.Rihtere
Lab. of Surface Physics *Dr.phys.*F.Muktepavela	
Lab. of Visual Perception *Dr.habil.phys.* I.Lacis	
Lab. of Organic Materials *Dr.habil.phys*. I.Muzikante	
Lab. of Electronic Engineering *Dr.* A.Kristins	

Table 2

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. Jurģis Grūbe, PhD student
5. Anastasija Jozepa
6. Andris Krumins, Prof., Dr.habil.phys.
7. Peteris Kulis, Dr.phys.
8. Aleksejs Kuzmins, Dr.phys.
9. Kaiva Lūse, PhD student
10. Inta Muzikante, Dr.habil.phys.
11. Juris Purāns, Dr.phys.
12. Uldis Rogulis, Dr.habil.phys.
13. Mārtins Rutkis, Dr.phys.
14. Andrejs Silins, Prof., Dr.habil.phys.
15. Linards Skuja, Dr.habil.phys.
16. Anatolijs Sharakovskis, PhD student
17. Andris Sternbergs, Dr.habil.phys.
18. Janis Teteris, Dr.phys.
19. Anatolijs Truhins, Dr.habil.phys.
20. Nils Veidemanis, A/S "Sidrabe"
21. Guntars Zvejnieks, Dr.phys.

Table 3

International Advisory Board of the Institute

1. Prof. Dr.J.Banys, University of Vilnius, Lithuania
2. Prof. Dr. Gunnar Borstel, University of Osnabruck, Germany
3. Prof. Niels E.Christensen (chairman), University of Aarhus, Denmark
4. Prof. Dr.R.Evarestov, St.Petersburg University, Russia
5. Prof. Claes – Goran Granqvist, Uppsala University, Sweden
6. 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 2011. 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 2011. 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 2011:

No	Author	Award
1.	Dr.habil.phys. J.Kotomin	Member of Latvian Academy of Science
2.	Dr.phys. M.Rutkis	The correspondent member of Latvian Academy of Science
3.	Dr.habil.phys. A.Truhins	Author of the best scientific achiewment (from Latvian Academy of Science)
4.	Dr.phys.J.Zhukovskii, R.Evarestov	Author of the best scientific achiewment (from Latvian Academy of Science)
5.	M.Dunce	The L'OREAL-UNESCO sholarship „For Women in science 2011"
6.	Dr.phys. A.Sharakovskis	Award of Latvian Academy of Science (The Ludvigs and Maris Jansons Prize, 2011)
7.	Dr.habil.phys. A.Sternberg	The Riga's Prize in science 2011

At the end of 2011, 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 2011 **four international conferences** have been organised at the Institute:

- Annual International conference "Functional materials and nanotechnologies", April 5 - 8, 2011, Riga, Latvia;
- The International Workshop "Nanostructured Zirconia for Optical Sensors", April 4-5, 2011, Riga;
- The International Workshop "Ceramic Membranes for Energy Applications", April 4-5, 2011, Riga;
- International Student Conference "Developments in Optics and Communications 2010", April 28 – 30, 2011, Riga, Latvia;

Table 4

INCOME OF ISSP, THOUSAND Ls, FROM 2005 - 2011

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Structural funds from EU
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**
2011	**2719,1**	**448,0**	**515,5**	**104,6**	**121,1**	**1530,0**

*) – investment for building reconstruction

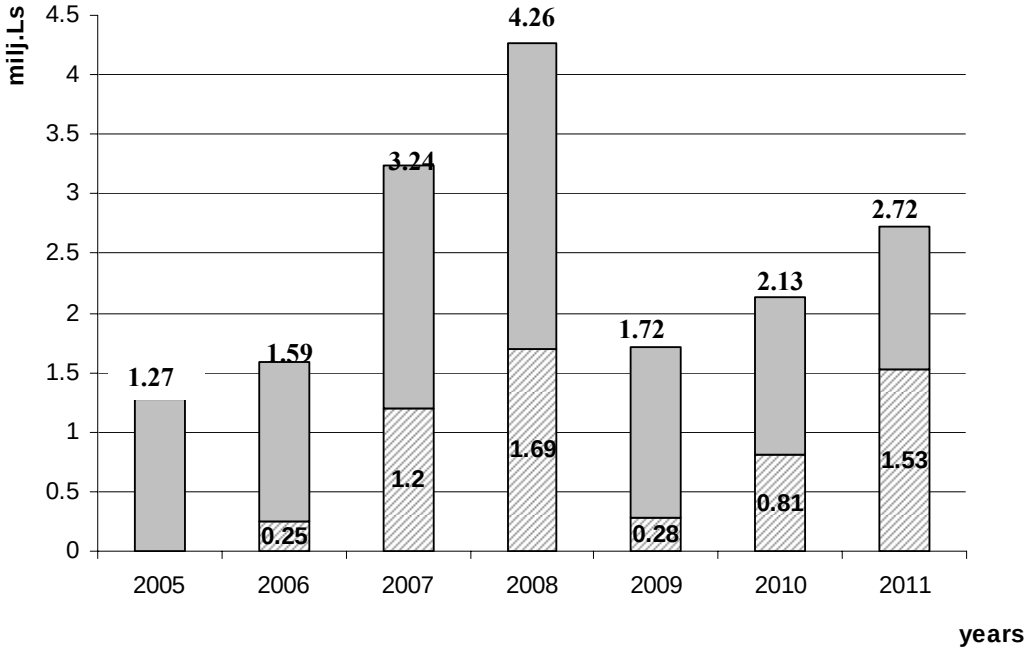

Fig.1. Total financing of the ISSP milj. LVL from 2005 to 2011

▨ - *financing from EU Structural funds*

The main source for **international funding** were seven EC 7th Framework Programme contracts:
- F-Bridge – 18.7 thous. EUR
- Catherine – 17.1 thous.EUR
- 3 EURATOM projects – 20.4 thous. EUR
- NASA-OTM project – 58.1 thous. EUR
- Reemigration grant (G.Vaivars) – 40.0 thous. EUR

Main achievments in 2011:

1. 143 SCI papers published by the staff of Institute;
2. 1 patent application;
3. 13 B.sc. thesis and 4 M.Sc. thesis in physics were defended under the supervision of our scientists;
4. E.Elsts, S.Fomins, J.Hodakovska, M.Shorohovs and J.Proskurins were acquired degree of doctor of physics (PhD);
5. The formation of "National Research Centre" for nanostructures and multifunctional materials, constructions and technologies by the ISSP .

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

Prof. Dr. A.Krumins

CRYSTALS PHYSICS

Head of Division 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, binary and complex rare earth fluoride nanocomposite materials prospective for the light emitters, detectors and visualization systems with enhanced quantum efficiency. Fluoride 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 binary and complex rare earth fluorides. The energy relaxation mechanisms were studied during up-conversion processes by means of spectral and time-resolved luminescence measurements in binary and complex rare earth fluorides containing Er, Eu, Nd ions.
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 fotonic 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 E. Elsts
4. Dr. phys. A. Fedotovs
5. Dr. phys. P. Kulis
6. Dr. phys. B. Polyakov
7. Prof., Dr. habil. phys. U. Rogulis
8. Dr. phys. A. Sarakovskis
9. Dr. habil. phys. M. Springis
10. Prof., Dr. habil. phys. I. Tale
11. Dr. phys. J. Trokss
12. Mg. phys. J. Jansons

PhD Students

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

Students

1. I. Brice
2. A. Antuzēvičs
3. G. Doke
4. O. Kiseļova
5. M. Voss

Scientific visits abroad

U. Rogulis (1 week, Germany)
E. Elsts (1 week, USA)
Dz. Berzins (1 week, Germany
I. Brice (1 week, Lithuania)
A. Voitkans (1 week, Germany)
A. Voitkans (1 week, Italy)

Cooperation

Latvia

Joint stock company “Alfa”

Germany

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

Romania

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

Main results

ANALYSIS OF Mn^{2+} EPR SPECTRAL SHAPES FOR STUDIES OF THE OXYFLUORIDE GLASS CERAMICS

A Fedotovs, Dz Berzins, O Kiselova, A Sarakovskis, U Rogulis

We investigated the EPR superhyperfine structure of the Mn^{2+} ion in the disordered BaF_2 crystalline media which tends to crystallize in the oxyfluoride glass-ceramics material. Obtained EPR spectra reveal explicit shf structure due to Mn^{2+} ion building into the BaF_2 lattice showing its usefulness as a probe in orientationally disordered and amorphous structures. Two types with explicit shf structure of Mn^{2+} ion characteristic EPR spectra were obtained in BaF_2 powder samples characteristic with broad (type 1) and narrow (type 2) hyperfine structure lines. Spectra of the ZnF_2-BaF_2 oxyfluoride glass-ceramics samples revealed explicit fine structure lines.

NOVEL SYNTHESIS OF UP-CONVERSION PHOSPHOR BASED ON RARE-EARTH DOPED $NaLaF_4$

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

In this work Er^{3+} doped $NaLaF_4$ material has been synthesized Along with the description of the synthesis route, luminescence spectra and decay kinetics of both traditional and up-conversion luminescence of Er^{3+} will be presented for different Er^{3+} doping levels. It will be shown that the main mechanisms involved in the creation of the up-conversion luminescence in $NaLaF_4$:Er^{3+} under excitation at about 975 nm are excited state absorption and energy transfer. Relative impact of either of the mechanisms in $NaLaF_4$:Er^{3+} depends on both the concentration of Er^{3+} and on the excitation wavelength: the increase of either the concentration or the excitation wavelength leads to the prevalence of energy transfer mechanism over excited state absorption mechanism.

MULTICOLOR UP-CONVERSION LUMINESCENCE IN RARE-EARTH DOPED $NaLaF_4$

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

In this work we tried to achieve multicolor up-conversion luminescence in low phonon energy material $NaLaF_4$ doped with different Er^{3+}; Tm^{3+} and Yb^{3+} concentrations. Up-conversion luminescence was measured and main luminescence bands from Er^{3+} and Tm^{3+} in red, green and blue spectral regions were observed. The relative intensities of the luminescence bands could be changed by changing the doping levels of rare-earth ions. Changes in the up-conversion luminescence color could be achieved by applying different infrared pump power density. The color coordinates of the multicolor up-conversion luminescence depending on doping level as well as on the pump power density were presented in CIE (x, y) chromaticity diagram (1931).

INTRINSIC DEFECT RELATED LUMINESCENCE IN ZrO_2

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

The studies of ZrO_2 and yttrium stabilized ZrO_2 nanocrystals luminescence as well as yttrium stabilized single crystal luminescence and induced absorption showed that the intrinsic defects are responsible for luminescence at room temperature. These defects form a quasi-continuum of states in ZrO_2 band gap and are the origin of the luminescence spectrum dependence on the excitation energy. Luminescence centers are oxygen vacancies related but not the vacancies themselves. At room temperature, in ZrO_2, deep traps for electrons and holes exist. The oxygen vacancies are proposed to be the traps for electrons.

LOCALIZATION DYNAMICS OF EXCITON LUMINESCENCE IN $In_xGa_{1-x}N$ 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 $In_xG_{1-x}N$ 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.

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.

Scientific publications

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2. B. Polyakov, L. Dorogin, S. Vlassov, I. Kink, A. Lohmus, A. Romanov, R. Lohmus. Real-time measurements of sliding friction and elastic properties of ZnO nanowires inside a scanning electron microscope. Solid State Communications, 151, 1244–1247, 2011.
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7. A. Voitkans, L. Dimitrocenko, S. Bartlin, I. Barke, K.-H. Meives-Broer, P. Kulis, I. Tale, Ex situ investigations of MOCVD-grown gallium nitride nanowires using reflection high energy electron diffraction, IOP Conf. Ser.: Mater. Sci. Eng. 23 (2011) 012038.
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Lectures on Conferences

27th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2011, February 14-16

1. J. Butikova, I. Tale, Estimation of the concentration of atoms using parameters of plasma in local thermodynamic equilibrium, - Abstracts of the 27th Scientific Conference ISSP LU, 2011, p. 7.
2. I. Tale, A. Voitkans, J. Butikova, Spectroscopy of Ga vapour concentration and dynamics in Tokamak plasma. Project WP10/PWI-05-0401/ULV/PS, - Ibid., p. 8.
3. J. Smits, A. Sarakovskis, G. Kucinskis, G. Bajars, J. Kleperis, Electrochemical properties, structure and morphologyof $LiFePO_4$ thin films annealed by different methods, - Ibid., p. 30.
4. J. Grube, G. Doke, M. Voss, A. Sarakovskis, M. Springis, Up-conversion luminescence in $NaLaF_4$ with different Er^{3+} concentrations, - Ibid., p. 52.
5. I. Brice, U. Rogulis, E. Elsts, A. Sarakovskis, G. Doke, Activated oxyflourides for solid-state lighting, - Ibid., p. 53.
6. G. Doke, M. Voss, J. Grube, A. Sarakovskis, M. Springis, Up-conversion luminescence of erbium and ytterbium doped $NaLaF_4$ material, - Ibid., p. 81.
7. Dz. Berzins, A. Fedotovs, U. Rogulis, A. Sarakovskis, EPR hyperfine structure of radiation defect in oxyflouride glass ceramics, - Ibid., p. 82.
8. A. Fedotovs, Dz. Berzins, O. Kiselova, A. Sarakovskis, Paramagnetic impurities for oxyflouride glass ceramics structure studies, -. Ibid., p. 83.
9. J. Jansons. Pusvadītāju fizikas problēmu laboratorijas izveides priekšnosacījumi. – Ibid., p. 92-96.

10. I. Tāle, Jonu kristālu pētījumi Pusvadītāju fizikas problem laboratorijā, - Ibid., p. 111-113.

International conference "Functional materials and nanotechnologies" FM&NT, Riga, 2011, April 5 -8

1. L. Dimitrocenko, P. Kulis, A. Sarakovskis, I. Tale, A. Voitkans, Dynamics of exciton creation and decay processes in composition – disordered InGaN thin films, - International conference „Functional materials and nanotechnologies" FM&NT 2011, Book of abstracts, ISSP LU, Riga, April 5 – 8, p 43.
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1. U. Rogulis, E. Elsts, J. Jansons, A. Sarakovskis, G. Doke, A. Stunda, K. Kundzins, Rare earth activated oxyfluoride glasses and glass-ceramics for scintillation

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I. Brice, U. Rogulis, E. Elsts, A. Šarakovskis, J. Grūbe, G. Doķe, Activated oxyfluorides for solid-state lighting, 54th Scientific Conference for Young Students of Physics and Natural Sciences, Open Readings 2011, Vilnius, LITHUANIA, 2011, PP-16, p. 96.

Popular Science Articles (in Latvian)

1. J. Jansons. LU fizikas docentam Egonam Zablovskim – 85. – „Zvaigžņotā Debess", 2011. gada pavasaris (211), 34. – 39. lpp.
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Doctoral thesis

E. Elsts "Spectroscopic Studies of Scintillator Materials: CsI:Tl, CdWO4:Mo and Tb activated oxyfluorides"

Bachelor thesis:

1. J. Bergmane „Rekristalizēta amorfa silicija plāno kārtiņu elektrofizikālās īpašības", vad. Guntis Mārciņš.
2. A. Romanova „Rekristalizēta amorfa silicija plāno kārtiņu struktūru veidošanās likumsakarības", vad. Guntis Mārciņš
3. I. Brice „Aktivitēti oksifluorīdi redzamās gaismas luminoforos" vad. Uldis Rogulis.

DEPARTMENT OF DISORDED MATERIAL PHYSICS

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

Solid state radiation physics Laboratory Head of laboratory Dr.habil.phys.L.Grigorjeva	Laboratory of amorphous materials spectroscopy Head of laboratory Dr.habil.phys. L.Skuja	Laboratory of Solid state optics Head of laboratory Dr.habil.phys. A.Trukhin

Laboratory of solid state radiation physics	Laboratory of amorphous materials spectroscopy	Laboratory of Solid state optics
Dr.habil.phys. L.Grigorjeva Dr.habil.phys. D.Millers Dr.K.Smits	Dr.habil.phys. A.Silins Dr.habil. L.Skuja	Dr.habil.phys. A.Trukhin
Technical staff Eng. A.Sitdikov	Students Raitis Sondors	
Ph.D students M.Shorokhov		
Students L.Bukonte; J.Rikveilis V.Liepina; L.Pukina		

Research area

The electronic properties of advanced materials for scintillators, light transformers, gas sensors, radiation detectors, photocatalysis, persistent phosphors, as well as high-performance optical glass for NIR to VUV spectral range are studied by means of spectroscopic methods including time-resolved spectroscopy.

Scientific Visits Abroad

1. Dr.habil.phys.L.Grigorjeva, Estonia (4 days)
2. Dr.habil.phys. D.Millers, Poland (3 days)
3. Dr.K.Smits, France (14 days)
4. Dr.habil.phys. D.Millers, France (14 days)
5. Dr.Habil.phys. L.Grigorjeva, France (14 days)
6. Dr.Habil.phys. L.Grigorjeva, Germany (7 days)
7. Dr.Habil.phys. L.Grigorjeva, France (6 days)
8. Dr.K.Smits. , The Nitherlands (5days)
9. Dr.habil. L.Skuja, Japan (59 days)
10. Dr.habil. L.Skuja, China (7 days)

Cooperation

Latvia
SIA "Baltic Scientific Instruments (Dr.V.Gostilo, M.Shorohov)
SIA RITEC
Riga Technical University, Institute of Inorganic Chemistry (Dr.habil.sc.ing. J.Grabis, Dr. Dz.Jankoviča)
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)
Kotel'nikov Institute of Radio-engineering and Electronics of RAS, Russia (Prof.,Dr. Konstantin Golant)

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 (Prof. K. Kajihara)

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

Experimental methods and equipment

Absorption spectroscopy. FTIR absorption spectroscopy: EQUINOX 55 (10000-400 cm^{-1} and 22000-7000 cm^{-1} spectral regions) was developed for dispersed materials.
Transient absorption under electron beam excitation.
Luminescence spectroscopy. Luminescence excitation by the following sources is available : a pulsed electron beam accelerator (10 ns, 270 keV, 10^{12} electrons/pulse), X rays, YAG:Nd laser (266 nm, 532 nm), nitrogen laser (337 nm), excimer lasers (248, 193 and 157 nm), deuterium and xenon lamps. Luminescence detection is performed using photomultipliers/monochromators and cooled CCD camera coupled with spectrograph. Time-resolved luminescence is detected by digital oscilloscopes, multichannel photon counters or time-correlated single-photon counting.

Vacuum ultraviolet spectroscopy: McPherson 234/302 200 mm monochromator with D_2 lamp with MgF_2-window serving as light source (120-250 nm). Excimer F2 pulsed laser (157 nm).
Raman and luminescence spectroscopy: Andor Shamrock303i spectrometer with Newton DU971N electron multiplying cooled CCD , NIR to UV spectral range. Hamamtsu mini spectrometer C10082CAH VIS –UV spectral range.
Energy-dispersive X-ray fluorescence microanalysis (EDAX Eagle III spectrometer, Rhodium X-ray source with microcapillary focusing lens, detected elements from Na to U, spatial resolution ~50 μm).

Main results

PHOTOLUMINESCENCE AND PHOTOCATALYTIC ACTIVITY OF ZINC TUNGSTATE POWDERS

L.Gigorjeva, D.Millers, J.Grabis, Dz.Jankoviča

$ZnWO_4$ powders with grain size in range 20 nm-10 μm have been synthesized by a simple combustion method and subsequent calcinations. The photocatalytic activities of powders were tested by degradation of methylene blue solution under UV light. The luminescence spectra and luminescence decay kinetics were studied and luminescence decay time dependence on powder average grain size was obtained. The correlation between self-trapped exciton luminescence decay time and photocatalytic activity of $ZnWO_4$ powders was shown. A model explaining the excitonic luminescence decay time correlation with photocatalytic activity was proposed.

THE TIME-RESOLVED LUMINESCENCE CHARACTERISTICS OF Ce AND Ce/Pr DOPED YAG CERAMICS OBTAINED BY HIGH PRESSURE TECHNIQUE

L.Grigorjeva, D.Millers, K.Smits, A.Sarakovskis, W.Lojkowski,
A. Swiderska-Sroda, W.Strek, P.Gluchowski

Transparent Ce and Ce/Pr doped YAG ceramics were prepared under high pressures (up to 8 GPa) and relative low temperature (450^{o}C). Grain size of the ceramics is less than 50 nm. However unknown defects or disorder strains on grain boundaries caused the additional absorption in these ceramics. The luminescence intensity, spectra and the decay time dependence on pressure applied during ceramic preparation were studied. Concentration of some intrinsic point defect was reduced under the high pressure applied for sintering process.
It is shown that formation time of the excited state of Ce luminescence depends on the pressure applied during ceramic sintering.

UP-CONVERSION LUMINESCENCE IN ZrO_2 NANOCRYSTALS

K.Smits, A.Sarakovskis, D.Millers, Dz.Jankovia, L.Grigorjeva

A set of undoped and Er/Yb doped ZrO_2 samples with different dopant concentrations were prepared and studied. The dopant concentration impacts to up-conversion luminescence intensity and luminescence temperature dependence. There are correlation between Er/Yb concentration and tetragonal or even structure stabilization as well as intrinsic defect

concentration. The role of intrinsic defects to up-conversion luminescence characteristics was shown.

LUMINESCENCE IN Eu DOPED ZrO_2 NANOCRYSTALS

K.Smits, L.Grigorjeva, D.Millers, Dz.Jankoviča

The time-resolved luminescence of undoped as well as europium doped (0.1 mol% - 20 mol%) ZrO_2 nanocrystals obtained by sol-gel synthesis were studied. The electronic excitations in zirconia are mobile, so with the increasing of activator concentration the intrinsic defects related luminescence decreases and intensity of activator luminescence increases until it reaches saturation. It is known that the Eu acts as phase stabilizer and as well Eu^{3+} is used as luminescence probe. The mechanisms of excited state creation and the possible models of luminescence centers are studied.

OXYGEN-EXCESS AMORPHOUS SiO_2 with ^{18}O-LABELED INTERSTITIAL OXYGEN MOLECULES

K.Kajihara, M.Hirano, L.Skuja, H.Hosono

Exchange between oxygen molecules embedded in amorphous SiO_2 (interstitial O_2) and oxygen atoms in the a-SiO_2 network is found to be remarkably slow at 500 °C. Thermal loading of $^{18}O_2$ at this temperature yields a-SiO_2 containing ^{18}O-labeled interstitial O_2 whose ^{18}O fraction is as high as ~90%. The ^{18}O fraction of interstitial
O_2 in this sample is quickly decreased by thermal annealing at or above 700 °C because of the oxygen exchange accompanied by the release of ^{16}O from the a-SiO_2 network. This finding indicates that the oxygen exchange starts at much lower temperatures than indicated by previous works, based on monitoring of the isotopic composition of oxygen atoms in the a-SiO_2 network.

EFFECTS OF TEMPERATURE ON ELECTRON PARAMAGNETIC RESONANCE OF DANGLING OXYGEN BONDS IN AMORPHOUS SILICON DIOXIDE

L.Skuja, K.Kajihara, M.Hirano, A.Silins, H.Hosono

The properties of electron paramagnetic resonance (EPR) signal of oxygen dangling bonds in amorphous SiO_2 ("non-bridging oxygen hole centers", NBOHC) in excimer laser-irradiated amorphous SiO_2 were studied in the temperature range 20K to 295K. NBOHCs strongly affect optical and chemical properties of amorphous SiO_2 -based (nano) structures and their surfaces. The behaviour of their EPR signal is complicated due to a nearly degenerate electronic ground state. It was found that EPR signal has a non-Curie (~1/T) T-dependence down to 40K, indicating that EPR-based concentration estimates routinely obtained at T=77K
underestimate the center concentrations at least by a factor of 1.7. The estimates of NBOHC concentration, based on EPR, are typically ~10 times lower than those derived from optical spectroscopy, evidently due to incomplete accounting for temperature, microwave saturation and due to degenerate ground state coupled to disorder effects. The EPR signal of NBOHCs shows a strong microwave saturation at T<40K which allows for a high-sensitivity

detection by 2nd-harmonic EPR registration techniques. Using it, the low intensity low-field wing of the
EPR signal was shown to extend to g values as large as g=2.4.

CRUCIAL DEPENDENCE OF EXCIMER LASER TOUGHNESS OF "WET" SILICA ON EXCESS OXYGEN

L.Skuja, K.Kajihara, M.Hirano, H.Hosono

Creation of point defects by ArF (6.4 eV) and F_2 laser (7.9 eV) irradiation in synthetic "wet" silica glass thermally loaded with interstitial O_2 molecules was studied by optical absorption, electron paramagnetic resonance and infrared absorption. The presence of excess oxygen caused a significant increase of laser-induced ultraviolet (UV) absorption, which was 4 times (7.9 eV-irradiation) and >20 times stronger (ArF
irradiation) as compared to O_2 -free samples. The spectral shape of photoinduced absorption nearly completely coincided with the spectral shape of oxygen dangling bonds (NBOHC) in 3 to 6.5 eV regions. The contribution of Si dangling bonds (E' centers) was less than few % and was not dependent on oxygen content. Peroxy radical defects were not detected. The photoinduced NBOHCs thermally decayed at 400...500 C. However, a subsequent brief 7.9 eV irradiation restored their concentration up to 70%. This sensitization can be in part attributed to generation of interstitial Cl 2 and HCl. These data show that oxygen stoichiometry is an important factor for maximizing the laser toughness of wet silica.

FRENKEL DEFECT PROCESS IN AMORPHOUS SILICA

K.Kajihara, M.Hirano, L.Skuja, H.Hosono

Point defects strongly influence optical properties of synthetic amorphous silica (synthetic a-SiO_2) used in excimer laser photolithography and their properties are intensively studied. Decomposition of an Si-O-Si bond into a pair of oxygen vacancy and interstitial oxygen species is an intrinsic defect process in a-SiO_2. It is similar to the creation of vacancy-interstitial pairs in crystalline materials and is regarded as "Frenkel defect process" in an amorphous material. Oxygens are also known to be emitted from a-SiO_2 surfaces under irradiation with vacuum-ultraviolet (VUV) light or electron beam. However, the anion part of the Frenkel pair in a-SiO_2 , interstitial
oxygen atom, lacks reliable spectroscopic signatures. Therefore, Frenkel process has been studied much less than another intrinsic defect process in a-SiO_2 , a simple cleavage of an Si-O bond, yielding a pair of silicon and oxygen dangling bonds. Interstitial oxygen molecule (O_2), a common form of the interstitial oxygen species in a-SiO_2, exhibits characteristic infrared photoluminescence (PL) at 1272 nm. This PL band allows interstitial O_2 to be detected selectively with a high sensitivity, and is useful in studying Frenkel defect processes in both a-SiO_2 and crystalline SiO_2 . The Frenkel process is dominant over the formation of the dangling bond pairs in high-
purity synthetic a-SiO_2 . Both these processes are influenced by the degree of the structural disorder of a-SiO_2 characterized by distribution of Si-O-Si angles. Fluorine doping promotes the structural relaxation and is useful in decreasing the concentration of "strained" Si-O-Si bonds, which have Si-O-Si bond angles widely different from the relaxed angle and are vulnerable to radiation. Moderate fluorine doping is effective in improving both UV-VUV transparency and radiation hardness, whereas heavy fluorine doping tends to enhance defect processes involving the Frenkel mechanism and to degrade the radiation hardness.

EXCHANGE BETWEEN INTERSTITIAL OXYGEN MOLECULES AND NETWORK OXYGEN ATOMS IN AMORPHOUS SiO_2 STUDIED BY ^{18}O ISOTOPE LABELING AND INFRARED PHOTOLUMINESCENCE SPECTROSCOPY

K.Kajihara, T.Miura, H.Kamioka, M.Hirano, L.Skuja, H.Hosono

Amorphous SiO_2 (a-SiO_2) thermally annealed in an oxygen atmosphere incorporates oxygen molecules (O_2) in interstitial voids. When the thermal annealing is performed in $^{18}O_2$ gas, interstitial $^{18}O_2$ as well as interstitial $^{16}O^{18}O$ and $^{16}O_2$ are formed due to the oxygen exchange with the a-SiO_2 network. The infrared photoluminescence band of interstitial O_2 was utilized to quantitatively analyze the oxygen exchange, taking into account the influences of common network modifiers in synthetic a-SiO_2 (SiOH,
SiF, and SiCl groups). The presence of network modifiers does not significantly change the average rate of ^{18}O transfer from interstitial O_2 to the a-SiO_2 network and its activation energy, suggesting that the network modifiers themselves do not serve as preferential oxygen exchange sites. When the concentration of SiOH groups is low, the oxygen exchange rate is distributed, indicating that only a small part of the network oxygen atoms participates in the oxygen exchange. However, the distribution of the oxygen exchange rate is distinctly narrow in the sample with high SiOH concentration. It is attributed to the redistribution of the network ^{18}O atoms and the modification of the a-SiO_2 network topology caused by reactions with mobile interstitial water molecules, which are transiently formed by dehydroxylation of paired SiOH groups. The activation energy for the average oxygen exchange rate is larger than that of the permeation of interstitial O_2 in a-SiO_2 . Furthermore, the average exchange-free diffusion length of interstitial O_2 below 900C ($\gtrsim$1 μm) is far larger than the scale of the interstitial voids in a-SiO_2 ($\lesssim$1 nm). These observations confirm that the oxygen exchange is not necessarily involved in the permeation of interstitial O_2.

VISIBLE TO VACUUM-UV RANGE OPTICAL ABSORPTION OF OXYGEN DANGLING BONDS IN AMORPHOUS SiO_2

L.Skuja, K.Kajihara, M.Hirano, H.Hosono

Synthetic silica glass with an optical absorption spectrum dominated by oxygen dangling bonds (nonbridging oxygen hole centers, or NBOHCs) and having negligible (<1%) contribution from the usually co-present Si dangling bonds (E'γ-centers), was prepared by room temperature ultraviolet photobleaching of high SiOH content (“wet”) silica, irradiated by F_2 laser (7.9 eV) at T=80 K. This allowed us to obtain the up-to-now controversial optical absorption spectrum of NBOHC in the ultraviolet and vacuum-ultraviolet (UV-VUV) region of the spectrum and to show that it is semicontinuous from 4 to 7.8 eV and cannot be represented by a pair of distinct Gaussian bands. Since NBOHC is one of the main UV-VUV range optical absorbers in silica, its spectral shape provides a tool to disentangle contributions of different color centers to optical losses in this spectral region.

LOCALIZED STATES IN SILICA. A SHORT REVIEW

A.Trukhin

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 recombination 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.

γ-RAY-INDUCED GeODC(II) CENTERS IN GERMANIUM DOPED α-QUARTZ CRYSTAL

A. Trukhin, A. Boukenter, Y. Ouerdane, S.Girard

Main luminescence of α-quartz crystal doped with germanium is luminescence of a self-trapped exciton near germanium. The luminescence characteristic for silica glass doped with germanium – so call GeODC – never was observed in as grown Ge-doped α-quartz crystal. Now we had performed experiment if GeODC like luminescence could appear after γ-irradiation of Ge-doped α-quartz crystal. The answer is positive: a new luminescence with two bands – a blue one with time constant about 100 μs under pulsed light of ArF laser (193 nm) and an UV one with fast decay ~1.5 ns under the same excitation appears and it is resembling the GeODC luminescence of silica glass. Beside under excitation of F_2 excimer laser (157 nm) the old STE luminescence remains in the sample irradiated. However, evident differences are obtained to the induced center with respect to known the twofold coordinated Ge center. The excitation with KrF laser does not provide decay time constant about 100 μs but provide blue luminescence with a faster decay about 4 μs. The pulses of ArF laser also excite this component of decay for the blue band. That we connect with multiformity of γ-ray created centers in amorphous areas of the Ge-doped crystal.

LUMINESCENCE IN GeO_2-SiO_2 FILMS FABRICATED BY SPCVD

A.Trukhin, K.Golant, J.Teteris

A line of Ge-doped silica films 10-20μ in thickness were synthesized by the surface-plasma chemical vapor deposition (SPCVD) on silica substrates. The content of Ge in different films was varied as $n{\cdot}GeO_2$-$(1-n)\cdot SiO_2$ with n changing from 0.02 to 1. No luminescence was observed in as received films under the excitation by 5 eV UV photons. It was the reason to conclude that the twofold coordinated germanium center is not formed immediately during the film preparation by SPCVD. However, subsequent heat treatment of the films by a CO_2 laser beam leads to the appearance of luminescence as well as to a huge grows of the absorption band at 5 eV, which indicates to the presence of twofold coordinated germanium centers. This observation correlates with the case of Ge implanted silicon dioxide thin films, in which luminescence of the twofold coordinated germanium was found to increase several hundreds times after the heat treatment . In pure (without silicon) GeO_2 SPCVD films the twofold coordinated germanium centers were not revealed even after heat treatment. However, under an ArF excimer laser (193 nm wavelength) excitation some luminescence is observed in the non-treated films with intensity increase at cooling down to 80 – 60 K. The decay kinetics of this luminescence significantly differs from that of the twofold coordinated germanium center, although its spectral content is similar.

Scientific publications

1. L.Grigorjeva, D.Millers, K.Smits, A.Sarakovskis, W.Lojkowski, A.Swiderska-Sroda, W.Strek, P.Gluchowski. The time-resolved luminescence characteristics of Ce and Ce/Pr doped YAG ceramics obtained by high perssure technique. Optical Mater., 2011 (article in Press).doi.:10.1016/j.optmat.2011.05.023.
2. K.Smits, L.Grigorjeva, D.Millers, A.Sarakovskis, J.Grabis, W.Lojkowski. Intrinsic defects related luminescence in ZrO_2. J.of Lumin., 2011, 131 (10) pp.2058-2062.
3. R.Zabels, F.Muktepavela, L.Grigorjeva. Deformation behavior of nanostructured ZnO films on glass. Thin Solid Films., 2011 (Article in Press), doi.:10.1016/j.tsf.2011.10.150.
4. A.N.Trukhin, K.Smits, A.Sarakovskis, G.Chikvaidze, T.I.Dyuzheva, L.M.Lityagina.Luminescence of dense, octahedral structured crystalline silicon dioxide (stishovite). J.of Lumin., 2011, 131 (11) pp.2273-2278.
5. A.N.Trukhin, K.Smits, G.Chikvaidze, T.I.Dyuzheva, L.M.Lityagina. Luminescence of silicon dioxide – silica glass, α-quartz abd stishovite. Cent. Eur. J. of Physics, 2011, 9 (4) pp.1106-1113.
6. A.N. Trukhin, Luminescence of localized states in silicon dioxide glass. A short review, Journal of Non-Crystalline Solids, 2011, 357 pp. 1931–1940.
7. A.N.Trukhin ,A.Boukenter ,Y.Ouerdane ,S.Girard, γ-ray induced GeODC(II) centers in germanium doped α–quartz crystal, Journal of Non-Crystalline Solids, 2011, 357 pp. 3288–3291.
8. L.Grigorjeva, D.Millers, J.Grabis, Dz.Jankovica. Photoluminescence and photo-catalytic activity of zinc tungstate powders. Cent. Eur. J. of Physics, 2011 9 (2) pp.510-514.
9. K. Kajihara, T.Miura, H.Kamioka, M.Hirano. L.Skuja, H.Hosono, Exchange between interstitial oxygen molecules and network oxygen atoms in amorphous SiO_2 studied by ^{18}O isotope labeling and infrared photoluminescence spectroscopy. Phys.Rev. B83, 064202 (2011).

10. L. Skuja, K.Kajihara, M.Hirano, H.Hosono, Crucial dependence of excimer laser toughness of "wet" silica on excess oxygen J. Non-Crystalline Solids v.357 p.1875–1878 (2011) (doi:10.1016/j.jnoncrysol.2010.12.047).
11. K. Kajihara, M.Hirano, L.Skuja, H.Hosono Oxygen-excess amorphous SiO_2 with ^{18}O-labeled interstitial oxygen molecules J. Non-Crystalline Solids v.357, No 8-9, p.1842-1845(2011).
12. K. Kajihara, M.Hirano, L.Skuja, H.Hosono Frenkel defect process in amorphous silica Proc. of SPIE Vol. 8077 80770R-1 (2011).
13. L. Skuja, K.Kajihara, M.Hirano, A.Silins, H.Hosono Effects of temperature on electron paramagnetic resonance of dangling oxygen bonds in amorphous silicon dioxide, IOP Conf. Series: Materials Science and Engineering 23 (2011) 012016
14. L. Skuja, K. Kajihara, M. Hirano, H. Hosono, Visible to vacuum-UV range optical absorption of oxygen dangling bonds in amorphous SiO_2, Phys.Rev.B 84, 205206 (2011) [9 pages].

Lectures in Conferences

International Baltic Sea Region Conference "Functional materials and nanotechnologies 2011 (FM&NT)", April 05-08, Riga, Latvia.

1. Dz.Jankovica, J.Grabis,L.Grigorjeva, D.Millers, K.Smits, L.Bukonte. Synthesis and characterization of Cerium and Europium Doped Nanocrystals. Book of Abstracts. P.97.
2. A.Swiderska-Sroda, K.Galazka, W.Lojkowski, T.Chudoba, A.Opalinska, K.Smits, L.Grigorjeva, D.Millers, C.Leonelli. Optical Oxigen Nano-sensor. Book of abstracts, p.24
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5. R.Zabels, F.Muktepāvela, L.Grigorjeva, K.Kundziņš. Effec of Nanopowder Morphology on the Properties of ZnO Sintered Ceramics. Book of abstracts, p.196.
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9. A.N.Trukhin, A. Boukenter, Y. Ouerdane, S.Girard, „γ-ray-induced GeODC(II) centers in germanium doped α-quartz crystal", Book of abstracts, p. 92.
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LU CFI 27th Scientific Conference, 2010, 17-19 Febr., Riga, Latvia

1. L.Bukonte, L.Grigorjeva, V.Tupureina, D.Millers, M.Knite. YAG un ZnO nanopulveru/plimēru kompozītu optiskās īpašības. Abstracts, p.38 (oral).
2. J.Rikveilis, L.Grigorjeva, D.Millers, K.Smits. Oksīdu nanopulveru fotokatalīzes efektivitātes pētījumi. (poster).
3. V.Liepiņa, Dz.Jankoviča, K.Smits, D.Millers. Luminiscento īpašību atkarība no aktivēta stroncija aluminăta sintēzes un pēcapstrādes (poster).
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11th International Conference on Inorganic Scintillators and Their Aplications.September., 11-16, 2011, Giessen, Germany.

1. D.Millers, K.Smits, L.Grigorjeva. Luminescence of cerium doped zirconi nanocrystals. Program and Abstract Book, P1.21.
2. L.Grigorjeva, D.Jankoviča, K.Smits, D.Millers, S.Zazubovich. Luminescence of Ce, Pr and Ce/Pr doped nanopowders. Program and Abstract Book, P2.13.

18th International Workshop on Room Temperature Semiconductor X-ray and Gamma-Ray Detectors, 23-29 October, 2011, **Valencia, Spain**

1. V.Ivanov, P.Dorogov, A. Loutchanski, L.Alekseeva, L.Grigorjeva, D.Millers. Impoving the performance of CdZnTe Detectors Using Infrared Stimulation. Abstracts, RTSD S-2462.
2. L.Aleksejeva, P. Dorogov, V.Ivanov, A. Loutchanski, L.Grigorjeva, D. Millers. Investigation of the Influence of Light Illumination on the Characteristics of CdZnTe Detectors. Abstracts, RTSD S-2463.

2th International Conference on Bio-Sensing Technology. 10-12 October, 2011, Amsterdam, the Netherland.

K.Smits, J.Liepins, M.Grube, M.Gavare, D.Jankovica, A.Sarakovskis. ZrO_2 nanocrystals as a temperature probe in baker's yeast Saccharomyces cerevisiae cells. Abstracts, P125.

The 19th University Conference on Glass Science August 3-5, 2011, Rensselaer Polytechnic Institute, Troy, New York 12180, USA

K.Kajihara, L.Skuja, H.Hosono ^{18}O labeled interstitial oxygen molecules as a probe to study reactions involving oxygen-related species in amorphous SiO_2.

16th Internat. Conf. "Radiation Effects in Insulators", REI-16, Beijing, China, August 15-19, 2011

L.Skuja, K.Kajihara, M.Hirano, H.Hosono Point defects in glassy/amorphous SiO_2 and related materials, paper I-3(invited), Abstract book, p.36.

Doctoral thesis

Mihails Šorohovs. TlBr crystal optical, electrical and surface properties investigation; X-ray and γ-ray detectors development. Rīga, 2011.

Master thesis

Laura Bukonte. Polimēru/oksīdu nanopulveru kompozītu luminiscentās īpašības, RTU, 2011

DEPARTMENT OF FERROELECTRIC PHYSICS

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

Research Areas

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.

Material preparation methods.
Synthesis and processing of bulk ceramics samples is based on solid state reactions of oxides and carbonates exploiting synthesis at atmospheric pressure as well as two-stage hot pressing technologies.

Characterization methods.
Include X-ray diffraction, atomic force microscopy, piezo-response force microscopy, electron scanning microscopy with EDX option, EPR and Raman spectroscopies, dielectric impedance and hysteresis measurement tools, piezoelectric properties and field induced deformation, electrocaloric effect, ellipsometry and reflectometry techniques, adaptive optics.

Research Topics:

- Phase transitions and ordering effects in "ordinary" ferroelectrics and ferroelectric relaxors along with new compositions, including multi-component systems containg 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 intrinsic localized excitations in nonlinear lattices: heuristic explanation of the nature of polar nano-regions in advanced complex oxides;
- Transition-element doping effects in ABO_3 perovskites;
- Synthesis and characterization of piezoelectric ceramics without lead;
- Physical 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 niobatetantalate ceramics;
- Elastic properties of ceramics derived from barium titanate;
- Research of new compositions for varios pratical applications and research of ferroelectric and relaxor state.

Scientific staff: Doctors

1. Dr. phys. Eriks Birks
2. Dr. phys. emeritus Karlis Bormanis
3. Dr. habil. phys. Vilnis Dimza
4. Dr. phys. Sergejs Fomins
5. Dr. phys. Eriks Klotins
6. Dr. habil. phys. Andris Krumins
7. Dr. phys. Maris Kundzins
8. Dr. phys. Anatoly Mishnev
9. Dr. habil. phys. Maris Ozolins

Scientific staff: Magisters

1. Mg. chem. Maija Antonova
2. Mg. chem. Anna Kalvane
3. Mg. phys. Karlis Kundzins
4. Mg. phys. Aina Plaude
5. Mg. phys. Zane Zaula

Graduate Students

1. Lelde Kundzina

10. Dr. habil. phys. Andris Sternberg
11. Dr. habil. phys. Juris Zvirgzds

PhD Students

1. Mg. phys. Marija Dunce
2. Mg. phys. Varis Karitans
3. Mg. phys. Kaiva Luse
4. Mg. Sc. ing. Ilze Smeltere

Technical staff

1. Ing. Maris Livins
2. Ing. Modris Logins

Programmes and projects

1. National Research program in Materialsciences:
   Development of novel multifunctional materials, signal processing and information technologies for competitive knowledge-based products.
   Project #1. Multifunctional materials for high-tech applications in conversion of radiation energy, information recording, storage, transfer and processing.
2. Project 10.0032-1.7. Development of research and technology potential for elaboration of new and nanostructured materials and related applications.
   Subproject: # Nanostructured complex oxides: fundamentals, experiment and applications.
   Subproject: # Surface and boundary effects of dielectrical, optical and mechanical properties in nanostructurated functional materials.
3. Project 09.1548. Physical processes in multilayer and multicomponental structures.
4. ERAF projects: Support of science and research.
   Subproject: # 088. Innovative glass coatings.
   Subproject: # 114. Development of innovative technology for obtaining solar grade silicon by electron beem method.
   Subproject: # 137. Technologies of material digital multispectral control and quality improvement.

Scientific Visits Abroad

Mg. chem. **Maija Antonova**

1. International Scientific Conference «Actual Problems of Solid State Physics», «Актуальные проблемы Физики твердого тела», Minsk, Belarus, October 18 – 21.

Dr. phys. emeritus **Karlis Bormanis**

1. XIX Russian conference on Physics of Ferroelectrics (ВКС – XIX), Moscow, Russia, June 20-23.
2. European Meeting on Ferroelectricity, EMF-2011, Bordeaux, France, June 26 – July 2.
3. International Conference Advanced Optical Materials and Devices, AOMD-7, Vilnius, Lithuania, August 28-31.
4. International Scientific Conference «Actual Problems of Solid State Physics», «Актуальные проблемы Физики твердого тела», Minsk, Belarus, October 18 – 21.

Mg. phys. **Marija Dunce**

1. European Meeting on Ferroelectricity, EMF-2011, Bordeaux, France, June 26 – July 2.

2. The 13-th International Conference „Advanced Materials and Technologies" and Summer School "European Doctorate in Physics and Chemistry of Advanced Materials": Palanga, Lithuania, August, 27-31.

Mg. phys. **Sergejs Fomins**

1. European Conference of Visual Perception, (ECVP-2011), Touluse, France, August.28–September 1.

Mg. chem. **Anna Kalvane**

1. International Scientific Conference «Actual Problems of Solid State Physics», «Актуальные проблемы Физики твердого тела», Minsk, Belarus, October 18 – 21.

Mg. phys. **Varis Karitans**

1. International Conference „Adaptive Optics: Methods, Analysis, Applications", Toronto, Canada, July 10-14.

Mg. phys. **Karlis Kundzins**

1. Workshop: INCA - Energiedispersive Analyse. Oxford Instruments GmbH, 65205 Wiesbaden, Gemany, May 11-13.

Dr. phys. **Maris Kundzins**

1. European Fusion Development Agreement Public Information Network meeting (EFDA PIN meeting), Greifswald, Germany, June 15-18.

Mg. phys. **Kaiva Luse**

1. 13th International conference-school "Advanced Materials and Technologies", Palanga, Lithuania, August 27-31.

Dr. phys. **Anatoly Mishnev**

1. XXII Congress and General Assembly of the International Union of Crystallography, Mardid, Spain, August 22-30.

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

1. International Conference Advanced Optical Materials and Devices, AOMD-7, Vilnius, Lithuania, August 28-31.

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

1. Piezo – 2011: Electroceramics for End Users VI, Sestriere, Italy, February 27 – March 3.
2. 12th Conference of the European Ceramic Society, ECERS XII, Stockholm, Sweden, June 19 – 24.
3. European Meeting on Ferroelectricity, EMF-2011, Bordeaux, France, June 26 – July 2.

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, February 09-10; May 02-03; October 04-05.

2. Meeting of Heads of Research Units of EURATOM Associations: Garching, Germany, September 07-08.
3. Meetings of the High Level Group on Nanoscience and Nanotechnologies: Brussels, May 25-26; June 15-16; October 03-04; December 13-14.
4. Meeting on Nanotechnology and applications: Brussels, March 02-04.
5. The 20th IEEE International Symposium on Applications of Ferroelectrics, Vancouver, Canada, July 23-29.
6. International Conference „Micro- and Nanoengineering“ (MNE-2011), Berlin, Germany, September 19-22.
7. Meeting of the EFDA Steering Committee: Munich, Garching, Germany, April 12-14; Warszaw, Poland, October 24-25.
8. COST Domain of Materials, Physics and Nanosciences: Committee Meeting in Tartu, Estonia, September 12-15.
9. Visit of M. von Laue – P. Langevin institute and CNPS, Grenoble, France, November 22-23.

Visitors from Abroad

1. Martinas Kinka, Vilnius University, Vilnius, April-May, 3 weeks.
2. Juras Banys, Vilnius University, Vilnius, April, 1 week.
3. Barbara Garbarz-Glos, Renata Bujakiewicz-Koronska and Wlodzimierz Šmiga, Institute of Physics, Krakow Pedagogical University, Krakow, April, 1 week.

Cooperation

Latvia

1. Riga Technical University, Faculty of Material Science and Applied Chemistry, Institute of Technical Physics (Prof. M. Knite, Prof. A. Ozols).
2. Riga Technical University, Biomaterial Innovation and Development Center (Dr. L. Berzina-Cimdina).
3. Daugavpils University, Innovative Microscopy Centre (Dr. E. Tamanis).
4. Ventspils highschool (Dr. J. Harja).
5. University of Latvia, Institute of Chemical Physics (Dr. D. Erts).
6. University of Latvia, Department of Chemistry (Mag. A. Zvirgzdinsh).
7. University of Latvia, Institute of Atomic Physics and Spectroscopy (Dr. hab. J. Spigulis).
8. Institute of Physics, University of Latvia (Prof. E. Blums, Dr. M.M. Maiorov).
9. A/S “Sidrabe”.
10. SIA “GroGlass SIA”.
11. SIA “Baltic Scientific Instruments”.
12. SIA „Fonons“.

Austria

1. University of Vienna, Faculty of Physics, Functional Materials (Prof. A. Fuith).
2. Vienna University of Technology, Institute of Atomic and Subatomic Physics (Prof. H.W. Weber).

Belorussia

1. Institute of solid state and semiconductor physics of NAS of Belarus (Dr. S.V. Trukhanov, Dr. Yu. Radyush).
2. Center of optoelectronic technology, NAS of Belarus (Dr. Yu.V. Trofimov}.

Czech Republic

1. Institute of Physics, Academy of Sciences of the Czech Republic, Prague (Dr. 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. J. Levoska, Dr. M. Tyunina, Dr. J. Hagberg).

Italy

1. Italian Institute of Technology, Corso Trento 21, Turin (Dr. I. 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, Dr.phys. R. Bujakiewicz-Koronska, Dr. W. Šmiga).
2. Institute of Molecular Physics, Polish Academy of Science, Poznan (Dr. E. Markiewicz).

Portugal

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

Russia

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

Ukraine

1. Poltava Quartz Glass Plant Ltd. (V. Panibratskiy)

Main results

NUMERICAL EVIDENCES OF POLARIZATION SWITCHING IN PMN TYPE RELAXOR FERROELECTRICS *

E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, and D. Engers

Extensive efforts to find unambiguous answer to what distinguishes relaxors from conventional freroelectrics have persisted since the 1983 [1] and are still an active field of research in condensed state theory. We present a conceptual and computational framework for chemically ordered $Pb(Mg_{1/3}Nb_{2/3}O_3)$ (PMN) relaxor ferroelectric distinguished by chemically ordered supercells violating disorder of the host lattice. Ingredients borrowed from the first principles calculations [2] include supercell lattice parameters whereas the thermodynamical arguments are restricted by invariance under permutations of ordered sites and zero spontaneous polarization of disordered sites.

Conceptual framework supporting both local nonzero and zero mean polarization of the supercells includes prepositions as follows: (i) total energy involves invariance under permutations of the supercells, (ii) double degenerate states for supercells are reproduced by symmetric Miller indices, and (iii) in a lattice of supercells the polarization is pseudorandom with zero mean for each component.

Computations are preceded over a simulation box of 8x8x8 supercells specified by eight varieties of the supercell polarization, symmetric Miller indices, pseudorandom distribution of polarization and zero mean for each component.

Statistics treated in canonical ensemble within the mean field approach reveals temperature development of polar nanoregions as an interplay between the (random) initial state polarization of supercells and their dipole-dipole interactions increased at cooling.

It allows us to quantify and explain the polarization switching of individual supercells examplified by the temperature development of supercell # 220 illustrated in Figure 1.

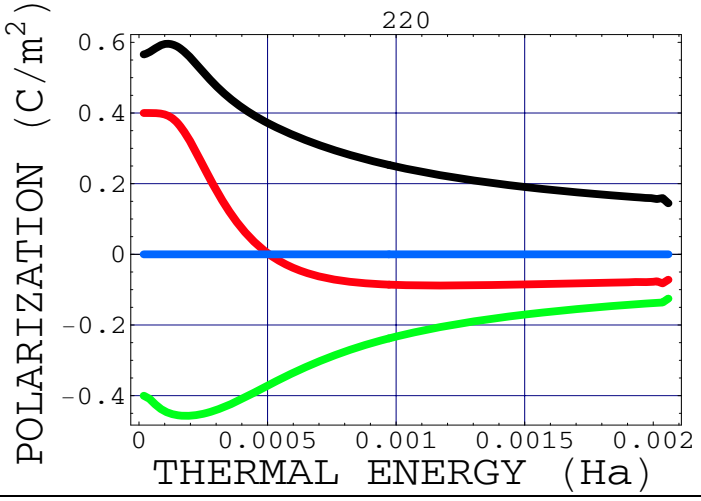

Figure 1. Temperature development of polarization for supercell #220 at cooling with P_x (green), P_y (red), P_z (blue) and $|\mathbf{P}|$ (black) plots.

Polarization switching which appear at thermal energy 0.0005 Ha is assigned to the dipole-dipole interaction increased at cooling.

While the approach considered here is restricted to the temperature invariance both the size and the volume fraction of supercells and, as a , it suggests a framework within which to rationalize and predict the complex behavior of PMN and related materials [3].

References: [1] Burns G., Dacol F.H. Solid State Commun. 1983, 48, 853.
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[3] E. Klotins, et al., Integrated Ferroelectrics, 2011, **123,** 32-39.

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POLAR NANOREGIONS IN $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN): INSIGHTS FROM SUPERCELL APPROACH *

E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, and D. Engers

Polar nanoregions play a central role in models of relaxor ferroelectrics characterized by chemical disorder on microscopic scale supporting ultra high parameters in technological applications.

The central and long term unresolved problem is to quantify and explain $A(B'B'')O_3$ complex oxides with two levels of disorder. At the level of elementary lattice the system is chemically disordered due the difference of ionic charges in B positions. This disorder is presumably violated in chemically ordered polar supercells, yet condensed randomly without common casual influence.

We report advancements going beyond the early empirical approaches and are borrowed from the first principles calculations [1] adressed to the $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) structured of $Pb^{2+}Mg^{2+}O_3^{2-}$ and $Pb^{2+}Nb^{5+}O_3^{2-}$ primitive cells with 2- and 1+ excess charge. The charge balance is achieved for a $15\,n$ $(n=1,2,..)$ atoms supercell embedded in disordered host lattice with no ferroelectric activity .

Essential topics developed in terms of coarse-grained Hamiltonian and mean field statistics simulations [2] helps to explain the role of energetically equivalent structural varieties of the supercells and their invariance under permutations as a source supporting random oriented residual polarization without adjustable parameters like random intracell and intercell interactions and quenched electric fields [3]. Representive details include both nonzero local and zero macroscopic polarization of the structure as well as the temperature change of the supercell anisotropy at cooling (Figure) and field cooling.

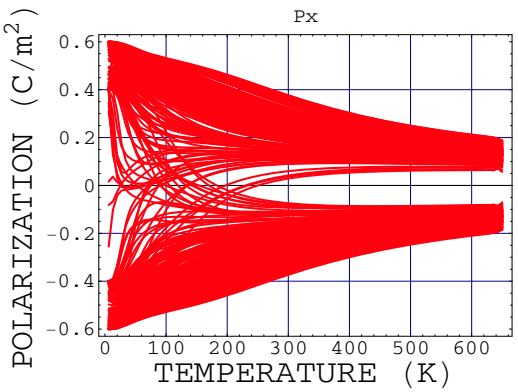

Figure. Representive example of zero field cooling for a model of 512 supercells. At high temperature the polarization of each supercell P_x (belonging to one of the eighth available local polarization vectors) approaches to zero. At cooling the polarization of individual supercells either increases, with the initial local polarization maintained, or undergoes local transition toward the opposite direction. Symmetry of polarization plots with respect to the zero polarization line approves zero total polarization.

Remaining questions, not fully understood and answered include increasing of the volume fraction of polar nanoregions with decreasing temperature and the pre-transitional phenomena evidenced by neutron [4,5] and NMR spectra [6] that are definitely incompatible with the implicit asssumption that the volume fraction of polar nanoregions correlates with the chemical ordering and is invariant with respect to the temperature.

Observation–matching answers to these questions are expected within a complementary approach accounting for the nonlinearity of intersite potential of supercells as an ingredient of dynamical interpretation of polar nanoregions [7] revealing remarkable property that the chemical disorder is in favor of spontaneous dipole moment so suggesting promissing lines of future research.

References

[1] S.A. Prosandeev et al., Phys. Rev. 2004, B 70, 134110.
[2] E. Klotins et al., Integrated Ferroelectrics, 2011, 123, 32-39.
[3] E. Klotins et al., Cent. Eur. J. Phys. 2011, 9, 2.
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[5] P.M. Gehring et al., Phys. Rev. B 2009, 79, 224109.
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[7] E. Klotins, Physica, 2010, E 42 , 614.

* *In cooperation with Institute Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, France.*

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

I. Smeltere, M. Atonova, A. Kalvane, and M. Livinsh

In the present work processing and characterization of lead free ceramics with a stoichiometric formula $(1-x)(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3$-$xBaTiO_3$ (x=0.01, 0.015, 0.02) were produced and have been studied. Ceramics were sintered via conventional ceramics processing method at temperatures 1150^o – 1220^oC 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.

X-ray diffraction analysis of the $(1-x)(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3$-$xBaTiO_3$ (x=0.01, 0.015, 0.02) (KNNS-xBT) ceramics confirmed single phase perovskite structure with monoclinic or tetragonal cell depending on x. No peak corresponding to the secondary phase was observed implying that KNNS and BT ceramics formed homogeneous solid solution.

The fracture microstructure of the $(1-x)(K_{0.5}Na_{0.5})Nb_{0..96}Sb_{0.04}O_3$-$xBaTiO_3$ (x=0.01, 0.015, 0.02) was investigated by SEM as shown in Figs. 1. a-c.

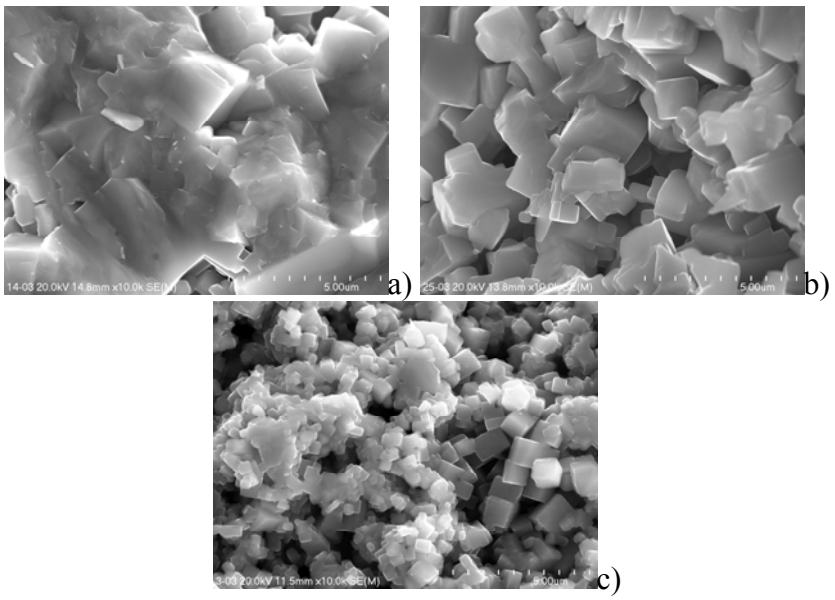

Figure 1. SEM micrographs of fractured surface of $(1-x)(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3$-$xBaTiO_3$ a) x=0.01; b) x=0.015; c) x=0.02

With increasing $BaTiO_3$ concentration in the composition the average grain sizes decrease; the shape of grains is rectangular although a little rounded. The fracture occurs along the grain boundaries except for the samples with x=0.01. 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. The obtained so-called "mappings" with EPMA revealed quite even distribution of elements on the polycrystalline material surface and at the same time confirmed the qualitative composition of examined samples.

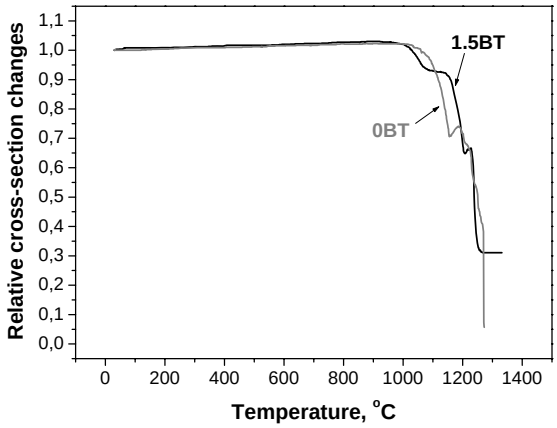

Figure 2. High temperature microscope analysis

Figure 2 shows the influence of $BaTiO_3$ addition on the sintering process of the ceramic body taken from the high temperature microscope measurements. $BaTiO_3$ has much higher sintering temperatures than Sb-substituted KNN we assume that BT engages in the sintering process later which is the reason of developing of the shoulder. It also makes the ceramics sintering interval broader which is significant for KNN-based materials.

The addition of $BaTiO_3$ effects the dielectric properties of the composition. The addition of 1 mol% of BT increases the value of dielectric permittivity ε and decreases T_c. In the same time BT decreases dielectric losses (Fig.3).

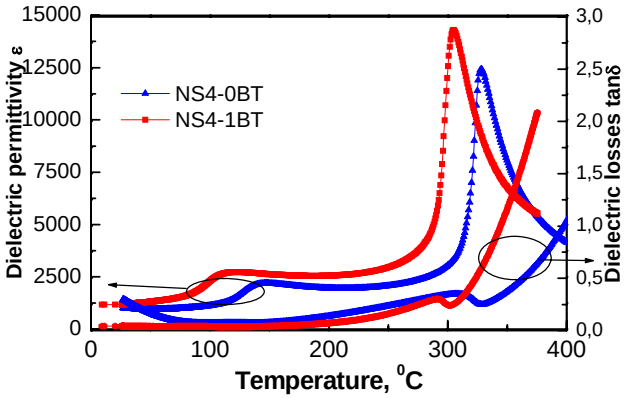

Figure 3. Dielectric permittivity ε and losses tanδ as a function on temperature

BEHAVIOUR OF THE REVERSE DIELECTRIC PERMEABILITY IN SBN-75 CERAMICS

K. Bormanis, A.I. Burkhanov*, S.V. Mednikov**, and Liu Thi Njan**

The dielectric nonlinearity in $Sr_{0.75}Ba_{0.25}Nb_2O_6$ (SBN-75) ceramics is observed. Earlier studies of polarisation switching in SBN-75 single crystals [1, 2] had shown essential decrease (as compared with ordinary ferroelectrics) of polarisation with each cycle in the thermal range of the relaxor phase, which had been related to "freezing" processes in disordered ferroelectrics.

Manifestations of similar processes were of interest in SBN-75 ceramics taking into account that dielectric permittivity ε' and dielectric loss ε'' are smaller compared with single crystal by more than order of magnitude if measured along the polar axis.

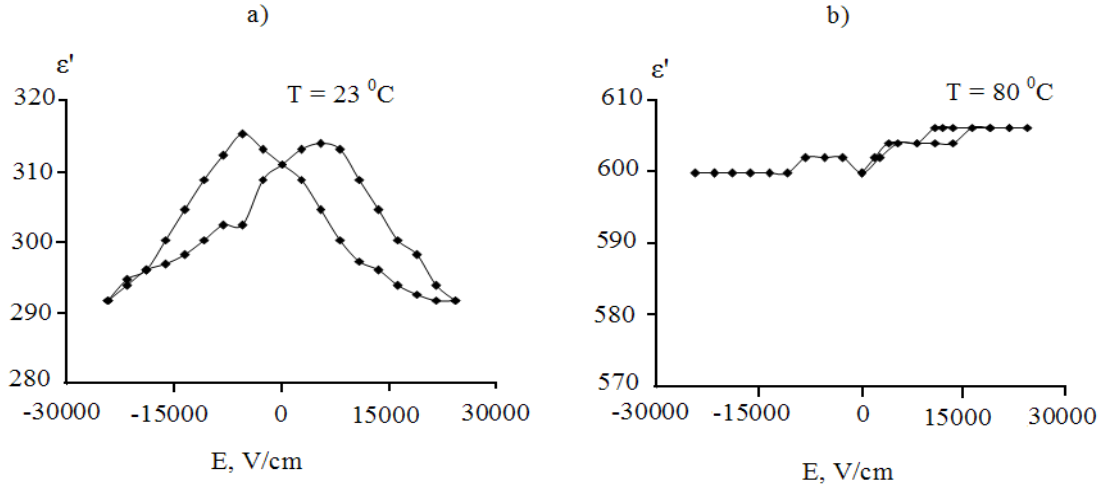

Figure 1. Field dependence of dielectric permittivity at different temperatures for SBN-75.

Behaviour of reverse ε' ($E_=$) at $T < T_m$ and at $T \geq T_m$ in SBN-75 ceramics is presented in Fig. 1. a and b, respectively. Behaviour of dielectric nonlinearity at $T < T_m$, different from single crystal, is similar to that of ordinary ferroelectrics – the $\varepsilon'(E_=)$ curve is closed while at $T \geq T_m$ the magnitude of ε' practically does not depend on the bias field $E_=$.

Possible effects of mechanical tension on features of dielectric nonlinearity in ceramics are discussed, suppression of relaxor properties in case of ceramic materials, in particular.

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THERMAL EXPANSION AND ELECTROMECHANICAL PROPERTIES IN $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ SOLID SOLUTIONS

M. Dunce, E. Birks, I. Aulika*, A. Fuith**, M. Antonova,
R. Taukulis, and A. Sternberg

The transfer from diffused to normal ferroelectric phase transition, passing different stages of relaxor behaviour, was found in $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ by research of

polarization and dielectric properties. Here thermal expansion and electromechanical properties are studied for these compositions.

Two methods were used in the studies of electric field-induced deformation - the classical resonance-antiresonance method, was used to determine piezoelectric coefficients for compositions, which are in FE state at room temperature. Whereas Michelson interferometer with an original method of interference analysis was used for measurements of electric field-induced deformation in quasistatic regime. The character of the obtained polarization dependence of the deformation corresponds to the place of the concrete composition in the phase diagram. It was stated that for compositions, which are in the relaxor state at room temperature, the deformation is proportional to polarization square, which allows us to determine values of electrostriction coefficient Q_{11}. The largest electric field-induced deformation of 0.054% was observed for composition NBT-ST-PT 0.4/0.52/0.08, which is close to morphotropic phase boundary between pseudocubic and tetragonal structure.

Studies of thermal expansion were used for characterization of the relaxor state. Thus attention was paid to determination of the Burns temperature (T_B), using measurements of thermal expansion. The measurements did not give us possibility to determine T_B precisely only from temperature dependence of the thermal expansion. However comparing NBT-ST-PT compositions with different character of the relaxation state allowed us to establish that all of these compositions have similar values of the thermal expansion coefficient at $T>400^oC$. From this we can conclude that in the mentioned temperature range the thermal expansion does not depend on local polarization, which is different for these compositions, and define $T_B \sim 400^oC$.

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RELATION OF DIELECTRIC PERMITTIVITY AND ELECTRIC FIELD DEPENDENCE OF POLARIZATION IN SOME RELAXORS WITH PEROVSKITE STRUCTURE

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

The dielectric nonlinearity is studied in ferroelectric relaxors $0.92PbMg_{1/3}Nb_{2/3}O_3$-$0.08PbTiO_3$ (PMN-PT) $0.4Na_{1/2}Bi_{1/2}TiO_3$-$0.5SrTiO_3$-$0.1PbTiO_3$ (NBT-ST-PT) and $Pb_{0.9075}La_{0.0925}(Zr_{0.65}Ti_{0.35})_{0.9775}O_3$ (PLZT). It is shown that above the temperature of dielectric permittivity maximum nonlinearity of dielectric permittivity corresponds to electric field dependence of polarization.

Decreasing of dielectric permittivity under DC electric field, characteristic for relaxors, is found in PMN-PT and NBT-ST-PT. Dependence of the distribution function of relaxation times, used for description of dielectric dispersion, is weakly influenced by electric field. A parallel shift of dielectric permittivity is observed in all frequency range, where dielectric dispersion exists. It is showed that the approach, usually used for description of P(E), does not correspond to the temperature dependence of dielectric permittivity. It is not confirmed that distribution of size of PNR is a reason for distribution of relaxation times.

Low nonlinearity coexists with expressed dielectric dispersion in PLZT. The nature of nonlinearity and characteristic bending of P(E) in this composition are explained by existence of internal bias field, caused by presence of Me^{3+} and oxygen vacancy defect dipole.

ELECTROCALORIC EFFECT IN $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ SOLID SOLUTIONS

J. Hagberg*, M. Dunce, E. Birks, M. Antonova, and A. Sternberg

Previously a gradual transfer from relaxor to ferroelectric state in dependence on concentration of constituents, passing different stages of relaxor behaviour, was established in triple solid solutions (1-x-y)$Na_{1/2}Bi_{1/2}TiO_3$-x$SrTiO_3$-y$PbTiO_3$ ((1-x-y)NBT-xST-yPT) by research of dielectric properties. The electric-field-induced first-order phase transition, characterized by double hysteresis loops, is found in a certain range of the compositions.

In this work the electrocaloric effect is studied in the solid solutions NBT-ST-PT in the concentration range of relaxor ferroelectric properties. The temperature and electric field dependences of the electrocaloric effect qualitatively correspond to the results, established earlier in other relaxor ferroelectrics.

High values of the electrocaloric effect are found at the electric-field-induced phase transition in the composition range, where the relaxor properties diminish in favour of the ferroelectric state. In compositions 0.4NBT-0.4ST-0.2PT and 0.4NBT-0.35ST-0.25PT these values reach ~1.1 ^oC at E=20 kV/cm in the region of the phase transition. Very different nature of ECE is found in compositions with low concentration of PT, where ferroelectric state can not be reached even under electric field. It was showed that the calculation of ECE in relaxor state according to traditional thermodynamic considerations does not correspond to the experimental results.

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PRINCIPLES OF DESIGNING CONTAINERS FOR THERMO-CHEMICAL TREATMENT OF HIGH PURITY COMPOUNDS

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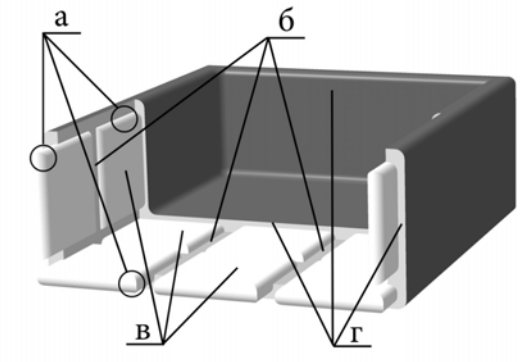
Mathematical modelling of the distribution of strain in layered quartz ceramics with protective coating of niobium pentoxide from two sides is tested. It is found that fragmentation of the basic layer (decreasing the area of the continuous boarder between layers) and smoothing of sharp edges of the base fragments should reduce the strains on the boundary between the substrate and coating and, correspondingly, enhance the thermal resistance of the samples.

Treatment of the niobium pentoxide coating by concentrated light flow (CLF) induces a network of fractal micro- and nano-size fractures that compensates the difference of thermal expansion between the layers. The absolute value of the negative coefficient of linear thermal expansion (CLTE) of Nb_2O_5 treated by CLF decreases while the curve of relative thermal expansion becomes more symmetric. Due to the fractal micro- and nano-size structures forming at treatment by CLF in optical oven the CLTE of tantalum pentoxide samples exhibits a region of negative or close to zero values. The fraction of nanometre-size fractures in case of Ta_2O_5 treatment by CLF is likely considerably larger as compared with Nb_2O_5.

The studies have demonstrated that possible control of bulk expansion of the material and fragmentation of the basic layer allow to obtain layered ceramics and products thereof possessing enhanced thermal resistance to withstand thermal cycling.



Experimental acoustic emission studies have confirmed the increase of thermal resistance of the samples by factor ~1.5. Smoothing the

edges of the fragments of the ceramic substrate provides additional increase of thermal resistance by ≈15 %. Containers for calcination of high purity grade niobium hydroxide made of fragmented ceramic substrate and coated by CLF-processed Nb_2O_5 have shown improved thermal resistance. Such containers, as shown in figure, withstand thousands of fast thermal cycles $T_{room} \leftrightarrow 1000$ ºC.

Figure. Container of structured quartz core and niobium pentaoxide coating: a – rounded corners, b – seams connecting segments (c) of quartz ceramics, d – protective coating of niobium pentaoxide.

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DIELECTRIC PROPERTIES AND CONDUCTIVITY OF FERROELECTRIC $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$ and $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ SOLID SOLUTIONS

K. Bormanis, M.N. Palatnikov[*], V.V. Efremov[*], N.V. Sidorov[*], and I.N. Efremov[*]

The ABO_3 ferroelectric (FE) solid solutions (SS) of perovskite structure on the basis of sodium niobate exhibit a number of properties interesting for application: relatively low values of density and dielectric permittivity, high ultrasonic velocity and good piezoelectric performance, and a wide range of mechanical Q-factor. Results of dielectric and conductance studies over the thermal range of 290 – 700 K and frequency range of 25 - 10^6 Hz in $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$ and $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ perovskite FESS are discussed. Electric properties and phase transition parameters of $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$ and $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ FESS are found to depend substantially on the way the initial mixture is synthesised. A first-order FE phase transition proceeds in the $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$ and $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ FESS within the observed range of temperature. The co-precipitated $Ta_{2y}Nb_{2(1-y)}O_5$ pentoxides being used for synthesis of the $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ FESS it is possible to achieve rather high values of dielectric permittivity at high frequencies while the Curie point shifts by ~ 75 K to a lower temperature as compared with $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$, synthesised from mechanical mixture of the Ta_2O_5 and Nb_2O_5 oxides, which cannot be explained by the minor difference in proportions of the ingredients in the final SS. Techniques of obtaining the initial oxides has also a substantial effect on the ion conductivity of the $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$ and $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ FESS. The activation energy of ion conductivity in the $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ FESS is lower while its value – considerably higher compared with $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$. The different thermal behaviour of the real part of dielectric permittivity and conductivity between the $Li_{0.07}Na_{0.93}Ta_{0.1}Nb_{0.9}O_3$ and the $Li_{0.07}Na_{0.93}Ta_{0.111}Nb_{0.889}O_3$ FESS are obviously related to the way of obtaining the initial oxides Ta_2O_5 - Nb_2O_5 and $Ta_{2y}Nb_{2(1-y)}O_5$.

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INFLUENCE OF OCULAR ABERRATIONS ON DIAMETER OF RETINAL BLOOD VESSELS[*]

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Lower-order and higher-order ocular aberrations influence not only visual perception but also appearance of retinal images. We suggest that apparent diameter of blood vessels may differ for various types of aberrations based on how the maps of point spread functions are

orientated to these vessels. We test our hypothesis by simulation methods and by using adaptive optics system on basis piezooptic segmented mirror. The optic wavefront correction was sufficient to create higher order aberrations as spherical and coma.There was moderate correlation between diameter ratio of two blood vessels assessed by two ophthalmologists. We conclude that ophthalmologist when examining fundus of an eye must pay attention to both patient's aberrations and also those of examiner.

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RAYLEIGHT EQUATION ANOMALOSCOPE FROM COMMERCIALLY AVAILABLE LEDs[*]

R. Trukša, S. Fomins

In early 1907 - Nagel offered new way to diagnose red - green colour vision defects, offering a device called anomaloscope. Using this equipment in practice it is possible to distinguish protanopia from deuteranopia also protanomaly from deuteranomaly with best available accuracy.

We used LEDs as light source because they can provide necessary brightness, narrow or almost narrow spectrum with significant maximum and low power consumption properties. LED anomaloscopes already have been provided by Woods et al [1], showing that this modification of device is good substitute for original Nagel anomaloscope. Our aim is to create and calibrate a power LED based anomaloscope for diagnosis of red-green colour vision defects. Other field of use of anomaloscope is a seasonal and overall variation of normal colour vision in Latvian population.

We tested two types of LEDs but no one of light sources provided necessary brightness or spectrum properties. One type of light sources produced 12-28.1 nm wide spectrum which is enough except green LEDs, because their spectrum should be about 10 nm wide. Colour mixture of available red and green primaries appeared saturated. Calculations showed retinal luminescence of 1.70- 2.30 logTd, but it is not enough for the photopic requirements. To solve the problem of brightness control - we decided to use power LEDs which can provide necessary retinal luminance. Only imperfection of these light sources is wider spectral half width. However, this can be narrowed by interference filters. The drawback of the linear potentiometer control for a control the brightness of red-green primaries is a lack of accuracy and dynamic depth. Direct control of LEDs by digital analog converter via PC serial port is an easy way. However, anomaloscope needs balanced control of primaries brightness, which could result in sophisticated schematics. To solve both problems we used microcontroller which allows to control up to 6 LEDs at same time with different PMW (pulse – width modulation) frequencies.

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MULTISPECTRAL ANALYSIS OF COLOR VISION DEFICIENCY TESTS[*]

S. Fomins, and M. Ozolinsh

Color deficiency tests are usually produced by means of polygraphy technologies and help to diagnose the type and severity of the color deficiencies. Due to different factors, as lighting

conditions or age of the test, standard characteristics of these tests fail, thus not allowing diagnosing unambiguously the degree of different color deficiency. Multispectral camera was used to acquire the spectral images of the Ishihara and Rabkin pseudoisochromatic plates in the visible spectrum. 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.
Spectral data was converted to cone signals, and successive mathematics applied to provide a simple simulation of the test performance. Colorimetric data of the each pixel of the test image can be calculated and distribution of color coordinates is presented. 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.
[*] *In cooperation with Optometry and Vision Science Department, University of Latvia.*

Lectures on Conferences

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69th Conference of University of Latvia. Riga, Latvia, January – March, 2011.

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2. A.Voitkāns, L. Dimitročenko, S. Bartling, K. Kundziņš, P. Kūlis. III grupas nitrīdu un to cieto šķīdumu nanostruktūru sintēze ar MOCVD metodi un to klasificēšana. Programma, 73. lpp.
3. O. Vilītis, M. Rutkis, K. Kundziņš, V. Zauls. Iekārta funkcionālu nanodiegu klājumu izgatavošanai. Programma, 73. lpp.

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5. V. Karitans, M. Ozolins, and K. Luse. Dependence of Wavefront Aberrations on Spectral Properties of Shack-Hartmann Wavefront Sensor. Book of Abstracts, p. 102.
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2. V. Karitans, and M. Ozolinsh. Vernier Acuity as a Function of Higher-Order Ocular Aberrations. Abstracts, p. 68.
3. S. Fomins, and U. Atvars. After-Images In Chromoluminance Space.
4. E. Skutele, and V. Karitāns. Producing of Ray Tracing Aberrometer for Studying Wavefront Deformations. Abstracts, p. 70.
5. M. Leontjeva, and G. Ikaunieks. Visual Acuity Improving With Methods Based on Perceptual Learning.
6. Z. Meskovska, and G. Ikaunieks. Effect of Straylight on Electroretinographic Response.
7. R. Trukša, and S. Fomins. Rayleight Equation Anomaloscope From Commercially Available LEDs. Abstracts, p. 86.
8. I. Zakutajeva, and S. Fomins. Wetting Angle of New and Worn Contact Lenses Identified by the Sessile Drop Technique.

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1. I.Smeltere, M.Antonova, M.Livinsh, and B.Garbarz-Glos. Electrical and mechanical properties of KNN based lead-free ceramics. Abstract No.103/353 (1078).
2. M. Palatnikov, O. Shcherbina, K. Bormanis, A. Frolov, N. Sidorov, and I. Smeltere. Thermo-Resistant Ceramic Coatings of Containers for Thermo-Chemical Treatment of High Purity Niobium Compounds. Abstract No.103/1180 (2273).

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1. M.N. Palatnikov, A.N. Salak, K. Bormanis, O.B. Scherbina, V.V. Efremov, N.V. Sidorov, I.N. Efremov, and N. Mironova-Ulmane. Structure and Elastic Properties of Sodium Niobate Ceramics Prepared at High Pressure. Abstract Tu3-31.
2. M.N. Palatnikov, K. Bormanis, V.V. Efremov, N.V. Sidorov, I.N. Efremov, and N. Mironova-Ulmane. Dielectric Properties of Lithium-Sodium Tantalate-Niobate Solid Solutions. Abstract Tu3-32.
3. K. Bormanis, A. Kalvane, A.I. Burkhanov, I.E. Tumanov, and N. Mironova-Ulmane. Dielectric properties of PMN+2%Li_2O at low and infra-low frequencies.Abstract Tu3-33.

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1. С.Н. Каллаев, З.М. Омаров, Р.Г. Митаров, А.Р. Билалов, К. Борманис, С.А. Садыков. Теплофизические свойства сегнетоэлектриков на основе цирконата-титаната свинца. Тезисы докладов, с. 28.
2. И. Смелтере, М. Антонова, А. Калване, К. Борманис, М. Ливиньш. Синтез и диэлектрические свойства твердых растворов легированных ниобатов калия и натрия. Тезисы докладов, с. 124.
3. А.И. Бурханов, А.М. Сережкин, К. Борманис, А. Калване. Диэлектрические свойства ферримагнитной керамики $Pb(Fe_{1/2}Ta_{1/2})O_3$ в широкой температурной области. Тезисы докладов, с. 129.
4. А.И. Бурханов, И.Е. Туманов, К. Борманис, А. Калване. Влияние примеси лития на низко- и инфранизкочастотные диэлектрические свойства керамики магниобата свинца. Тезисы докладов, с. 131.

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1. M. Palatnikov, O. Shcherbina, K. Bormanis, V. Sandler, and N. Sidorov. Formation of a Stoichiometric Layer and a New Polar Phase at Vapour Transport Equilibration of Lithium Tantalate Single Crystals. Abstract P9-4.
2. N.V. Sidorov, M.N. Palatnikov, D.V. Evstratova, and K. Bormanis. Features of the Patterns Emerging at Irradiation of Congruent Photo-Refractive Lithium Niobate Crystals. Abstract P9-13.
3. M. Dunce, E. Birks, M. Antonova, M. Kundzinsh, V. Zauls, and A. Sternberg. Electrocaloric Effect in $N_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ Solid Solutions. Abstract P3-2.
4. R. Grigalaitis, J. Banys, E. Tornau, D. Kiselev, I. Bdikin, A. Kholkin, K. Bormanis, and A. Sternberg. Visualization of Nanodomains in PMN-PT Ceramics by Piezoresponse Force Microscopy. Abstract P3-9.
5. Š. Svirskas, M. Ivanov, Š.Bagdzevičius, J. Banys, M. Dunce, M. Antonova, E. Birks, and A. Sternberg. Broadband Dielectric Spectroscopy of $0.4Na_{1/2}Bi_{1/2}TiO_3$ – $(0.6\text{-}x)SrTiO_3$ – $xPbTiO_3$ Solid Solutions. Abstract P3-12.
6. S. Bagdzevicius, R. Grigalaitis, J. Banys, A. Sternberg, and K. Bormanis. Broadband Dielectric Investigation of Sodium Potassium Niobate Ceramic Doped 8% of Antimony. Abstract P3-14.
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8. K. Bormanis, A. Kalvane, A.I. Burkhanov, and A.M. Serezhkin. Dielectric Nonlinearity in $Pb(Fe_{1/2}Ta_{1/2})O_3$ Ceramics. Abstract P3-30.
9. I. Smeltere, A. Kalvane, M. Antonova, and M. Livinsh. Microstructure and Electrical Properties of Ta-Substituted KNN Lead-Free Ceramics. Abstract P6-11.

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1. M. Dunce, E. Birks, M. Antonova, and M. Kundzinsh. Electric Field Dependence of Dielectric Permittivity and Polarization in Some Relaxors with Perovskite Structure. Abstracts, P72.
2. K. Luse, A. Pausus, M. Ozoliņš, and V. Karitans. Evaluation of Commercial Retroreflector Optical Properties. Abstracts, P38.

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Vilnius, Lithuania, August 28-31, 2011.

1. N.V. Sidorov, A.V. Syuy, M.N. Palatnikov, and K. Bormanis. Photo-Refractive Light Scattering and Photorefraction in Ferroelectric Lithium Niobate Single Crystal. Abstracts, p. 18.
2. M. Palatnikov, K. Bormanis, O. Shcherbina, V. Sandler, N. Sidorov, and I. Efremov. Development of a Layers and a Polar Phases at Vapour Transport Equilibration of Lithium Tantalate Crystals. Abstracts, p. 19.
3. E. Skutele, and V. Karitans. Producing of Ray Tracing Aberrometer for Studying Wavefront Deformations. Abstracts, p. 48.
4. K. Luse, M. Ozolins, and M. Tukisa. Retroreflection of Warning Sign Materials at Varios Entrance and Observation Angles. Abstracts, p. 58.

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2. N.V. Sidorov, M.N. Palatnikov, V.M. Voskresensky, O.R. Starodub, V.T. Kalinnikov, K. Bormanis, A. Sternberg, E.P. Fedorova, and L.A. Aleschina. Ordering of Structural Units and Cluster Formation in Lithium Niobate Crystals. Proceedings 1, 251-253.
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56. С.Н. Каллаев, К. Борманис. Теплоемкость сегнетокерамики PLZT-9 в области размытого фазового перехода. Актуальные проблемы Физики твердого тела. Сборник докладов Международной научной конференции 18-21 октября 2011 г., Минск, Издатель А.Н. Варксин, 1, 280-282.

57. М.Н. Палатников, В.А. Сандлер, О.Б. Щербина, Н.В. Сидоров, К. Борманис, А. Штернберг. Образование слоев различного состава и новой полярной фазы при обработке монокристаллов $LiTaO_3$ в парах лития. Актуальные проблемы Физики твердого тела. Сборник докладов Международной научной конференции 18-21 октября 2011 г., Минск, Издатель А.Н. Варксин, 1, 335-337.

58. С.А. Садыков, А.Ш. Агаларов, С.Н. Каллаев, С.М. Алиева, К. Борманис. Электролюминесценция керамики $(Pb_{0,91}La_{0,09})(Zr_{0,65}Ti_{0,35})O_3$ с нанополярной структурой. Письма в ЖТФ, 2012, 38, 3, 17-24.

59. С.А. Садыков, А.Ш. Агаларов, С.Н. Каллаев, К. Борманис. Переключение поляризации в релаксорной ЦТСЛ керамике в сильном импульсном электрическом поле. Труды Междунар. симпозиума ODPO-14, Лоо, 2011, 2, 99-102.

60. И.Е. Туманов, А.И. Бурханов, К. Борманис, А. Калване. Влияние Li_2O на характер диэлектрического отклика керамики PMN. Материалы Международной научно-технической конференции, INTERMATIC-2011, Москва, МИРЭА, 2011, 2, 135-138.

Doctor theses

Sergejs Fomins „Shape and Color in Image Recognition", presented 2011.
Varis Karitans „Influence of optical and neural factors on quality ofthe perceived image", submitted.

Dr. phys. Vladimir Pankratov – senior researcher
Dr. habil. phys. Stanislav Chernov – state emeritus
MSc. Liana Shirmane (PhD student) – assistant
MSc. Darja Jakimovica (PhD student) – assistant (until April)

Research Area and Main Problems

Our research interests are focused on investigation optical ant time-resolved luminescence properties of prospective nano- and macroscopic inorganic materials (insulators and semiconductors) in the vacuum ultraviolet spectral range using synchrotron radiation.

International Cooperation

Germany: Prof. Claus Feldmann (Karlsruhe Institute of Technology)
Prof. Heinz von Seggern (Darmstadt University of Technology)
Dr. Joerg Zimmermann (Darmstadt University of Technology)
Dr. Aleksei Kotlov (HASYLAB at DESY (Hamburg))
Denmark: Prof. Arne Nylandsted Larsen (Aarhus University)
Prof. Brian Bech Nielsen (Aarhus University)
Poland: Prof. Wieclaw Strek (Wroclaw)
USA: Prof. Arnold Burger (Fisk University**,** Tennessee)
Prof. R.T. Williams (Wake Forest University, North Carolina)

Scientific visits abroad

Dr. V. Pankratov: Karlsruhe Institute of Technology (Karlsruhe, Germany) (7 days); Aarhus University (Aarhus, Denmark) (1 month); DESY (Hamburg, Germany) (5 weeks), E-MRS Spring Meeting (Nice, France) (1 week), IWASOM-2011 Conference (Gdansk, Poland) (1 week).

L. Shirmane: DESY (Hamburg, Germany) (5 weeks), IWASOM-2011 Conference (Gdansk, Poland) (1 week).

Scientific publications

1. V. Pankratov, A.I. Popov, L. Shirmane, A. Kotlov, C. Feldmann, $LaPO_4$:Ce,Tb and YVO_4:Eu nanophosphors: Luminescence studies in the vacuum ultraviolet spectral range, J. Appl. Phys. 110 (2011) 053522 (7 pages)
2. V. Pankratov, V. Osinniy, A. Nylandsted Larsen, B. Bech Nielsen, Si Nanocrystals in SiO_2: Optical Studies in the Vacuum Ultraviolet Range, Phys. Rev. B, 83 (2011) 045308 (5 pages)
3. V. Pankratov, A.I. Popov, A. Kotlov, C. Feldmann, Luminescence of Macro- and Nanosized $LaPO_4$:Ce,Tb Excited by Synchrotron Radiation, Optical Materials, 33 (2011) 1102-1105
4. A. Kalinko, A. Kotlov, A. Kuzmin, V. Pankratov, A.I. Popov, L. Shirmane, Electronic Excitations in $ZnWO_4$ and $Zn_xNi_{1-x}WO_4$ using VUV Synchrotron Radiation, Cent. Eur. J. Phys. 9 (2011) 432-437
5. E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, D. Engers, Polar nanoregions in $Pb(Mg_{1/3}Nb_{2/3})O_3$(PMN): insights from suprcell approach, Cent. Eur. J. Phys. 9 (2011) 438-445

6. E. Klotins, A.I. Popov, V. Pankratov, L. Shirmane, D. Engers, Numerical evidences of polarization switching in PMN type relaxor ferroelectrics, Integrated Ferroelectrics, 123 (2011) 32-39

Presentations at scientific conferences, congresses, meetings, schools and workshops

I. ISSP Conference (Riga, Latvia, February, 2011)

1. V. Pankratov, A.N. Larsen, B.B. Nielsen, ZnO nanocrystals/SiO_2 multilayer structures fabricated by RF-magnetron sputtering, Abstracts p. 42.
2. V. Pankratov, V. Osinniy, A.N. Larsen, B.B. Nielsen, Si nanocrystals in SiO_2: Optical studies in the vacuum ultraviolet range, Abstracts p. 43.
3. V. Pankratov, A.I. Popov, S.A. Chernov, C. Feldmann, Mechanism for enrgy transfer processes between Ce^{3+} and Tb^{3+} in $LaPO_4$:Ce, Tb nanocrystals by time-resolved luminiscence spectroskopy, Abstracts, p. 44.
4. V. Pankratov, L. Shirmane, A.I. Popov, A. Kotlov, C. Feldmann, Luminescence of nano- and macrosized $LaPO_4$:Ce,Tb excited by synchrotron radiation, Abstracts p. 45.
5. V. Osinniy, V. Pankratov, A.N. Larsen, B.B. Nielsen, Vertical charge-carrier transport in Si nanocrystal/SiO2 multilayer structures, Abstracts p. 46.
6. L. Shirmane, V. Pankratov, A.I. Popov, A. Kotlov, C. Feldmann, Luminescnece properties of YVO_4:Eu^{3+} nanocrystals under synchrotron radiation, Abstracts p. 47.
7. L. Shirmane, V. Pankratov, W. Strek, W. Lojkowski, Peculiarities of luminescent properties of cerium doped YAG transparent nanoceramics, Abstracts p.48.

II. International conference "Functional materials and nanotechnologies" FM&NT-2011 (April 05-08, 2011, Riga, Latvia)

1. I. Karbovnyk, V. Lesivtsiv, I. Bolesta, S. Velgosh, I. Rovetsky, V. Pankratov, A.I. Popov Optical Properties of BiI_3 Nanoclusters Embedded in CdI_2 Layered Crystals, Abstracts), Book of Astracts p. 116.
2. A.I. Popov, V. Pankratov, D. Jakimovica, E. Klotins, L. Shirmane, A. Kotlov, Luminescence Properties of $BaZrO_3$ under Synchrotron Radiation, Book of Abstracts, p. 117.
3. A.I. Popov, V. Pankratov, V. Bratus, A. Kotlov, Electronic Excitation and Luminescence of 3C-SiC Pure and Neutron Irradiated Silicon Carbide, Book of Abstracts, p. 118.
4. A.I. Popov, V. Pankratov, A. Lushchik, E. Klotins, L. Shirmane, V.E. Serga, L.D. Kulikova, A. Kotlov, VUV Luminescence of MgO, Book of Abstracts p. 119.
5. P.V. Savchyn, V.V. Vistovskyy, A.S. Voloshinovskii, V. Pankratov, A.I. Popov, A. Kotlov, Luminescence of Eu^{2+}-doped $LaCl_3$ microcrystals incorporated in the NaCl host, Book of Abstracts p. 122.

III. E-MRS Spring Meeting (Nice, France) (May 2011)

1. V. Pankratov, A.I. Popov, E.A. Kotomin, Polarons in Complex Oxides, E-MRS Spring Meeting, Abstracts: L2-15.
2. A.I. Popov, E.A. Kotomin, V. Pankratov and J. Maier, Generalization of Rabin-Klick diagram for a whole family of alkali halides, E-MRS Spring Meeting, Abstracts: L2-16

IV. NATO Advanced Research Workshop: Nanodevices and Nanomaterials for Ecological Security, Jūrmala, Latvia, (June 2011)

1. V. Pankratov, A.I. Popov, L. Shirmane, A. Kotlov, C. Feldmann, Luminescence properties of nanosized phosphors under synchrotron radiation.
2. A.I. Popov, V. Pankratov, L. Shirmane, A. Kotlov, Synchrotron radiation studies on luminescence properties of macro- and nanosized $MgAl_2O_4$.

V. International Workshop of Advanced Optical Materials (IWASOM) 2011, Gdansk, Poland, (July 2011)

1. V. Pankratov, L. Shirmane, A.I. Popov, A. Kotlov, C. Feldmann, Luminescence properties of $YVO_4:Eu^{3+}$ nanocrystals under synchrotron radiation, Book of Abstracts p. 63.
2. V. Pankratov, L. Shirmane, A.I. Popov, A. Kotlov, P. Glohowski, W. Strek, Luminescence of $MgAl_2O_4:Cr^{3+}$ nanocrystals under synchrotron radiation, Book of Abstracts p. 84.

The Main results

Si NANOCRYSTALS EMBEDDED IN SiO_2: LUMINESCENCE PROPERTIES IN THE VACUUM ULTRAVIOLET SPECTRAL RANGE

V. Pankratov
V. Osinniy A. Nylandsted Larsen, B. Bech Nielsen (Aarhus University, Denmark)
A. Kotlov (HASYLAB at DESY, Germany)

The huge interest in silicon nanocrystals (Si NCs) during more than 10 years is caused by their unique fundamental physical properties and their promising applications. In the present study the optical and luminescence properties of Si NC in the UV-VUV spectral range were studied with pulsed synchrotron radiation from the DORIS III storage ring of DESY (Hamburg, Germany). The SUPERLUMI experimental station of HASYLAB was used for the measurements of emission, excitation and transmission spectra.

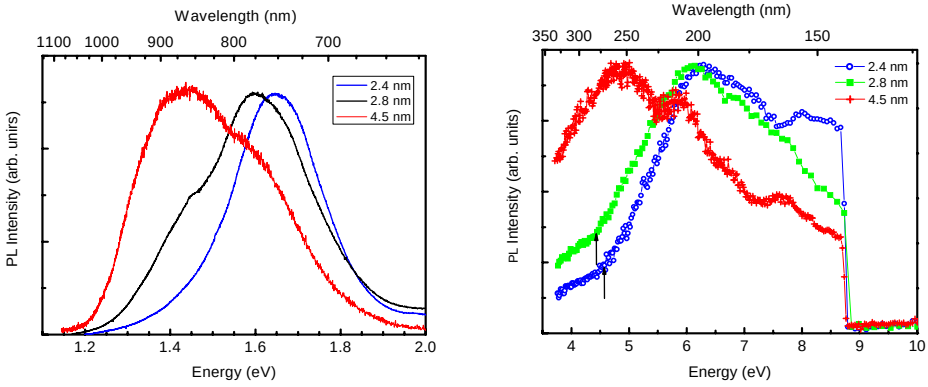


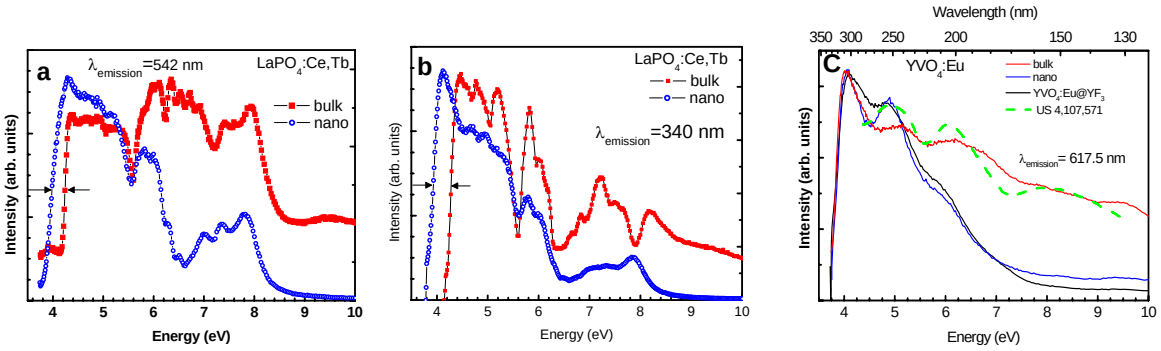
Fig.1: PL spectra for Si NCs with different diameters under 150 nm (8.27 eV) excitation at 8 K (left). PL excitation spectra for Si NCs with different diameters are depicted in the right graph [V. Pankratov et al., Phys. Rev. B **83** (2011) 045308].

The dependence of the photoluminescence excitation spectra on the nanocrystals size was experimentally established for the first time (Fig.1). It is shown that the photoluminescence excitation and absorption spectra are significantly blueshifted with decreasing Si nanocrystal size. A detailed comparison of photoluminescence excitation and absorption spectra with data from theoretical modeling has been done. It is demonstrated that the experimentally determined blueshift of the photoluminescence excitation and absorption spectra is larger than the theoretical predictions. The influence of point defects in the SiO_2 matrix on the optical and luminescence properties of the embedded Si nanocrystals was clearly established and demonstrated. Moreover, it is demonstrated that no energy transfer takes place between the SiO_2 and Si nanocrystals when the excitation energy is higher than the band-to-band transition energy in SiO_2.

$LaPO_4$:Ce,Tb AND YVO_4:Eu NANOPHOSPHORS: LUMINESCENCE STUDIES IN THE VACUUM ULTRAVIOLET SPECTRAL RANGE

V. Pankratov, L. Shirmane, A.I. Popov
A. Kotlov (HASYLAB at DESY, Germany)
C. Feldmann, (Karlsruhe Institute of Technology, Germany)

Comparative analysis of the luminescent properties of nanocrystalline $LaPO_4$:Ce,Tb and YVO_4:Eu luminescent materials with macrocrystalline analogues, commercially produced by Philips, has been performed under excitation by pulsed vacuum ultraviolet (VUV)



synchrotron radiation, ranging from 3.7-40 eV. Special attention was paid to VUV spectral range, which is not reachable with commonly used lamp and laser sources.
Fig. 2. Comparison of excitation spectra of Tb^{3+} (a) and Ce^{3+} (b) emissions for bulk and nanosized $LaPO_4$:Ce,Tb. Excitation spectra of Eu^{3+} emission in the bulk, nanosized, and nanosized YF_3-covered YVO_4:Eu at 10 K in 3.5–10 eV (c) spectral range [V. Pankratov et al., J. Appl. Phys. 110 (2011) 053522].

It was demonstrated that nanoparticles' surface can drastically change emission and excitation spectra of nanopowders, comparing with corresponding bulk materials (Fig 2.). Especially significant distinctions between excitation spectra for nano and bulk materials were observed under relatively high energy excitation (exceeding 10 eV). It was suggested that surface-related loss processes, namely electron-hole pairs' non-radiative annihilation at the surface, are responsible for the suppression of energy transfer processes from the host lattice to impurity ions and, subsequently, for rare-earth emission degradation under high energy excitations in nanosized materials.

DEPARTMENT OF SEMICONDUCTOR MATERIALS

SEMICONDUCTOR MATERIALS

AND SOLID STATE IONICS

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, electron-beam technology
- Material characterization by spectroscopic methods (Raman scattering, FTIR spectroscopy, optical and X-ray absorption, EXAFS, XANES), electrical and electrochemical impedances, AFM, TGA/DTA, etc
- Solid state ionics:
  - electro-, photo-, thermo-, chemo- or gaso-chromic phenomena in transition metal oxides
  - structural changes due to ion intercalation
  - lattice dynamics and structural and electronic phase transitions
  - solid state reactions at interfaces electrode – solid electrolyte
  - gases and ions sensing phenomena and detection technologies
- Functional coatings and multi layer electrochemical systems
- Hydrogen absorption phenomena in metals, semiconductors and insulators
- Development of hydrogen generation equipment and new nano structured materials for hydrogen storage
- New measurement technologies and instruments with artificial intellect (encl., eNose)
- Development methods and techniques for quality and reliability testing for lead –free joints of PCB
- Hydrogen technologies (production, storage, transportation, application); renewable energy technologies (solar, wind, static electricity, water, microbial fuel cells);
- Development of cathode materials for Lithium thin film batteries;
- Gas sensors and sensor arrays; odour recognition and removal with adsorbent and low temperature plasma discharge technologies.
- Tritium analysis

Research Topics

- Ion transfer in solids, over two phase interfaces and composites as well as structural changes due to ion intercalation, lattice dynamics and structural and electronic phase transitions.
- Ion transfer problems related to electro-, photo-, chemo-, thermo-chromic phenomena in transition metal oxides as well as to solid state reactions at interfaces electrode – solid electrolyte.
- Application of electrical and electrochemical impedances for characterization of ionic systems, nanostructured and porous materials, composites.
- Development of nanostructuring methods for functionalization of plate glass and fiber glass surfaces as well investigation influence of ultrasound on leaching processes, pores structure and ion exchange of glass fibers.
- Application of thermal analyses (TGA/DTA) and sorptometry for investigation of porous materials and absorbing capacity of functional species.
- Investigation of stability of materials for electrochemical multi layer systems and electrochromic coatings as well as intergrain activity in solid electrolyte layers based on polymer composites.
- Development methods and techniques for functilization
- 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 transport and stationary applications; for energy storage and electricity/heat generation; synthesis and research of new materials for hydrogen technologies (electrodes in electrolysers and microbial fuel cells, structured nanomaterials for photoelectrolysis, hydrogen storage media, polymer membranes and membrane-electrode assemblies for fuel cells);
- Lithium intercalation materials and their application for thin film rechargeable battery; the technologies for electricity generation from renewables (solar, wind, static electricity, water, algae and microorganisms);
- Gas sensors and sensor arrays for gas and odour monitoring; odour recognition and removal with adsorbents and ozone technologies; development of technologies .
- Investigations of tritium release properties of neutron-irradiated beryllium.
- Development of innovation technology for producing of solar silicon using electron-beam technology
- Mathematical modeling of silicon melting by electron beam

Scientific staff:	Technical staff:	Postgraduate students:	Students:
1. Dr. phys. A.Azens	1. K. Alsbergs	1. A. Anspoks	1. P. Aizpurietis
2.Dr.chem. G. Bajars	2. J. Balodis	2. I. Dimanta	2.. A. Ēcis
3. Dr.phys. G.Chikvaidze,	2. L. Jēkabsons	3. J. Dimants	3. A. Gruduls
4. Dr.phys. J.Gabrusenoks	4. A. Kursitis	4. I. Dirba	4. R.Janeliukštis
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6. Dr.phys. J. Hodakovska	6. K.Vilnis	6. J. Timoshenko	6. A. Krūmiņa
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11.. Dr.phys A.Kuzmins			11. A. Šivars
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13. Dr.phys. E.Pentjuss			13. L.Veļķere
14. Dr.hab.phys. J.Purans			13. A. Zīle
15. Dr.phys. V.Ogorodņiks			14.J.Zandersons
16. Dr.chem. G.Vaivars			15. M.Zubkins
17. Dr.chem. A.Vitins			

Laboratories of Semiconductor Material Department

Laboratory of Solid State Ionics – Head of Laboratory Dr. phys. A.Lusis

Laboratory of EXAFS Spectroscopy – Head of Laboratory Dr. hab. phys.J.Purans

Laboratory of Hydrogen and Gass Sensors – Head of Laboratory Dr.J.Klepers

Cooperation

Latvia

7. University of Latvia (LU):
   - Faculty of Physics and Mathematics.
   - Faculty of Chemistry (Dr. A.Vīksna) &
   - Faculty of Biology (Prof. I.Muiznieks)
   - Faculty of Medicine
   - Faculty of Economics and Management (Prof. B.Sloka)
   - Institute of Chemical Physics (Dr. G. Kizane)
3. Riga Technical University (RTU):
   - Institute of Silicate Materials (Prof. G.Mežinskis).
   - Institute of Inorganic Chemistry (Dr. J. Grabis, Dr. E.Palcevskis, Dr. A. Dindune)
   - Institute of Idustrial Electronics and Energetic (Prof. L.Ribickis).
   - Institute of Textile Material Technologies and Design (Prof. I.Baltiņa)
   - Institute of Biomaterials and Biomechanics (Dr. I.Lasenko)
4. Latvia University of Agriculture, Research Institute of Agricultural Machinery,
5. Institute of Physical Energetics, Riga
6. Latvian Electrical Engineering and Electronics Industry Association (LEtERA)
7. Latvian Electroindustry Business Innovation Centre (LEBIC).
8. Latvian Association for Textile and Clothing Industry
9. Latvian Hydrogen Association

10. Housing and Environment Department of Riga City Council, Riga,
11. JSC “Valmiera Glass Fiber”
12. JSC “Sidrabe”
14. JSC „Riga Electric Machine Building Works”,
13. SIA „EMU PRIM”,
14. SIA “Adviser Union”
15. IC „Plazma PL”,

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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. Dipartimento di Fisica, Università di Trento (Trento, Italy).
2 IFN-CNR, Institute for Photonics and Nanotechnologies, Section "ITC-CeFSA" of Trento, Italy.
3 Università della Calabria (Arcavacata di Rende, Italy).

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

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.

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

Ukraine
State Scientific Recearch Institute “HELIUM”, Vinnitsa, Ukraine – Dr. V. Panibratskiy

Participation in Research Projects:

Latvian:
1. ESF Project "Nanomaterials for perspective energy effective solutions", No. 2009/0202/1DP/1.1.1.2.0/09/APIA/VIAA/141 (2009-2013).

2. ESF Project "Nanomaterials for perspective energy effective solutions", No. 2010/0272/2DP/2.1.1.2.0/09/APIA/VIAA/088 (2010-2013).

3. ERDF project Nr.2010/0243/2DP/2.1.1.1.0/10/APIA/VIAA/156, subproject "Vacuum coatings for solar energy collector" (2011-2013).
4. ERDF project „Development of innovation technology for producing of solar silicon using electron-beam technology" Nr.2010/0245/2DP/2.1.1.1.0/10/APIA/VIAA/114 (2010-2013)..

5. ERDF project "Innovative glass coatings" No. 2010/0272/2DP/2.1.1.1.0/10/APIA/VIAA/088 (2010-2013).

7. National Research Program "Innovative multifunctional materials, signal processing and informatic technologies -IMIS", task No. 1.21 – Investigation functionalization of glass fiber fabrics.

8. 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"

9. 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", subproject No.1.4. "Functional caoatings, processes and technologies for modification physicochemical properties of materials**"**

10. 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", subproject "Funcionalization flax and hemp fibers with metal an metal oxides coatings".

11. Grant from Latvian Council of Science Nr.09.1580 "Structure of nano-oxide materials and self-organization in stochastic media.

12. 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"

13. 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"

14. Grant from Investment and Development Agency of Latvia "Development and pilot-project implementation on eco-effective transport system in Latvia"

15. Grant from Riga City Council and SwedBank "Hydrogen based heater for vehicle salon and engine"

16. Grant from Student Council of University of Latvia "Synthesis and properties of TiO2 oriented nanotube layer"

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).

3. The European joint undertaking “Fusion for Energy” (F4E) work programme 2009 “Test Blanket Modules”. Contract reference: F4E-2009-GRT-030 Action 3. Coordinator at the University of Latvia: Gunta Kizane.

4. JET Fusion Technology programme. Field: Plasma facing components. Task No.: JW9-FT-3.46. Task title: “Analysis of tritium distribution in plasma facing components”. Deliverable D3 “The tritium release from untreated plasma exposed tiles under the simultaneous action of temperature, radiation and magnetic field”. Principal investigator: Dr.chem. Gunta Ķizāne.

Didactic work at the University of Latvia

1. Course Fizi5028 "Structure and Description of Nanomaterials" at the Latvian

University (A.Kuzmin).

2.Course Fizi7009 „Solid State Structure” at the Latvian University (A.Kuzmin).

3. Supervision (A.Lusis) of student Rims Janeliukštis (Faculty of Physics and mathemativs, University of Latvia) for a bachelor’s thesis on the topic “Modification of physical and chemical properties of glass fibers“, the bachelor’s thesis was defended in June 2011.

4. Supervision (A.Lusis) of student Janis Zandersons (Faculty of Physics and mathematics, University of Latvia) for a bachelor’s thesis on the topic “Methods and processes for functionalization textile fibers“, the bachelor’s thesis was defended in June 2011

5. Supervision of student Andris Matīss (Faculty of Chemistry, University of Latvia) for a bachelor’s thesis on the topic “Tritium release from neutron irradiated beryllium pebbles under action of temperature”, the bachelor’s thesis was defended in June 2011.

Main results

LATTICE DYNAMICS OF $WOCl_4$

J.Gabrusenoks

The $WOCl_4$ structure consists of pyramidal $WOCl_4$ units which are linked by linear asymmetric O- - - W----O bridges to polymeric $(WOCl_4)_n$ chains. The vibrational modes of $WOCl_4$ have been investigated. Calculations have been performed by using hybrid exchange density functional theory to determine equilibrium geometries and phonon frequencies. The Grimme dispersion correction for energy and gradient has been used in combination with B3LYP functional. The CRYSTAL09 computer code was used.

Experimental and calculated values of lattice constants and phonon frequencies are:

	Lattice constants,A		Phonon frequencies,cm^{-1}		
	a	b	Libration of chains	W - Cl	W - O
experiment	8,48	3,99	70	400	877
calculation	8,53	3,95	85	409	845

METAL COATINGS ON FABRICS FOR TECHNICAL APPLICATIONS

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

Metal coatings are widely used for functionalization of fabrics for different technical applications. The fabrics are porous medium versus plastic films, foils or sheets. The porous media usually adsorbs various chemical substances from the environment. One of them is water therefore content of moisture in fabrics have to be controlled before functionalization.

The electrical impedance spectroscopy is good method to study water in fabrics. The impedance spectra of system M/F/M are complicate due to heterogeneous constitution of system. There are problems with interpretation impedance data. There is need for appropriate physical models too. One way to solve the problem is to find relations between the systems M/F/M constitution, pore and metal type and the content of moisture.

In present work both sides of glass (GF) and flax (FF) fabrics were coated with metal (M = Ni, Cu or Al) and electrical impedance spectra of the systems M/F/M were studied. The leaching of glass fibers have been used to obtained porous fibers and fabrics on the micro and nano level. The flax fibers and fabrics are natural porous. Fabrics were coated with metal (Ni, Cu or Al) by DC magnetron sputtering in 100% Ar atmosphere.

Impedance analyzer HP 4194A with dielectric test fixture HP 16451B (electrode area S= 11.3 cm^2) was used.. The impedance spectra of metal coated fabrics are senstive to moisture and depend on content of absorbed water (Fig.1).

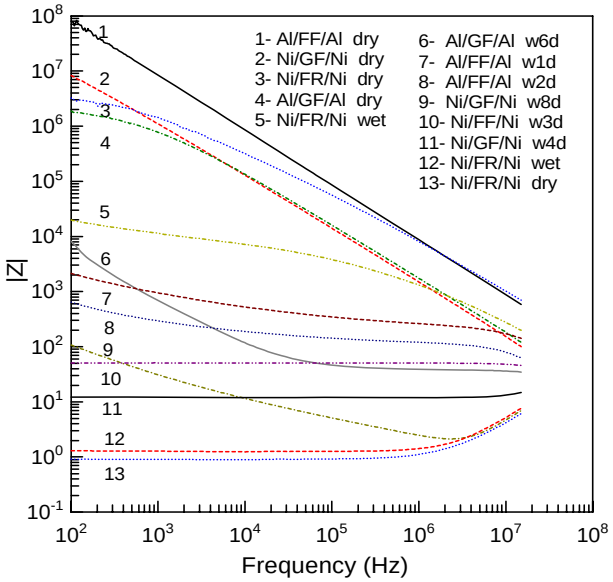

Fig.1. Impedance spectra of metal coated glass and flax fabrics (GF; FF) and foam rubber (FR) sheets. Number in curve labels (w1d-w8d) is number of days for sample in chamber with RH=100%.

Regardless of whether impedance |Z| value is big or small for the freshly made sample the absorption of water can reduce or increase the |Z| values. The deposited metal particles in porous surface formed electronically conducting channels with some percolation threshold, which could be changed by concentration and size of metal particles and water content. H_2O

molecules separate metal particles and provide ionic conductivity.Further more detailed studies for functionalization of nanostructured technical glass fibers and fabrics with metal coatings are required to explain how adsorbed H_2O 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.

SYSTEM FOR TEST OF THERMO-MECHANICAL PROPERTIES OF GLASS AND HEMP YARNS

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

For the development of new products based on technical textiles, which will be functionalized by vacuum coating technologies, is important test influence of functionalization technology on thermo-mechanical properties of textile yarns.
For that the system for test of thermo-mechanical properties of glass, flax and hemp yarns was build on instrument "*Mecmesin* model "MultiTest 1-*i*" with software EMPEROR" base. The temperature of furnace (Fig. 2) is ccontroled with Fuji Electric Micro-controller PXR3.
System specification:

- The long of yarn or test have been 20 cm.
- Load/force up to 250 N
- Maximal tension speed 500 mm/s
- Temperature 20 – 700 ^{0}C.

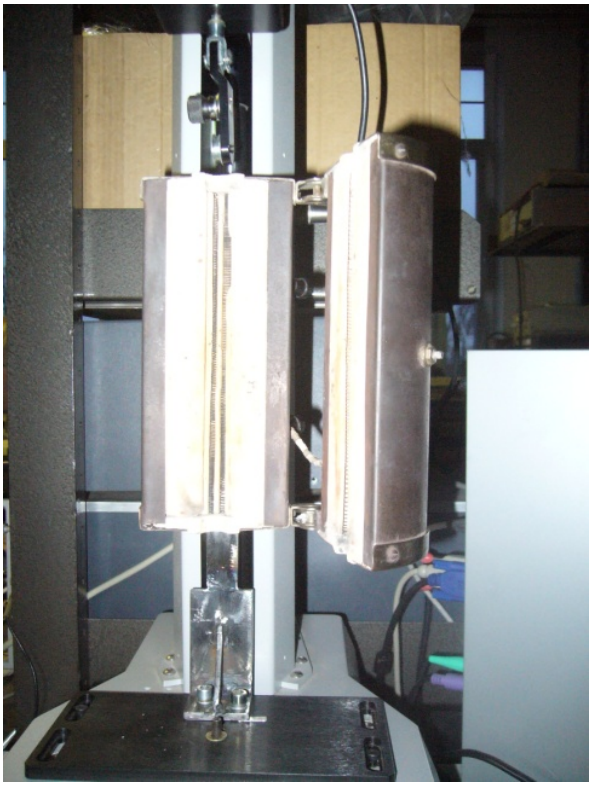

Fig.2. Yarn thermo-mechanical test system

PREPARATION OF TiO_2 THIN FILMS BY PARTICULATE SOL-ELECTROPHORETIC DEPOSITION

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

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

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

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

Obtained TiO_2 thin films were characterized by phase composition, morphology and their microstructures using X-ray diffraction, Raman spectroscopy, as well as transmission electron microscopy and scanning electron microscopy.

This work was financially supported by European Regional Development Fund project No.2010/0243/2DP/2.1.1.1.0/10/APIA/VIAA/156.

RESEARCH AND DEVELOPMENT OF MATERIALS AND DEVICES FOR HYDROGEN ENERGY TECHNOLOGIES

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Using inductive voltage pulses to power electrolysis cell allows reducing the total power necessary for electrolysis [1]. A great advantage of the proposed pulse electrolysis is that the charging of electrolytic cell lasts for a relatively shorter period than the following discharge using stored energy. Square pulses from the generator were applied to the field transistor connected in series with the DC power source. The end front of rectangular signal in the secondary winding of bifilarly wound transformer induced very sharp inductive pulse with high amplitude and opposite polarity with respect to applied voltage. Pulse of induced reverse voltage (the width <1 microsecond, amplitude 3-300 V) is passed through the blocking diode to the electrolytic cell. Results showed that the current pulse direction changes from negative to positive with the increasing concentration of electrolyte. The authors believe that such kinetics can occur when the electrochemical charging process in the cell is separated from a Faradic charge transfer process. At applying a sharp pulse the water electrolysis cell behaves as a capacity with a high Q-factor, while the Faradic discharge manifests itself by a discharge tail, when the power stored during cell charging in short pulse is used.

Our research with biohydrogen production is directed to find and test applicable bacterial isolates and different local substrates for hydrogen production. Experimental reactor test-system is built with separate glass chambers for simultaneous measurements of gases in liquid phase (hydrogen and oxygen) and gas phase (hydrogen, methane, carbon dioxide) to determine hydrogen production rate in fermentation process. Parallel gas analysis is made with the RGAPro-100 mass-spectrometer connected to the experimental test-system. Experiments were made with different isolates: *Aneurinibacillus aneurinilyticus, Clostridium sporogenes, Enterobacter asburiae, Enterobacter cloacae, Eubacterium limosum, Kluyvera*

ascorbata, Paenibacillus pabuli (isolates from Microbial Strain Collection of Latvia), E.coli BW25113 hyaB hybC hycA fdoG frdC ldhA aceE::kan (from prof. T.K.Wood, USA). Glucose, lactose and glycerol were used as substrates, concentration varied between 15 to 240 mM. After fermentation processes following results were obtained in liquid and gaseous phase: Escherichia coli BW25113 hyaB hybC hycA fdoG frdC ldhA aceE::kan produced hydrogen with rate 3 mmol/L/h, using 30mM glucose as substrate and 0, 04 mmol/L/h, using 60 mM lactose as substrate in gaseous phase. Clostridium sporogenes produced 1,5 mmol/L/h hydrogen in gaseous phase and 1,42 mmol/L/h hydrogen in liquid phase using 240 mM glycerol as substrate.

For successful hydrogen storage purposes the great concern is the development of materials, including zeolites, in which hydrogen might be stored without high energy consumption. Our research is focused on hydrogen adsorption facilitated with spillover from catalyst sites porous oxide substrate. The spill-over of hydrogen involves a transfer of electrons to acceptors within the support; this process modifies the chemical nature of the support and can also activate a previously inactive material and/or induce subsequent hydrogen physisorption. Sievert type and thermogravimetric measurements of zeolite/Pd and glass/metal hydride (MH) samples proved that the created composite material absorbs more hydrogen per weigh unit than both components separately. Unexpected observation was the deeper hydrogen absorption is induced in metal alloy, due contact between metal alloy and oxide material substrate – not only α and β hydride phases are reached, but also phase. Using the method of cooling the zeolite samples in the hydrogen atmosphere, it is found that values of 3-5 wt% of stored hydrogen can be easily achieved. We are looking for an explanation of this effect.

Latvian Hydrogen Association (LHA) was established on 2005 with aims to disseminate the ideas and conceptions about hydrogen economy between politicians and local municipalities; to promote and support the research, development and education activities in hydrogen energy technologies; to stipulate the realization of hydrogen energy demonstration projects and implementations of innovations in the market, trying to link business and research institutions. Five years experience shows that t is not easy to promote hydrogen technologies in country with proportion of renewable energy resources 30–35% already and with goal to increase them to 40% by 2020. LHA is trying to join hydrogen and renewable energy technologies in research, education and innovation activities. If all is clear in the science and topical areas of hydrogen related researches, then go to education issues is more difficult – necessary to teach not only children and students, but also politicians, government officials, businessmen and even traditional engineers from energy branch. Therefore LHA is organizing now the Latvian Hydrogen and Fuel Cell Technology Platform trying to identify and attract merchants from different companies. LHA is promoting also different innovations, like the use of hydrogen as supplement to fuel for oil saving and reduction of exhausts in vehicles, by organizing the team of researchers from different fields: management, marketing, physics, chemistry and biology to examine the best ways for fuel economy.

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

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Institute of Solid State Physics of University of Latvia;
Ingrida Bremere
Baltic Environmental Forum;
Martins Menniks
City Development Department of Riga City Council;
Arturs Viksna, Agnese Osite, Dmitrijs Pavlicuks
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Air quality in the city of Riga is evaluated from direct monitoring results and from accounting registered air pollutants in the city. It is concluded that from all air polluting substances listed in the European Commission directives, only nitrogen dioxide NO_2 and particulate matter PM10 exceed the limits. In assessing the projected measures to improve air quality in Riga, it can be concluded that the implementation of cleaner fuels and improvements in energy efficiency of household and industrial sectors will decrease particle pollution, but measures in the transport sector will also contribute to reducing air pollution from nitrogen oxides. In assessing the projected measures to improve air quality in Riga, it can be concluded that the implementation of cleaner fuels and improvements in energy efficiency of household and the industrial sectors will give greater effect to decrease air pollution by particles, but the planned measures in the transport sector will contribute to reducing air pollution from nitrogen oxides.

FUNCTIONAL MATERIALS FOR RESISTIVE SWITCHING MEMORIES FP6 MATERA – ERA-NET Materials Project

Project contact person: Dr. habil. phys. J. Purans

The aim of the project is to develop the basic science and technology for new functional ternary oxides for the use as future resistive switching memories at the nanoscale level (20 nm). Since extended defects as dislocations or defect clusters with nanoscale dimensions are considered to be the single resistive switching units in doped ABO_3-perovskites, one has to gain deeper understanding of the complex correlation between defect structure, elementary and defect distribution and switching properties.
Within the project, we indent to solve this challenging task by bundling the research activities of 3 different leading European groups which have a complementary expertise in the field of perovskite materials. The fabrication of $SrTiO_3$ thin films, doped with different transition metals (Fe, Nb) have been performed by Pulsed Laser Deposition in the Forschungs-zentrum Jülich. In order to clarify the spatial distribution of doping atoms, thin films as well as single crystals have been analyzed by means of sophisticated spectroscopic techniques, e.g. synchrotron based x-ray absorption spectroscopy (XAS) by the experimental partner at the Institute of Solid State Physics University of Latvia.
This work has been supported by ab initio calculations of the formation energies of defects and cation segregation by the theoreticians in the Institute of Solid State Physics University of Latvia.
For a given defect/cluster configuration, the resistive switching properties have been investigated in the Jülich group by means of the elaborate electrical characterization as well as by conductive-tip atomic force microscopy. In order to clarify the switching mechanisms,

these investigations have be supported by scanning tunnelling microscopy (STM) with atomic resolution as well as by x-ray photoelectron spectroscopy (XPS) and scanning Auger electron spectroscopy (AES) in the Katowice group.
As a result of intensive research, a microscopic model for resistive switching was develop and a fabrication a thin film device with improved switching performance was proposed.

SOLAR THERMAL ENERGY STORAGE MATERIAL DEVELOPMENT USING THE SOL-GEL AND VACUUM COATING TECHNOLOGY

ERDF Project: 2010/0243/2DP/2.1.1.1.0/10/APIA/VIAA/156

Project manager: G. Mežinskis
Institute of Silicate Materials, Riga Technical University,
Subproject manager: A. Lūsis
Institute for Solid State, University of Latvia,
Subproject manager: J. Kalnačš
Institute of Physical Energetics, Latvian Academy of Sciences,

The project aims to solar thermal energy storage material development based on significantly advanced technology for concentrated solar energy collector (CSEC). The project implementation activities associated with new, innovative CSEC absorption materials and production technologies that will provide alternative energy sources – to use solar radiation more efficiency. Development is based on the enamel and sol-gel technology as well as vacuumtechnology for CSEC collector multilayer coating manufacturing.

ADVANCED GLASS COATINGS

ERDF project Nr. 2010/0272/2DP/2.1.1.1.0/10/APIA/VIAA/088

Project manager: J.Purans

Innovative functional glassy coatings from the standpoint of modern technologies have a potential of novel and unexpected aspects, taking into account new physical properties, which is possible to achieve in the modern manufacturing process via control and manipulation of glassy coating at both macro- and nanoscale. We could mention here antireflective, low heat conductivity, electroconducting and other types of coatings, which play an increasing role in the energy effective applications, solar panels etc. In this Project Institute of solid state physics (Institute) will solve physical and technological problems, and create a new commercial products for export with a high added value.

Many modern energetical devices employ optically transparent coatings produced from electroconducting oxides (TCO) as one of key elements. There emerges a commercial possibility to develop equipment for production of such TCO coatings. Previously such the equipment for production of TCO coatings was based on expensive indium oxide (ITO) as a starting material for production of coatings with a high quality. The Institute wants to develop novel basic technologies, with much cheaper TCO coating production, which could be incorporated into the new coating quipments.

In the framework of the project the Institute plans to develop a new sputtering technology and solution investigations for different TCO materials on the basis of High Power Impulse Magnetron Sputtering (HIMIPS), and to investigate basic industrial operation principles, which could be employed as effective and economically profitable technology in AS „Sidrabe” in order to develop vacuum coating devices. Our Project will result in a

complicated industrial research, in order to clarify a possibility to use HIPIMS sources for sputtering and developing cheap and high quality vacuum coatings.

DEVELOP AN INNOVATIVE TECHNOLOGY FOR SOLAR-GRADE SILICON BY ELECTRON BEAM METHOD

ERDF Project Nr.: 2010/0245/2DP/2.1.1.1.0/10/APIA/VIAA/114
Project manager: G. Chikvaidze

Development of innovative technology to obtain a high purity silicon suitable for production of solar elements is performed in the frame of ERAF Project. Remelting and purification of metallurgical silicon using electron-beam technology have been made. Samples of silicon prepared with this technology were investigated using mass-spectrometry method (ICP-MS), Scaning Electrom Microscope, X-ray difractometer, Raman spectrometer, FTIR spectrometer.

Results: Metallurgical silicon with purity of 4N, produced in Kazakhstan is sufficient for production of Solar grade Silicon if we use the electron-beam technology. Oxidative refining carried out using of electron-beam remelting has significant advantage over merely technology by vacuum EB remelting. This method allows us to get out of silicon with a purity of 4N, the Solar Grade Silicon with purity of 6N (99,9999%) that can be used for Solar energetics. The modelling of the melting process of silicon by electron beam in a water-cooled cruicible have been performed. A simplified model for modeling the melt flow and heat transfer under law –frequency traveling magnetic field influence in the crucible with electron beam heating is described

TRITIUM RELEASE FROM THE PEBBLE-BED ASSEMBLIES NEUTRON-IRRADIATED BERYLLIUM PEBBLES UNDER ACTION OF TEMPERATURE

A. Vītiņš, G. Ķizāne*, A. Matīss*, E. Pajuste*, V. Zubkovs*

* *Institute of Chemical Physics, University of Latvia*

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 (∅≈1 mm) irradiated for 294 full power days from 17 April 2003 to November 2004 to the neutron fluence of $3\text{-}4\times10^{25}$ m^{-2} (E>0.1 MeV) at temperature 523-823 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 β=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_2 of 14-15 L/h. One PBA Be pebble was investigated in each tritium release experiment.

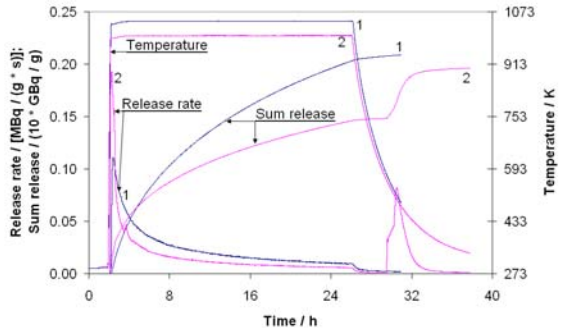

Fig. 1. Tritium release rate and tritium sum release from the PBA Be pebbles heated at the given temperature: curve 1 – a ramp of up to 36 K/min to an anneal temperature of 1043-1045 K; curve 2 – a ramp of up to 41 K/min to an anneal temperature of 999-1001 K. The PBA Be pebbles had the following masses (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 – 0.73, 2.09, 74.8%; 2 – 1.21, 1.96, not determined.

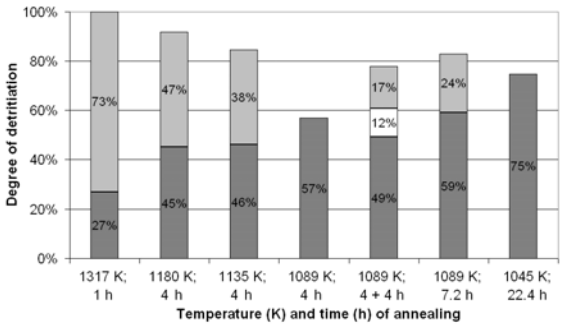

Fig. 2. Degrees of detritiation of the PBA Be pebbles achieved as a result of annealing under the given temperature and time. Series 1 (dark grey) – the degree of detritiation (27-75%) achieved before the start of the burst release. Series 2 (white) - the degree of detritiation (12%) achieved before the start of the burst release in the second annealing. Series 3 (light grey) – the degree of detritiation (17-73%) achieved after the start of the burst release.

Tritium release from PBA Be pebbles on annealing at 1045 and 1000 K for 22.4 h is shown in Fig. 1. The two pebbles investigated under the temperature programmes given in Fig. 1 had quite different tritium release patterns. One noticeable difference is a higher maximum tritium release rate for the pebble annealed at lover temperature (curve 2) than that at higher temperature (curve 1). At 1045 K, no burst release of tritium took place (curve 1). However, after annealing at 1000 K, burst release of tritium took place after cooling down to 560 K (curve 2). The pebble annealed at 1000 K (curve 2) was not dissolved in acid, but was used for microscopy, where it was found that visible cracks were formed and the porosity started to appear in the pebble. Degrees of detritiation achieved on annealing are summarized in Fig. 2. Contributions of the tritium release by atomic diffusion before the burst release and the tritium release after the burst release event are estimated in the total degree of detritiation.

Conclusions:

1. The total tritium inventory in the PBA Be pebbles was found to be 2-4 GBq/g. It may be considered as a reasonable estimation for tritium accumulation in the helium-cooled pebble bed test blanket module (HCPB TBM) Be pebbles for the neutron fluence achieved at the end of PBA irradiation 1.5-2 × 1025 m-2 (E > 1 MeV).
2. Two distinct stages of tritium release – a stage of gradual release and a stage of abrupt release peaks are clearly distinguishable in the tritium release of the PBA Be pebbles on annealing. These two stages may be related to the tritium release by atomic diffusion and bubble venting respectively.
3. Increasing the temperature of the beryllium pebble bed at neutron irradiation from 523-823 K to 1000-1045 K may reduce the tritium inventory in the beryllium pebbles by factor of ≥ 2.

4. Assuming that the tritium release at the end parts of the anneals is limited by diffusion if the burst release is absent, the effective values of the tritium diffusion coefficients were determined for the PBA Be pebbles as 2.6 × 10-13 m2/s for 1045 K and 5.1 × 10-13 m2/s for 1089 K.

Acknowledgement: This study was carried out with EFDA financial support (Technology Task TW5-TTBB-006-D08).

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2. A.Lusis, E.Pentjuss, J.Balodis, R. Janeliukštis, J.Zandersons. Application of metal coatings for functionalization of technical fibers and fabricēs, *Proceedings of the International conference"BalticSilica 2011*" (Riga, Latvia, May 23-25, 2011)
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3. M.Vanags, G.Bajārs, J.Kleperis, A.Lūsis. Procesi uz katoda un anoda ūdens impulsu līdzstrāvas elektrolīzē. Cathode And Anode Behaviour During Pulsed Dc Electrolysis Of Water; Abstracts of the 27th Scientific Conference of Institute of Solid State Physics of University of Latvia, Riga, February 14 – 16, 2011, p. 13;
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14. V. Zubkovs, A. Vītiņš, G. Ķizāne, E. Pajuste, A. Matīss, Comparison of tritium distribution in different neutron irradiated beryllium pebbles. Abstracts of the 27th Scientific Conference of Institute of Solid State Physics of University of Latvia, Riga, February 14 – 16, 2011, P. 75;

2. International Conference FM&NT Functional Materials and Nanotechnologies 2011, ISSP University of Latvia, Riga, April 5-8, 2011. Book of Abstracts:

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2. A.Lusis, E. Pentjuss, J. Gabrusenoks , J. Balodis: Impedance Spectroscopy Use of Flax and Hemp Fiber Functionalization Studies, International Conference "Functional materials and nanotechnologies FM&NT – 2011", April 5 – 8, 2011, Riga, Latvia.
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4. J.Kleperis, J.Linitis, A.Kalis, L.Grinberga. Photo-activity Research of Nano-Structured TiO2 Layers: Influence of Plasmon Light Absorption on Hydrogen Evolution Intensity. Book of Abstracts of International Conference FM&NT Functional Materials and Nanotechnologies 2011, ISSP University of Latvia, Riga, April 5-8, 2011, PO-34, p. 124;
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A.Lusis, E.Pentjuss, J.Balodis, R.Janeliukštis, J.Zandersons: Application of metal coatings for functionalization of technical fibers and fabrics

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1. A.Lusis, E.Pentjuss, G.Bajars, J.Gabrusenoks: Metal coatings on porous glass fiber fabrics for applications in electrochemical devices. Book of abstracts: (P-269).
2. Bajars G., Smits J., Kucinskis G., Kleperis J., Lusis A.: Electrochemical impedance studies of thin film composite LiFePO4/C Book of abstracts: (O-298).

5. 11th International Congress on Hydrogen Production ICH2P-11, Thessaloniki, Greece, June 19-22, 2011; Conference Abstracts Proceedings in CD form:

1. I.Klepere, A.Gruduls, V. Nikolajeva, J. Kleperis. „Bio-hydrogen production by anaerobic and facultatively anaerobic bacteria pure cultures using various substrates in experimental testsystems." Paper No 318BIO; 11th International Congress on Hydrogen Production ICH2P-11, Thessaloniki, Greece, June 19-22, 2011; Conference Abstracts Proceedings in CD form, 5 pages;
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3. J.Dimants, B.Sloka, J.Kleperis, I.Klepere Renewable Hydrogen Market Development: Forecasts and Opportunities for Latvia. Paper No 319GOV; 1th International Congress on Hydrogen Production ICH2P-11, Thessaloniki, Greece, June 19-22, 2011; Conference Abstracts Proceedings in CD form, 5 pages;
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6. Conference of Young Scientists on Energy Issues 2011 (CYSENI 2011); Kaunas (Lithuania), May 24 - 25, 2012:

V. Zubkovs, E. Pajuste, G. Kizane, A. Vitins, A. Matiss, Tritium localization in the bulk of neutron irradiated beryllium pebbles. CYSENI 2011, In Conference of Young Scientists on Energy Issues 2011 (CYSENI 2011), ISSN 1822-7554, 2011, X-538-544;

7. 4th World Hydrogen Technology Convention, 14th-16th September 2011 Scottish Exhibition and Conference Centre, Glasgow, Scottland:

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2. M. Vanags, J. Kleperis, G. Bajars, A. Lusis. Analysis Of Inductive Current Pulse Dynamics In Water Electrolyses Cell. Conference Abstracts 4th World Hydrogen Technology Convention, 14th-16th September 2011 Scottish Exhibition and Conference Centre, Glasgow, Scottland, UK p.68;

8. International Conference Current Issues in Management of Business and Society Development – 2011, May 5-7, 2011, University of Latvia, Riga (Latvia):

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9. 13th International Conference-School „Advanced Materials and Technologies", August 27 - 31 2011, Palanga, Lithuania:

V. Zubkovs, O. Paskova, A. Matiko, G. Kizane, E. Pajuste. Issues Related to Tritium Inventory in the neutron Irradiated Beryllium Pebbles. In 13-th International Conference-School „Advanced Materials and Technologies", August 27 - 31 2011, Palanga, Lithuania, p.144.

10. The COMSOL Conference 2011 Stuttgart (Germany), October 26-28, 2011:

I. Dirba, and J. Kleperis. Modeling of a Switchable Permanent Magnet Magnetic Flux Actuator. Abstracts of The COMSOL Conference 2011 Stuttgart (Germany), October 26-28, 2011: http://www.comsol.com/conference2011/europe/presentations/

11. The 15th International Conference on Fusion Reactor Materials (ICFRM-15), Charleston, South Carolina, USA, October 16-21, 2011:

A. Vītiņš, G. Ķizāne, A. Matīss, E. Pajuste, V. Zubkovs. Tritium release from the Pebble-Bed Assemblies neutron-irradiated beryllium pebbles under action of temperature. (Poster presentation by A. Vītiņš.) Abstract 15-231 is available online at: http://www.ornl.gov/icfrm15/pdf/scientificprog/ABSTRACTS/15-231%20Aigars%20Vitins.pdf

Studentu darbi

1. Aizstāvēts promocijas darbs (2011.g. 1. martā) fizikas doktora specialitātē: Jūlija Hodakokovska „Membrānas un membrānas-elektrodu kompleksa materiālu pētījumi pielietojumiem degvielas šūnās" (vad. J.Kleperis) , 2011

2. Sagatavots un iesniegts aizstāvēšanai promocijas darbs fizikas doktora specialitātē: Mārtiņš Vanags „Ūdens sadalīšanās procesu izpēte, izmantojot sprieguma impulsu un plazmas izlādes metodes" (vad. J.Kleperis), 2011

3. Aizstāvēts maģistra darbs LU Fizikas un matemātikas fakultātē: Imants Dirba „Teorētiskā modeļa izveide un optimālo materiālu izvēle pārslēdzamas magnētiskās plūsmas elektriskajām mašīnām" (vad. J.Kleperis), 2011

4. Aizstāvēts fizikas bakalaura darba LU Fizikas un matemātikas fakultātē: Rimas Janeliukštis „Stikla šķiedras fizikālķīmisko īpašību modificēšana" 2011. Vadītājs A.Lūsis

5. Aizstāvēts fizikas bakalaura darbs LU Fizikas un matemātikas fakultātē: Jānis Zandersons „Tekstilšķiedru funkcionalizēšanas metodes un procesi". 2011 Vadītājs A.Lūsis.

6. Aizstāvēts maģistra darbs LU Bioloģijas fakultātē: Ilze Klepere „Ūdeņraža veidošanās dažādu substrātu anaerobās fermentācijas testsistēmās" (vad. I.Muižnieks) 2011

7. Aizstāvēts bakalaura darbs LU Fizikas un matemātikas fakultātē: Arturs Kālis „Nanostrukturētu fotoaktīvu pārklājumu iegūšana un to morfoloģijas, struktūras un īpašību izpēte" (vad. J.Kleperis), 2011

8. Aizstāvēts dizainera maģistra darbs RTU Tekstilmateriālu tehnoloģiju un dizaina institūtā: Līva Veļķere „Kaņepju šķiedru termo-mehāniskās īpašības". Vadītāji: I.Baltiņa un A.Lūsis.

9. Aizstāvēts bakalaura darbs LU Bioloģijas fakultātē: Artūrs Gruduls „Bioreaktoru sistēmas prototipa izveide un optimizācija eksperimentālu pētījumu veikšanai ar fermentējošiem ūdeņraža un metāna gāzes producentiem" (vad. J.Kleperis), 2011

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	PhD students	MSc and BSc students
1. Dr. hab. E. Kotomin	13. D. Bocharov	15. O. Lisovskii
2. Dr. hab. V. Kuzovkov	14. A. Gopejenko	16. P. Merzlakovs
3. Dr hab. Yu.Shunin		17. A. Shirmane
4. Dr. O. Dumbrajs		18. A. Sorokin
5. Dr. R. Eglitis		
6. Dr. D. Gryaznov		
7. Dr. V. Kashcheyevs		
8. Dr. Yu. Mastrikov		
9. Dr. S. Piskunov		
10. Dr. A. Popov		
11. Dr. Yu. Zhukovskii		
12. Dr. G. Zvejnieks		

Scientific visits abroad

1. Dr. hab. E. Kotomin, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (9 months), University of Beijing, China (1 week)
2. Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (2 month), Karlsruhe Institute of Technology, Germany (1.5 months).
3. Dr hab. V. Kuzovkov, Northwesten University, USA (3.5 months)
4. Dr. D. Gryaznov, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (10 months)
5. Dr. Yu. Mastrikov, University of Maryland, USA (4 months), Institute for Materials Research-I, Karlsruhe, Germany (6 weeks).
6. Dr. S. Piskunov, University of Duisburg-Essen, Germany (2 weeks).

7. Dr. A. Popov, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (6 weeks), University of Beijing, China (1 week), National University of Lviv, Ukraine (1 week), Institute of Physics, Tartu, Estonia (2 weeks)
8. Dr. Yu. Zhukovskii, St. Petersburg State University, Russia (6 weeks), Institute for Materials Research-I, Karlsruhe, Germany (1 month), Institute of Nuclear Problems, Belarusian State University, Minsk (2 weeks), Institute of General and Inorganic Chemistry, Russian Academy of Science, Moscow (1 week).

International Cooperation

Belarus	1. Belarusian State University (Prof. S.A. Maksimenko)
Finland	2. Helsinki University of Technology (Dr. T. Kurki-Suonio)
France	3. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober)
Germany	4. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 5. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov) 6. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. Van Uffelen). 7. Max Planck Institut für Plasmaphysik, Garching (Dr. V. Igochine, Prof. Dr. K. Lackner, Dr. R. Mayer-Spasche, Prof. Dr. H. Zohm) 8. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk) Institut für Materialforschung I (KIT), Karlsruhe (Dr. A. Möslang) Department of Theoretical Chemistry, University of Duisburg-Essen, (Prof. E. Spohr)
Greece	11. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. K. Avramides)
Israel	12. Ben Gurion University, Beer Sheeva (Prof. A. Aharony, Prof. D. Fuks)
Italy	13. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Kazakhstan	14. Gumilyov National University, Astana (Prof. A. Akilbekov)
Japan	15. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	16. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Poland	17. Warsaw University, Dept of Chemistry (Dr A. Huczko)
Romania	18. University of Craiova (Dr. D. Constantinescu)
Russia	19. St. Petersburg State University (Prof. R.A. Evarestov) 20. Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (Prof. P.N. Dyachkov)
UK	21. Imperial College London (Prof. M.Finnis) 22. University College London (Prof. A.L. Shluger)
Ukraine	23. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)
USA	24. Northwestern University, Evanston, Illinois (Prof. M.Olvera de la Cruz) *25. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)*

Main Results

A. Electronic structure calculations for advanced materials

FIRST-PRINCIPLES NANO-SCALE SIMULATIONS OF CARBON NANOTUBES GROWTH UPON NI AND ALUMINA CATALYSTS

Yu.F. Zhukovskii, S. Piskunov, G. Zvejnieks, E.A. Kotomin,
S. Bellucci (*Laboratori Nazionali di Frascati, Italy*)

Within the EC FP7 CATHERINE project, in collaboration with Dr. S. Bellucci (Laboratori Nazionali di Frascati, Italy) and *Faculty of Computing (University of Latvia)* we have performed large-scale *ab initio* simulations on 2D periodic models of C/Ni(111) (The 5×5 SC model of nickel substrate, Fig. 1) and C/θ-Al_2O_3(010) nanostructures, which can describe peculiarities of the initial stage of growth for the SW CNT bundle upon the catalyst particle.

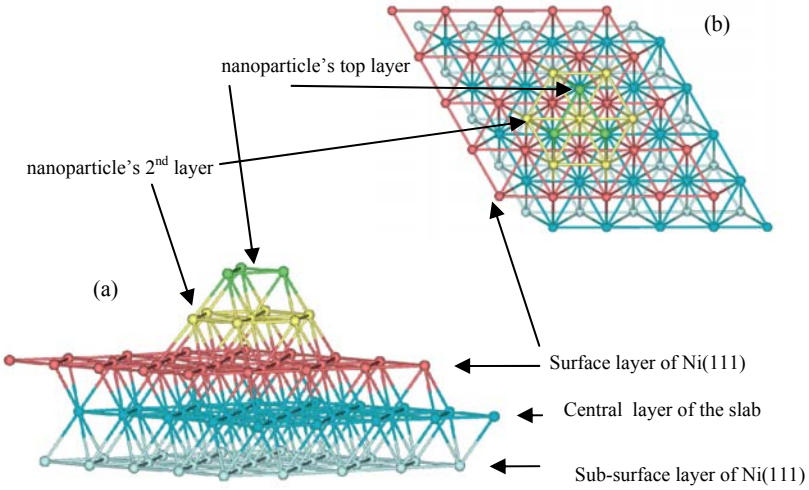

Fig. 1. Schematic illustration of nanostructured Ni(111) catalyst: (a) side view and (b) top view. Each surface plane is shown with different color to guide eyes. The lower light-blue plane is a mirror plane of symmetrically terminated 5-layer slab.

The network of adsorbed carbon atoms, which transforms to the nanotube structures, arise after the dissociation of hydrocarbon molecules *e.g.*, CH_4, flowing towards the substrate when using the CVD method. We estimate the dissociation energies for CH_4 molecules atop both substrates (see Fig. 2 for details) according to the total energy balance of the two-step dissociation mechanism:

$$(CH_4)_{ads} \rightarrow (CH)_{ads} + 3H_{ads,} \quad (1a)$$

$$(CH)_{ads} \rightarrow C_{ads} + H_{ads} \quad (1b)$$

The calculated energies of a complete dissociation (E_{diss}) have been found to be 2.33, 2.17, and 6.40 eV for perfect Ni(111), nanostructured Ni(111), and θ-Al_2O_3(010) substrates, respectively.

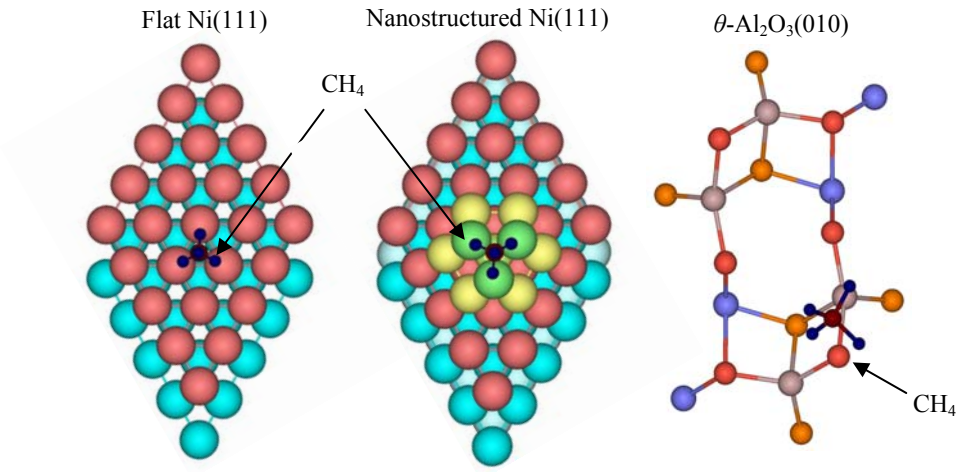

Fig. 2. Schematic illustration of CH_4 dissociation on both Ni(111) and θ-Al_2O_3(010).

As the result of our simulations, we predict an increase of catalytic activity of nanostructured Ni(111) surface, due to nanofacet formation that potentially can play a role in a predictable growth of CNT (Fig. 3). The key stage of carbon nanotube growth from catalyst is an initial swelling of an island consisting of carbon hexagons and pentagons formed from C_{ads} atoms atop the substrate up to creation of semi-fullerene.

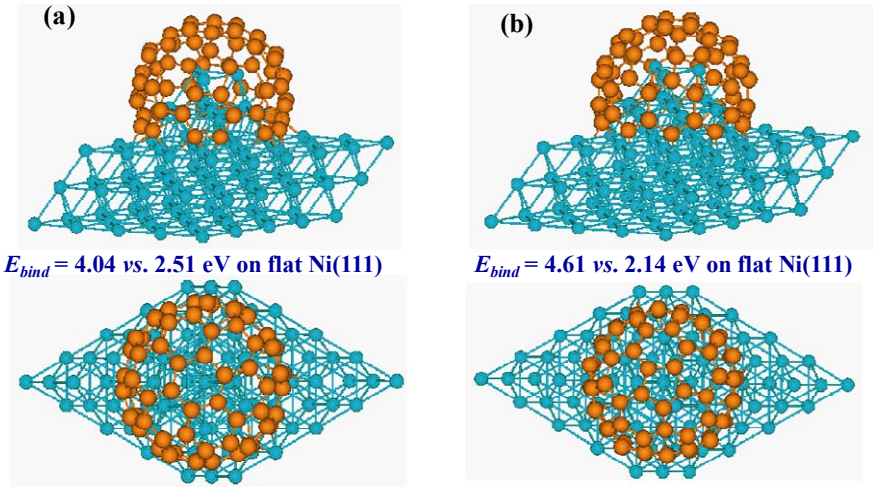

Fig. 3. Aside (upper) and atop (lower) views of 2D supercells containing CNT of either *ac* (a) or *zz* (b) type chirality upon the nanostructured Ni(111) surface.

Our results predict quite effective and reproducible mechanism of growth for carbon nanotubes upon the nickel nanostructured substrate. In absence of catalyst nanoparticles upon the bottom of the nanopores inside alumina membrane the carbon structures could grow from the walls towards the centers of nanopores: either carbon nanoscrolls or rather thick amorphous (soot-like) microtubes. At the bottom level of the multi-scale modeling, *ab initio* methods can be used for determining the electronic structure of the assumed carbon-metal nanocomposites.

FIRST-PRINCIPLES CALCULATIONS ON SINGLE- AND DOUBLE-WALL INORGANIC NANOTUBES AND THEIR STRUCTURAL ANALYSIS

Yu.F. Zhukovskii, S. Piskunov,
R.A. Evarestov, A.V. Bandura (*Department of Quantum Chemistry, St. Petersburg University, Russia*),
E. Spohr (*Department of Theoretical Chemistry, University of Duisburg-Essen, Germany*)

Within the line group irreducible representations developed *in collaboration with Prof. R.A. Evarestov and Dr. A.V. Bandura (St. Petersburg University, Russia)* the one-periodic (1D) nanostructures with rotohelical symmetry have been considered for symmetry analysis of single- and double-wall (SW and DW) boron nitride and titania nanotubes (BN and TiO_2 NTs) formed by rolling up the stoichiometric two-periodic (2D) slabs of hexagonal structure with the same or opposite orientation of translation and chiral vectors. We have simulated the two sets of commensurate double-wall BN NTs and TiO_2 NTs (Fig. 4) with armchair- or zigzag-type chiralities: $(n_1,n_1)@(n_2,n_2)$ or $(n_1,0)@(n_2,0)$, respectively.

a) optimized model of double-wall (6,6)@(12,12) *ac*-TiO_2 NT;

b) optimized model of double-wall (10,0)@(20,0) *zz*- TiO_2 NT.

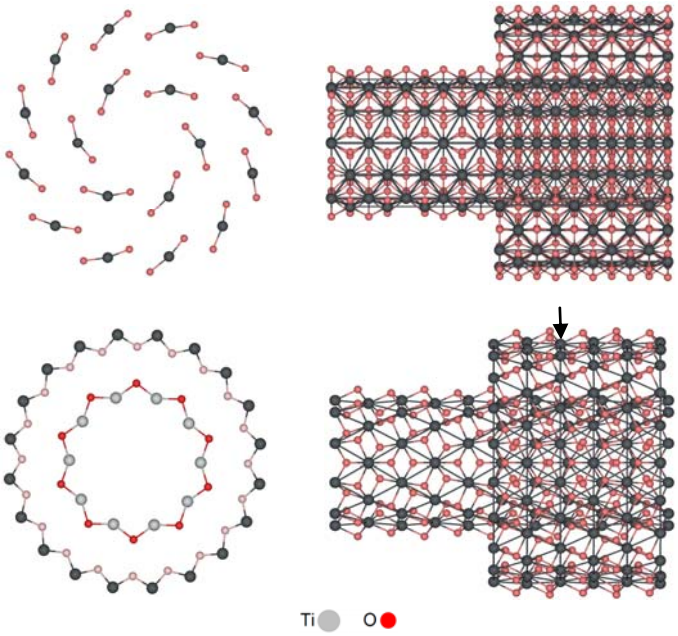

Fig. 4. Cross-sections and aside images of hexagonal DW TiO_2 NTs corresponding to optimized diameters (*i.e.*, left and right parts of models a) and b), respectively) for armchair and zigzag chiralities. For *zz*-DW NT (b), there are also shown atoms of the nearest ring behind the cross-section (as considerably more light circles).

Due to a noticeably larger ionic contribution to inter-wall interaction between three-layer O-Ti-O shells within DW TiO_2 NTs their polarization effects are certainly larger than those in double-wall boron nitride nanotubes which results in the higher electron density localization as compared to DW BN NTs. Considerable interaction between the walls in optimal DW NT configurations results in a decrease of band gaps in double-wall nanotubes as compared to those for SW NTs (this decrease is a more pronounced for DW TiO_2 NTs).

One-dimensional nanostructures synthesized from complex ternary oxides with a perovskite structure have attracted considerable recent interest due to their unique physical properties and promising novel functionalities as compared to bulk materials. At room temperature

$SrTiO_3$ possesses a high symmetry cubic structure and, thus, serves as an excellent model material for a wide class of ABO_3 perovskites. Consequently, understanding the behavior of $SrTiO_3$ on the nanoscale is significant for fundamental studies, as well as for shape-controlled synthesis of perovskite nanostructures with predictable properties. Based on *ab initio* calculations performed *in collaboration with Prof. E. Spohr (University of Duisburg-Essen, Germany) and Faculty of Computing (University of Latvia)* we predict that the most energetically stable NTs can be rolled up from (110) nanosheet of rectangular morphology:

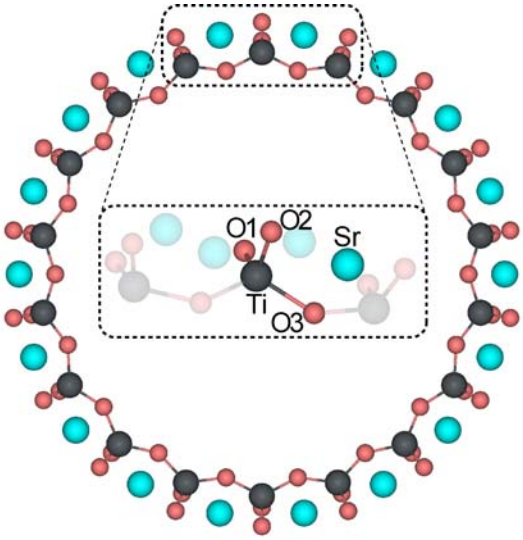

Fig. 5. Atomic structure of the most energetically stable $SrTiO_3$ nanotube.

The increase of the Ti–O bond covalency in the outer shell of strontium titanate NT may lead to an enhancement of adsorption properties which means that they can be used in gas-sensing devices. Quantum confinement effects lead to the widening of the NT band gaps, thus, making them attractive for band gap engineering, *e.g.,* in photocatalytic applications.

THEORETICAL SIMULATIONS ON ELECTRIC PROPERTIES FOR JUNCTIONS OF METALLIC ELECTRODES WITH CARBON NANOTUBES AND GRAPHENE NANORIBBONS

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

In collaboration with Dr. S. Bellucci (Laboratori Nazionali di Frascati, Italy) within the EC FP7 CATHERINE project, we have developed the model of *'effective bonds'* in the framework of both cluster approach based on the multiple scattering theory formalism and Landauer theory, which can allow us to predict the resistivity properties for C-Me junctions taking into account chirality effects in the interconnects of single-wall (SW) and multi-wall (MW) CNTs (Fig. 6) as well as single-layer (SL) and poly-layer (PL) GNRs (Fig. 7) with the fitting metals (Me= Ni, Cu, Ag, Pd, Pt, Au) on predefined geometry of carbon nanostructure. We have also developed the model of inter-shell interaction for the MW CNTs, which allows us to estimate the transparency coefficient as an indicator of possible 'radial current' losses.

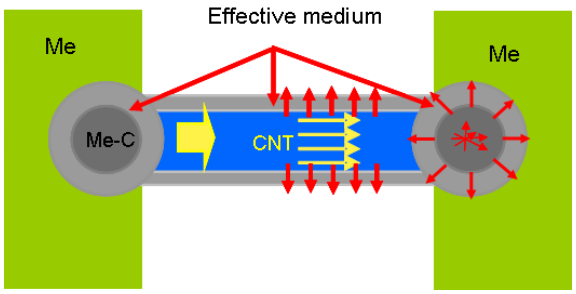

Fig. 6. Model of CNT - Me interconnect.

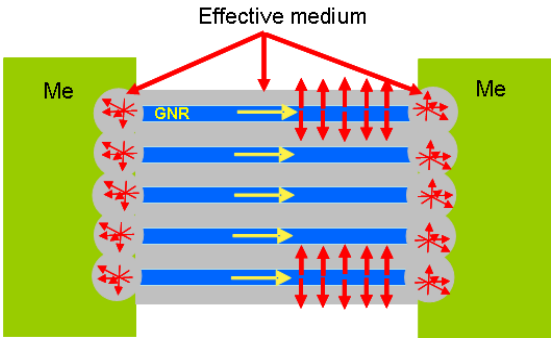

Fig. 7. GNR (polylayered) - Me interconnect.

Figs. 8 and 9 show the generalized results of simulations on resistance of junctions between various metallic substrates with SW CNT and SL GNR, respectively. It is clear that Ag and Au substrates are more effective electrically while Ni is rather a 'worse' substrate for interconnect, although it yields the most effective catalyst for CNT growth.

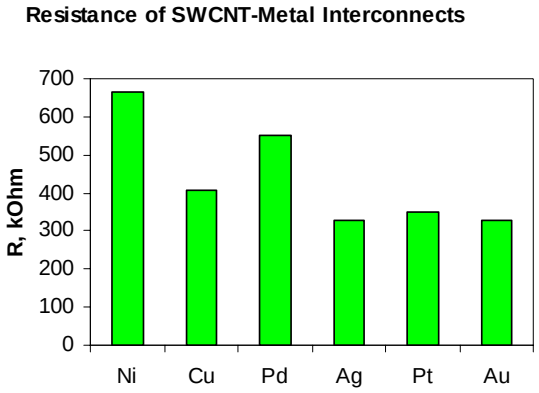

Fig. 8. Resistances of Me interconnects with zigzag-type SW CNT (diameter ~1 nm)

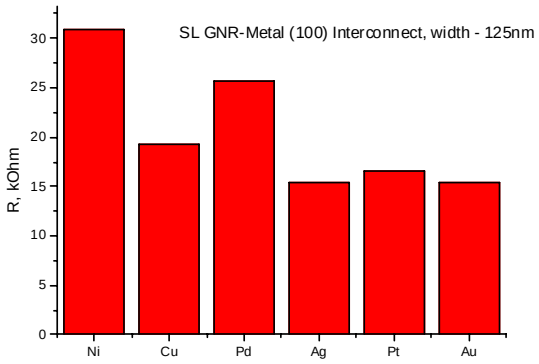

Fig. 9. Resistances of Me interconnects with the SL GNR (width ~125 nm)

Conductance and other current-voltaic parameters depend on the morphology of the nearest shells in MW CNTs and PL GNRs, which results in complications for technological synthesis. Nevertheless, the corresponding nanodevices possess the stable electric characteristics. We are able now to create a database of combinations for different CNT-Me and GNR-Me junctions taking into account a set of parameters, namely: angle of chirality, CNT diameter, numbers of walls or layers, type of metal substrate (Me), orientation of densely-packed metal substrate, *e.g.*, (100), (111) or (110). Thus, we are able to predict interconnect properties for various configurations of SW and MW CNTs as well as SL and PL GNRs.

MECHANISM OF OXYGEN MIGRATION AND INCORPORATION UPON PERFECT AND DEFECTIVE URANIUM NITRIDE (001) SURFACE

D. Bocharov, D. Gryaznov, Yu.F Zhukovskii, E.A. Kotomin,
P. Van Uffelen (*EC Institute for Transuranium Elements, Karlsruhe, Germany*)

For the first time, we have performed detailed first-principles simulations of perfect and defective uranium mononitride (UN) surfaces and their interaction with oxygen, *in collaboration with EC Institute for Transuranium Elements (Karlsruhe, Germany) and*

Faculty of Computing (University of Latvia). This is relevant for understanding mechanism of UN nuclear fuel exidation in air. Due to a mixed metallic-covalent nature of the chemical bonding in UN, we predicted a high affinity of adsorbed O towards the UN(001) surface. Indeed, the E_{bind} values of 6.9-7.6 and 5.0-5.7 eV *per* O adatom atop the surface U or N atoms, respectively, are accompanied by 0.5-1.2 *e* charge transfer from the surface towards the O adatom (Fig. 10). The positively charged surface U atom goes outwards, minimizing its distance with the adsorbed O atom while the N atom is strongly displaced from the adsorbed O atom inwards the slab, due to a mutual repulsion between N and O.

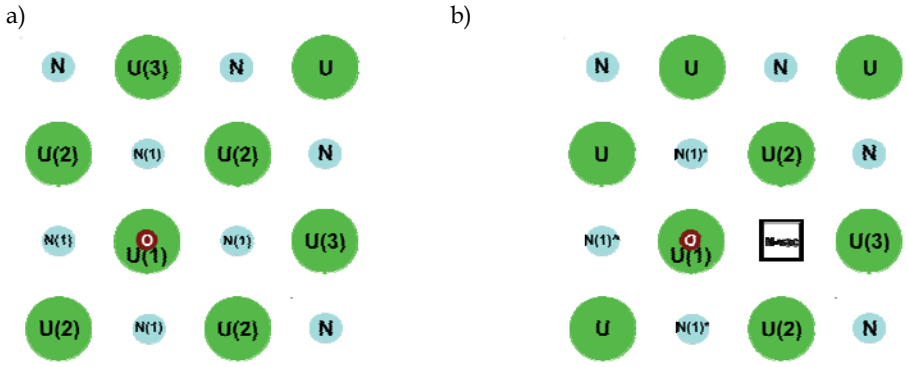

Fig. 10. Schematic top view of O adatoms located atop the surface U atom without (a) and with (b) N vacancy in the proximity of adsorbed O atoms. Numbers in brackets enumerate non-equivalent surface atoms.

Three main migration paths of O upon the UN(001) surface (Fig. 11) are as follows: *1*: between U atom and the nearest N atom, *2*: between the two neighboring U atoms, *3*: between neighboring N atoms. The most favorable migration trajectory has been optimized to be the line joining the sites atop the nearest surface U atoms and the hollow sites between them (path 2). The corresponding energy barriers found (0.36 eV for the 5-layer slab and 0.26 eV for the 7-layer slab) indicate a high mobility of adsorbed O atoms upon UN. The energy barriers along other two migration trajectories are substantially larger.

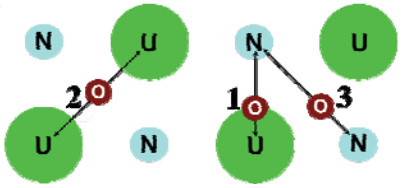

Fig. 11. Different oxygen migration paths upon the UN(001) surface (top view).

Both formation energies of uranium and nitrogen vacancies as well as binding energies of oxygen atoms and molecules adsorbed atop the defective UN(001) surface have been estimated too. Presence of the surface nitrogen vacancy closest to the surface U atom (U_{surf}) results in a low-barrier incorporation of migrating O adatom from position atop U_{surf} towards this vacancy, which can be considered as a trap. Based on the results of calculations discussed above the following stages of oxygen interaction with the UN surfaces were indentified to explain its easy oxidation: (*i*) chemisorption of molecular oxygen, (*ii*) spontaneous breaking of the O_2 chemical bond after molecular adsorption, (*iii*) location of the two newly formed O adatoms atop the adjacent surface U atoms, (*iv*) high mobility of adsorbed O atoms along the surface, (*v*) low-barrier incorporation of O into N-vacancies, *(vi)* stabilization of O atom

inside the N-vacancy, (*vii*) further incorporation of O in pre-existed sub-surface N-vacancies as a result of inter-layer diffusion.

AB INITIO SIMULATIONS OF IMPURITY CLUSTERS IN ODS STEELS

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

The understanding of the mechanisms and kinetics of yttria nanoparticle formation in the steel matrix is required of the development of the oxide dispersed strengthened (ODS) steels. The implementation of the ODS steel for fusion- and advanced fission-reactor blanket structures results in increase of the operation temperature by ~100°C which makes this material very promising these reactors. On the other hand, the mechanical properties and radiation resistance of ODS steels are sensitive to the size and spatial distribution of the oxide precipitates. Therefore, it is necessary to perform a large-scale theoretical modeling of the Y_2O_3 formation. Large-scale first principles calculations have been performed *in collaboration with Dr. A. Möslang and Dr. P.V. Vladimirov (Institut für Materialforschung I, Karlsruhe, Germany)* for the γ-Fe lattice containing Y-Y, Y-V_{Fe}, V_{Fe}-V_{Fe}, Y-O (Fig. 12) and O-O pairs as well as different configurations of three-atom clusters Y-O-Y (Fig. 13) and Y-V_{Fe}-Y. These calculations are [illegible]e-wise interaction energies necessary for further [illegible]DS growth.

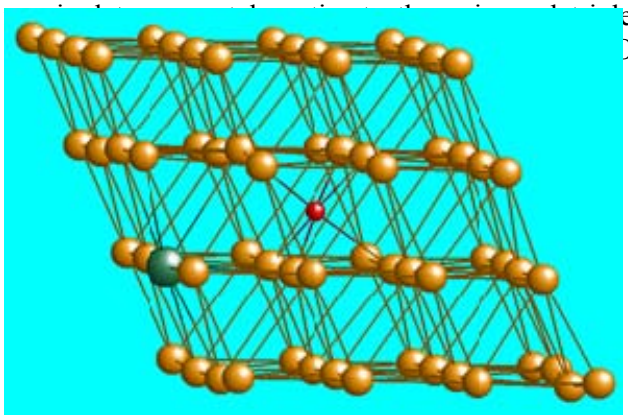

Fig. 12. Relaxed 2nd coordination sphere for configuration of Y-O_{int} pair.

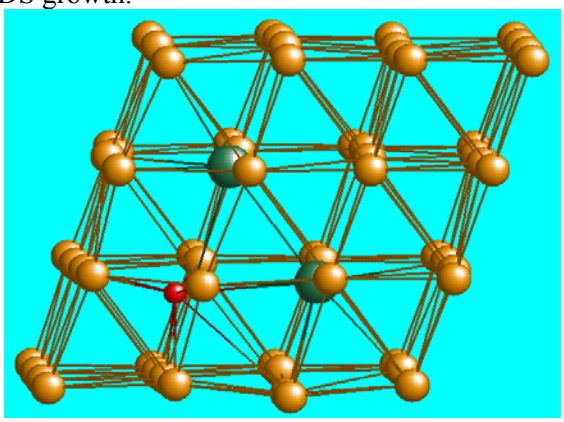

Fig. 13. Relaxed configuration of 2Y-O substitute atoms.

The analysis of the pair-wise interactions calculations show that a certain attraction occurs between the Y substitute atom and Fe vacancy, while no bonding occurs between two Y atoms at any distances. The calculations of the interactions between yttrium and oxygen substitute atoms as well as between two oxygen substitute atoms show similar behavior with the highest binding energies at the distance of 1-NN and the decrease of the binding energy with the increase of the inter-defect distance. No significant bonding has been found between the two Fe vacancies located at different distances.

At the same time, we predict location of Fe vacancies in the proximity of impurity atoms. The calculations on different Y-O-Y cluster configurations clearly show that not only the presence of oxygen atom is required to form certain binding between impurity atoms but also the presence of Fe vacancies favors the growth of the Y_2O_3 precipitates inside the iron crystalline matrix. This has been proven by the calculations of interactions inside the Y-V_{Fe}-Y cluster for which the binding energy has been found to be rather large.

FIRST PRINCIPLES CALCULATIONS OF OXYGEN VACANCY FORMATION AND MIGRATION IN $BA_{1-X}Sr_XCo_{1-Y}Fe_YO_3$ PEROVSKITES

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

Based on first principles DFT calculations, we analyzed oxygen vacancy formation and migration energies as a function of chemical composition in complex multicomponent (Ba,Sr)(Co,Fe)O_3 perovskites which are candidate materials for SOFC cathodes and permeation membranes. The atomic relaxation, electronic charge redistribution and energies of the transition states of oxygen migration are compared for several perovskites to elucidate the atomistic reason for the exceptionally low migration barrier in $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ that was previously determined experimentally. The critical comparison of $Ba_{1-x}Sr_xCo_{1-y}Fe_yO_3$ perovskites with different cation compositions and arrangements shows that in addition to the geometric constraints the electronic structure plays a considerable role for the height of the oxygen migration barrier in these materials. These findings help to understand the fast oxygen permeation and exchange properties of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ as well as some of its limitations

PHONON CALCULATIONS IN CUBIC AND TETRAGONAL PHASES OF $SrTiO_3$: A COMPARATIVE LCAO AND PLANE WAVE STUDY

D. Gryaznov, E.A. Kotomin,
R.A. Evarestov (St. Petersburg State University, Peterhof, Russia)
E. Blokhin, J. Maier (Max-Planck Institute for Solid State Research, Stuttgart, Germany)

The atomic, electronic structure and phonon frequencies have been calculated in a cubic and low-temperature tetragonal $SrTiO_3$ phases at the *ab initio* level. We demonstrated that the use of hybrid exchange-correlation PBE0 functional gives the best agreement with experimental data. The results for the standard Generalized Gradient Approximation (PBE) and hybrid PBE0 functionals are compared for the two types of approaches: a linear combination of atomic orbitals (CRYSTAL09 computer code) and plane waves (VASP 5.2 code). Relation between cubic and tetragonal phases and the relevant antiferrodistortive phase transition is discussed in terms of group theory and illustrated with analysis of calculated soft mode frequencies at the *Γ*- and *R*-points in the Brillouin zone. Based on phonon calculations, the temperature dependence of the heat capacity is in a good agreement with experiment. This approach is promising for defect modeling in many advanced materials under high operational temperatures.

FIRST-PRINCIPLES CALCULATIONS OF THE ATOMIC AND ELECTRONIC STRUCTURE OF PEROVSKITE SURFACES

R.I. Eglitis

The *ab initio* calculations of polar $CaTiO_3$ (111) surface were performed. Surface relaxation, rumpling, energetics, optical band gaps, and charge distribution are obtained using the computer code CRYSTAL and a hybrid exchange-correlation functionals. Using a hybrid B3LYP approach, the surface relaxation for the two possible Ti and CaO_3 (111) surface terminations are calculated. For both Ti and CaO_3-terminated CaTiO3 (111) surfaces upper layer atoms relax inwards, while the second layer atoms, with the sole exception of CaO_3-terminated surface Ca atom, relax outwards. The alculated surface relaxation energy for Ti-

terminated surface is more than five times larger than the surface relaxation energy for CaO3-terminated surface. The surface energy for Ti-terminated surface (4.18 eV/cell) is smaller, than the surface energy for CaO_3-termination (5.86 eV/cell).
We calculated also properties of the $SrZrO_3$ (001) surfaceBoth SrO and ZrO_2 terminations were considered. On the (001) surfaces all upper and third layer atoms relax inward, while outward relaxations of all atoms in the second layer are found with the sole exception of SrO-terminated $SrZrO_3$ (001) surface second layer O atom. Calculated surface rumpling for the SrO-terminated SrZrO3 (001) surface (6.77 % of the lattice constant) is by a factor of ten larger than the surface rumpling for the ZrO_2-terminated surface (0.72 % of a_o). A considerable increase in the Zr-O chemical bond covalency near the $SrZrO_3$(001) surface as compared to the bulk is predicted.

FIRST-PRINCIPLES SIMULATIONS ON THE *F* CENTER AGGREGATION IN BAF_2

R.I. Eglitis
H. Shi (School of Science, Beijing Institute of Technology, Beijing, China),
R. Jia (Bergische Universität Wuppertal, Germany)

The *F* center (an electron trapped by a fluorine vacancy) and *R* center (a defect composed of three F centers) in BaF_2 crystal have been studied using density functional theory (DFT) with hybrid exchange-correlation DFT-B3PW functional. Our calculations show that the *F*-center transfer barrier is equal to 1.83 eV. The association energy calculations on R centers indicate energy gain with respect to three isolated *F* centers. During *F*-center aggregation, a considerable covalency arises between two neighbor fluorine vacancies with trapped electrons. Three incompletely paired electrons trapped in the R center have an up-down-up spin arrangements and induce three defect levels in the gaps between valence bands (VB) and conduction bands (CB) for both α- and β-spin polarized band structures, respectively. More defect bands lead to more complex electron transitions, which were classified into two F- and four M-like transitions. The DOS calculations clearly reveal the components of defect bands.

FIRST-PRINCIPLES CALCULATIONS OF THE ELECTRONIC DENSITY OF STATES FOR SUPERIONIC Ag_2CdI_4 CRYSTALS

A.I. Popov
S. Velgosh, I. Karbovnyk, I. Bolesta, O. Bovgyra
(Ivan Franko National University of Lviv, Ukraine)
W. Ciepluch-Trojane, B. Andriyevsky (Faculty of Electronics and Computer Sciences,
Koszalin University of Technology, Poland)
I.V. Kityk (Czestochowa Technical University, Czestochowa, Poland)

Over the past few decades an enhanced interest takes place to the studies of silver-containing fast ionic conductors. These crystals are, first of all, of interest due to phenomena of the reversible transformation of luminescence centers structure as well as mobile silver ions concentration changes within the local irradiated region of the crystals.

This work completes our thorough investigation of Ag_2CdI_4 solid electrolyte. In addition to previous results of electrical, optical and thermal properties of this model compound and following recent report on its microstructure studied by SEM, impedance spectroscopy and fractal dimension analysis as well as infrared spectra and phonon density of states calculation,

herewith we focused on the band energy structure calculations of the Ag_2CdI_4 single crystals and determination of partial densities of states in the valence band.
Energy band dispersion calculations have been performed for Ag_2CdI_4 superionic within a framework of local density approximation (Perdew–Zunger parameterization) exploiting the first-principles CASTEP computer code. The *ab-initio* electronic structure simulations
were performed for both types of ε-Ag_2CdI_4 crystalline structures. Principal optical functions as well as the density of electronic states in the spectral range of inter-band optical transitions (2.5 eV–20 eV) were determined. Theoretically calculated absorption coefficients derived from the obtained band structure are compared with appropriate experimental data.

B. Kinetics of processes with self-organization

PATTERN FORMATION KINETICS FOR CHARGED MOLECULES ON SURFACES AND INTERFACES: MICROSCOPIC CORRELATION FUNCTION ANALYSIS

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

The kinetics of pattern formation and phase separation in a closed system of two types of oppositely charged molecules with competing short- and long-range interactions on surfaces/interfaces was studied combining three methods: a microscopic formalism of the joint correlation functions, Reverse Monte Carlo, and non-equilibrium charge screening factors. The molecular ordering occurs on the background of the Ostwald ripening and thus is strongly non-equilibrium. It is demonstrated how initial random distribution of molecules is changed for loose similar-molecule aggregates, with further reorganization into dense macroscopic domains of oppositely charged molecules (Fig. 14). Pattern formation process is characterized by the correlation length which monotonically increases in time.

The kinetics of pattern formation was also studied for reversible $A+B\rightarrow 0$ reaction of mobile oppositely charged molecules at the interface. Using formalism of joint correlation functions, non-equilibrium charge screening and reverse Monte-Carlo methods, it is shown that labyrinth-like percolation structure induced by (even moderate-rate) reaction is principally non-steady-state and is associated with permanently growing segregation of similar reactants and aggregation of similar reactants into domains. A role of short-range and long-range reactant interactions is discussed.

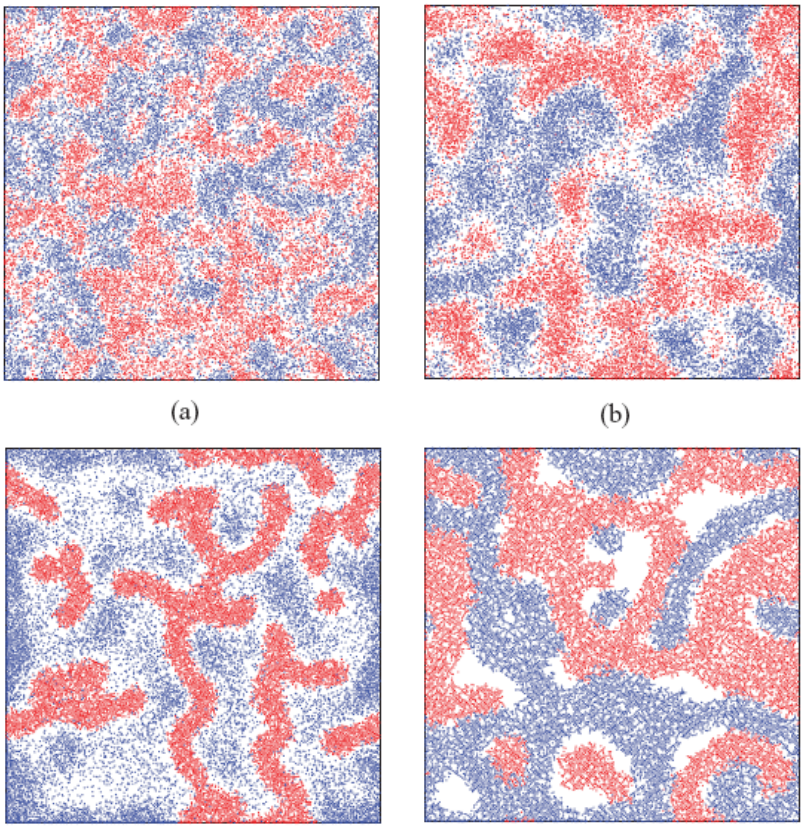

Fig. 14. Fragments of the characteristic snapshots obtained using the reverse Monte Carlo for the correlation functions

In collaboration with Northwestern University, Evanston, USA, the effects of non-equilibrium charge screening in mixtures of oppositely charged interacting molecules on surfaces are analyzed in a closed system. The dynamics of charge screening and the strong deviation from the standard Debye-Hückel theory are demonstrated via a new formalism based on computing radial distribution functions suited for analyzing both short-range and long-range special ordering effects. At long distances, the inhomogeneous molecule distribution is limited by diffusion, whereas at short distances (of the order of several coordination spheres) by a balance of short-range (Lennard-Jones) and long-range (Coulomb) interactions (Fig. 15). The non-equilibrium charge screening effects in transient pattern formation are further quantified. It is demonstrated that use of screened potentials, in the spirit of the Debye-Hückel theory, leads to qualitatively incorrect results.

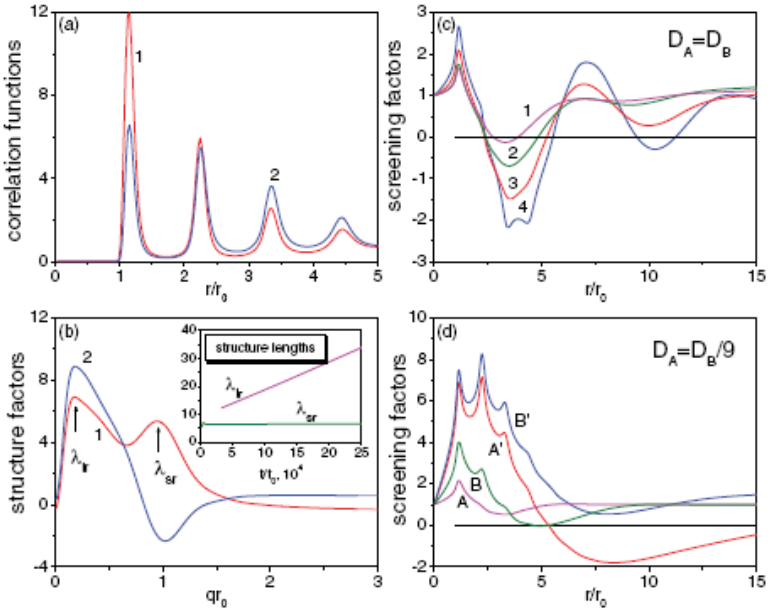

Fig. 15. Ionic binary systems with Lennard-Jones and Coulomb interactions at low temperatures for intermediate density: (a) the joint correlation functions; (b) the partial structure factors; (c) and (d) the non-equilibrium screening factors.

C. Physics of Plasma

A LOW-DIMENSIONAL MODEL SYSTEM FOR QUASI-PERIODIC PLASMA PERTURBATIONS

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[3]Max-Planck Institut für Plasmaphysik, Association Euratom-IPP, Germany

Larger scale plasma instabilities not leading to an immediate termination of a discharge often result in periodic nonlinear perturbations. A simplest possible model is suggested for description of the system with drive and relaxation processes with different time scales. The model is based on two equations: the first being responsible for the relaxation dynamics and the second one for the drive (Fig. 16). The model can be generalized to describe the pellet injection.

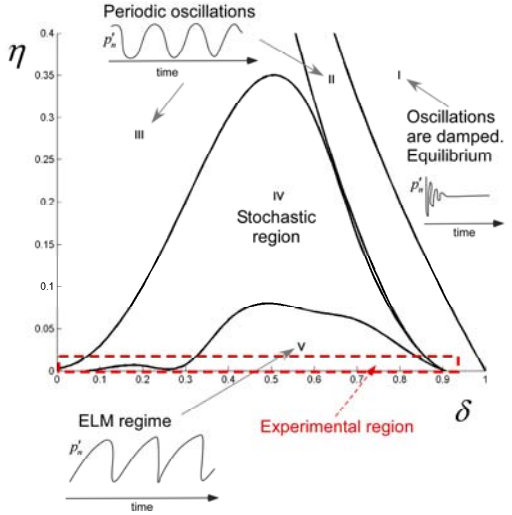

Fig. 16. Dynamical zones of oscillations in the parameter space

UNDERSTANDING COMPLEX MAGNETOHYDRODYNAMIC ACTIVITIES WITH A RELAXATION IN THE HT-7 TOKAMAK

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[3]Institute of Solid State Physics, Association Euratom-University of Latvia, Riga, Latvia

A new relaxation instability with complex magnetohydrodynamics (MHD) activities is found in the HT-7 tokamak operational region, which manifests itself in bursts of hydrogen alpha-ray radiations, electron cyclotron emission and soft x-ray (SX) radiations on outer channels, as well as complex MHD perturbations, but without hard disruptions. It is found that a stochastic annular belt resulted just before the relaxation due to the m/n = 5/3 island overlapping with m/n = 2/1 and m/n = 3/2 islands (Fig. 17).

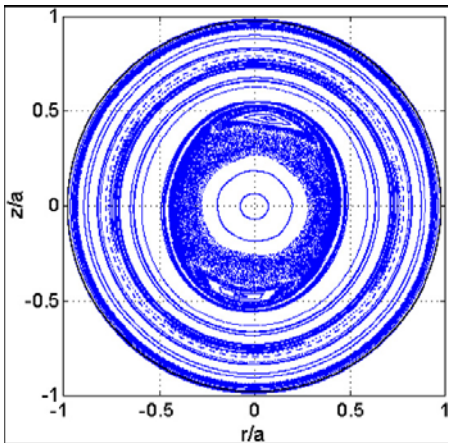

Fig. 17. The Poincare mapping where a stochastic annular belt of magnetic field lines could be observe

CT OF POSSIBLE REFLECTIONS ON THE OPERATIONS OF EUROPEAN ITER GYROTRONS

O Dumbrajs

Theory describing the effect of reflections on operation of gyrotrons with radial output is applied the ITER 170 GHz 2 MW coaxial cavity gyrotron, which is under development, and to the 170 GHz 1 MW cylindrical cavity gyrotron as a fall back solution.

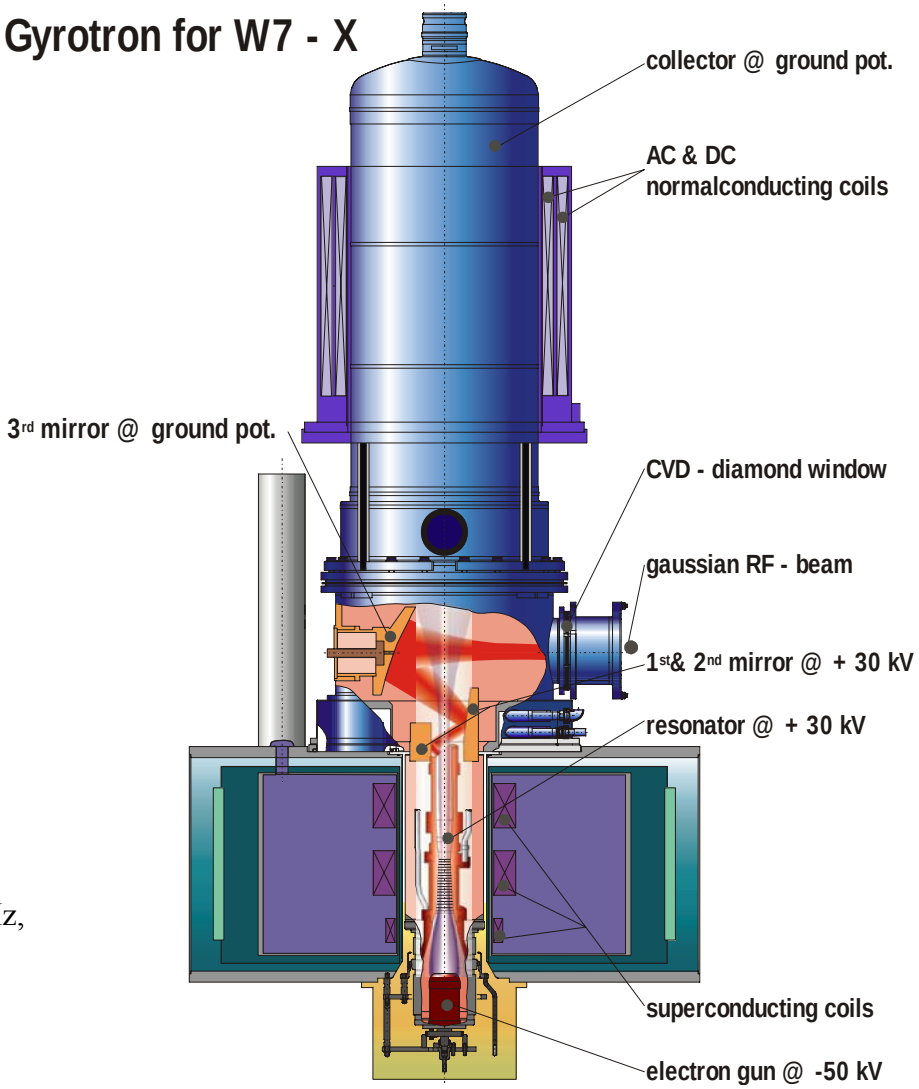

Fig. 18. European 140 GHz, 1 MW, CW Gyrotron

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20. R.I. Eglitis, "Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces as well as Nb impurity segregation towards the SrTiO3 surface". Abstracts: p. 67.
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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 lithoghraphy for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed. The methods for fabrication of subwavelength-gratings and surface-relief features with nanometer scale have been developed.

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Main Results

SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

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

OPTICAL RECORDING IN AMORPHOUS CHALCOGENIDE THIN FILMS

Janis Teteris

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

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

HOLOGRAPHIC LITHOGRAPHY IN AMORPHOUS CHALCOGENIDE THIN FILMS

J.Teteris, J.Aleksejeva and M.Reinfelde

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

SURFACE RELIEF FORMATION DURING HOLOGRAPHIC RECORDING

U.Gertners and J.Teteris

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

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

NANOSTUCTURED SURFACES FOR OPTICAL ANTIREFLECTION

J.Aleksejeva and J.Teteris

The demand for optically antireflective layers during last years has increased. Particularly such high demand is in the branches where large surfaces will be covered

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

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

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

OPTICAL RECORDING IN AZOBENZENE CONTAINING POLYMER FILMS

A. Gerbreders and J. Teteris.

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

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

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

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10. A.Gerbreders, J.Aleksejeva, J.Teteris, The Synthesis if Different Azo-Polyurethane Polymers for Optical Record. *Intern. Conf. TM&NT (Functional materials and nanotechnologies 2011,* Riga, Latvia, April 5-8, 2011, Book of abstracts,. p.152.
11. J.Aleksejeva, A.Gerbreders, M.Reinfelde, J.Teteris, Photoinduced birefringence in azo-dye doped polyurethane, *International Young Scientist Conference "Developments in Optics and Communications 2011",* Riga, Latvia, April 23-25, 2011, Book of abstracts, p. 60.
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13. J.Teteris, Photoinduced mass transport in amorphous chalcogenide and organic polymer films, *5th Intern.Conf. on Amorphous and Nanostructured Chalcogenides (ANC-5)*, Bucharest, Romania, June 26-July 1, 2011, Book of abstracts, p. 7.
14. M.Reinfelde, J.Teteris, Surface relief and polarization holographic grating formation in amorphous As-S-Se films, *5th Intern.Conf. on Amorphous and Nanostructured Chalcogenides (ANC-5)*, Bucharest, Romania, June 26-July 1, 2011, Book of abstracts, p. 37.
15. J.Aleksejeva, A.Gerbreders, U. Gertners, M.Reinfelde, J.Teteris, Polarization holographic recording in azo-benzene doped polyurethane polymer films, *5th Intern.Conf. on Amorphous and Nanostructured Chalcogenides (ANC-5)*, Bucharest, Romania, June 26-July 1, 2011, Book of abstracts, p. 40.
16. A.Gerbreders, J.Aleksejeva, J.Teteris, The synthesis of different variants of azo-polyurethane polymers for optical record, *5th Intern.Conf. on Amorphous and Nanostructured Chalcogenides (ANC-5)*, Bucharest, Romania, June 26-July 1, 2011, Book of abstracts, p. 45.
17. J.Teteris, J.Aleksejeva, E.Laizane, Photo-induced mass transport in azobenzene containing organic polymers, *The 12th European Conf. on Organized Films (ECOF 12),* Sheffield, United Kingdom, 17-20 July, 2011, Book of abstracts, p. 52.
18. J.Teteris, J.Aleksejeva, U.Gertners, Photoinduced mass transport in amorphous chalcogenide and organic polymer films, *24th Intern. Conf. on Amorphous and Nanocrystalline Semiconductors (ICANS24),* Nara, Japan, 21-26 August, 2011, Book of abstracts, p. 38.
19. U.Gertners, J.Aleksejeva, J.Teteris,, Photo-induced structural transformations in chalcogenide vitreous semiconductors, *24th Intern. Conf. on Amorphous and*

Nanocrystalline Semiconductors (ICANS24), Nara, Japan, 21-26 August, 2011, Book of abstracts, p. 143.
20. J.Aleksejeva, A.Gerbreders, U.Gertners, M.Reinfelde, J.Teteris, Polarization and Surface Relief Gratings in Disperse Red1 Doped Polyurethane Thin Films, *24th Intern. Conf. on Amorphous and Nanocrystalline Semiconductors (ICANS24),* Nara, Japan, 21-26 August, 2011, Book of abstracts, p. 169.
21. A.Gerbreders, Photosensitive Polyurethanes for Optical Record, *The 7th Intern. Conf. on Photonics, Devices and Systems (Photonics Prague 2011)*, Prague, Czech Republic, August 24-26, 2011, Book of abstracts, p.94.
22. U.Gertners, Direct Photo-Induced Surface-Relief Formation in Thin Layers of Chalcogenide Vitreous Semiconductors, *The 13th Intern. Conf."Advanced materials and technologies",* Palanga, Lithuania, 27-31 August, 2011, Book of abstracts, p.46.
23. J.Aleksejeva, A.Gerbreders, J.Teteris, Surface relief and polarization grating formation in azo-dye containingpolymer films, *Intern. Conf."Advanced optical materials and devices" (AOMD-7),* Vilnius, Lithuania, August 28-31, 2011, Book of abstracts, p. 10.
24. J.Teteris, Photoinduced mass transport in organic and inorganic polymers, *Intern. Conf."Advanced optical materials and devices" (AOMD-7),* Vilnius, Lithuania, August 28-31, 2011, Book of abstracts, p. 11.
25. A.Gerbreders, J.Aleksejeva, J.Teteris, Azo-polyurethane polymers for optical record, *Intern. Conf."Advanced optical materials and devices" (AOMD-7),* Vilnius, Lithuania, August 28-31, 2011, Book of abstracts, p. 21.
26. V.Kolbjonoks, V.Gerbreders, J.Teteris, Fabrication of gratings on chalcogenide As-S-Se thin films using electron beam, *Intern. Conf."Advanced optical materials and devices" (AOMD-7),* Vilnius, Lithuania, August 28-31, 2011, Book of abstracts, p. 23.
27. V. Kolbjonoks, V.Gerbreders, J.Teteris, A.Bulanov, E.Tamanis, Electron beam lithography on As-S-Se films, 8th Intern Conf. "HoloExpo-2011", 29 September- 01 October 2011, Proc. p.410-412.
28. M.Reinfelde, J.Teteris, Surface structuring by direct holographic recording, 8th Intern Conf. "HoloExpo-2011", 29 September- 01 October 2011, Proc. p.219-223.
29. J.Teteris, Photoinduced mass transport in organic and inorganic polymers, *V Ukrainian scientific Conf. on physics of semiconductors (USCPS-5)*, Uzhgorod, Ukraine, 9-15 October 2011,

LABORATORY OF VISUAL PERCEPTION

Head of Division Dr.habil.phys., Prof.I.Lacis

Research Area and Main Problems

Laboratory is a joint between colleagues in institute and department of Otometry and vision science of the University. Most of Department's Master thesis have been accomplished due to collaboration between units. All representatives of laboratory research staff and PhD students are members of department lecturers. The Optometry Master's program of the University has been established and is functioning to a large extent based on integration of research and study. The leading academic colleagues conduct research, also engaging students in scientific work. In 2011 more than 15 Bachelor's and 12 Master's thesis have been completed under supervision of laboratory researchers.

Research in laboratory is focused on following problems:

Visual evoked potentials related to visual perception;

- Aberrations of the eye and its impact on visual perception and retinal image quality;
- Color vision in visual perception and elaboration of new color vision tests;
- Aging and its impact on visual perception;
- Visual perception in road safety and new retroreflective materials;
- Kinematics of the Eye in describing cognitive processes;
- Vision in light scattering conditions, stray light and vision impairment;
- Subjective fixation disparity affected by dynamic asymmetry, resting vergence, and nonius bias.

Scientiffic staff
Prof. Ivars Lacis
Prof. Maris Ozolins
Asoc.prof. Gunta Krumina
Dr. phys. Gatis Ikaunieks
Dr.phys. Sergejs Fomins

PhD students
MSc. Varis Karitans
MSc. Aiga Svede
MSc. Ieva Timrote
MSc. Evita Kassaliete

Master student
BSc. Anete Pausus

Collaboration

Estonia
Tallin Health care college, Department of Optometry, (MSc. Vootele Tamme)

France
Laboratoire Regional des Ponts et Chaussees de Clermont-Ferrand (Dr. M. Colomb)

Germany
Institut fur Arbeitsphysiologie an der Universitat Dortmund (Dr. Wolfgang Jaschinski)

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

Scientific publications

1. Svede A, Hoormann J, Jainta S, Jaschinski W. (2011). Subjective fixation disparity affected by dynamic asymmetry, resting vergence, and nonius bias. *Invest Ophthalmol Vis Sci*., 52(7), 4356-4361.
2. K. Luse, M. Ozolins, V. Karitans, I. Jekabsone "Effect of position of retroreflective signs on recognition of pedestrian in reduced visibility conditions". Abstr. Int.Conf. „*DOC`2011*", Riga, p. 26 (2011).
3. S.Fomins, M.Ozoliņš, G.Krūmiņa, I.Lācis „Analysis of Rabkin Color Deficiency test under different illumination." Abstr. Int.Conf. „*Functional Materials and Nanotechnologies FMNT– 2011*", Riga, p.101 (2011).
4. M. Ozolinsh, I. Martín, D. Lauva, and V. Karitans „Howard-Dolman test at different opponent colour stimuli." *Journal of Modern Optics,* iFirst published on: 18 March 2011, DOI: 10.1080/09500340.2011.559313
5. E. Skutele, V. Karitans "Producing of ray tracing aberrometer for studying wavefront deformations". Abstr. Int.Conf. „*DOC`2011*", Riga, p. 70 (2011).

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 such as AlN, h-BN, AlGaN and some related materials such as Al_2O_3. Recently it was shown that 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. Our interests 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 materials mentioned above for elaboration of new luminescent materials for energy saving compact luminescent light sources. 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 (researcher)

Students - Technicians

1. Jana Grigorjeva (technician)
2. Roberts Kirsteins (technician)
3. Zanna Jevsjutina (technician)

Collaborations

Latvia

Institute of Inorganic Chemistry, Riga TU (Prof. J.Grabis)
Institute of Solid State Physics, University of Latvia

USA

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

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 investigations and results

PHOTOLUMINESCENCE OF Al_2O_3 NANOPOWDERS OF DFFERENT PHASES

L.Trinkler, B.Berzina, Z.Jevsjutina

Photoluminescence was studied in six samples of Al_2O_3 nanopowders produced from the same initial material by calcination in the 800-1400 ºC temperature range. At temperature around 1200 ºC phase transition in aluminum oxide lattice occurs; the samples produced at temperatures up to 1200 contain mainly δ phase, while those obtained at 1400 ºC contain pure α phase. In all studied samples of nominally pure aluminum oxide nanopowders photoluminescence is observed in red-infrared spectral range and determined by trace level concentrations of uncontrolled impurities. It was found that phase transition is accompanied with modification of the emission spectrum: a broad diffuse band centered around 750 nm presumably ascribed to emission of Fe^{3+} ions is characteristic for photoluminescence of the samples of δ phase, while narrow band emission of Mn^{4+} is observed in the samples of α phase. Aside from that emission of Cr^{3+} ion is observed in all studied samples with the difference that intensity, position and shape of emission bands are characteristic either to transient forms or to α phase of aluminum oxide. Switching of the active luminescence centers in the samples of the same composition with phase transition is tentatively explained by change of the crystal field symmetry affecting probability of electron transitions in impurity centers.

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

SPECTRAL CHARACTERZATION OF BULK h-BN AND MULTIWALL NANOTUBES

V.Korsak, B. Berzina, L.Trinkler

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. Two main predominant luminescence bands at 320 nm and 400 nm were established. Complex spectral investigations including luminescence and its kinetics measurements allow reveal luminescence mechanisms and defect structure forming luminescence centers.

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

LOW TEMPETATURE LUMINESCENCE OF AlN

L.Trinkler, B. Berzina, J.Grigorjeva

Photoluminescence of AlN ceramics and macro and nanopowders 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.

LUMINESCENCE STUDIES OF TERNARY AlGaN NANORODS AND NANOLAYERS

B.Berzina, L.Trinkler, J.Grigorjeva

Ternary compound AlGaN consists of two wide band gap components AlN and GaN with different band gaps E_g (6,2 eV and 3,2 eV, respectively) forming solid solution with common E_g depending on reciprocal concentration of Al and Ga atoms in material. Therefore, variation of concentration of Al and Ga components in $Al_{1-x}Ga_xN$ allows obtain material with variable band gap corresponding to wide spectral range of ultraviolet light providing its application in light emitting devices.

Spectral characterization of synthesized materials (nanorods and thin layers) synthesized at Taiwan National University was performed. The luminescence spectra were measured within wide temperature range from 8 K up to 300 K under sample excitation with laser light pulses at 266 nm and 310 nm. It was found that the exciton related luminescence band is observed within the spectral range of 320 nm – 400 nm and location of its maximum depends on value x characterizing the $Al_{1-x}Ga_xN$ material.

These studies were performed within a support of Mutual Funds Taiwan-Latvia-Lithuania Cooperation Project: “One-dimensional Nanostructures of Ternary AlGaN and metal doped-Zinc Oxide with Tunable Bandgaps: Growth, Characterization and Optical Properties”

Scientific Publications

1. L.Trinkler, B.Berzina, D.Jakimovica, J.Grabis, I.Steins *“Peculiarities of photoluminescence of Al2O3 bulk and nanosize powders at low temperature”*. Optical materials, 33 (2011), 817-822. doi:10.1016/j.optmat.2010.12.020

2. L.Trinkler and B.Berzina *“Luminescence properties in AlN ceramics and its potential application for solid state dosimetry”*. (pp. 59-82) A chapter in book Advances in Ceramics - Characterization, 82 Raw Materials, Processing, Properties, Degradation and Healing. ISBN 978-953-307-504-4, 370 pages, Publisher: InTech, Croatia, August 2011 http://www.intechopen.com/articles/show/title/luminescence-properties-of-aln-ceramics-and-its-potential-application-for-solid-state-dosimetry

3. V. Korsaks, B. Berzina, L. Trinklere. *“Low temperature 450 nm luminescence of hexagonal boron nitride”*. Latvian Journal of Physics and Technical Sciences N1 (2011) 55-60.

Lectures on Conferences

27th LU Scientific Conference of Institute of Solid State Physics, University of Latvia, February 14 - 16, 2011, Riga, Latvia

1. J.Grigorjeva, V.Korsaks, L.Trinkler, B.Berzina. "*Low temperature luminescence of AlN powders"*. Book of Abstracts, 2011, p.54.
2. Z. Jevsjutina, L.Trinkler and B.Berzina. *"Dependence of Al2O3 luminescence on temperature and grain size"*. Book of Abstracts, 2011 p. 55.

International Conference FM&NT; Functional materials and nanotechnologies 2011; Institute of Solid State Physics University of Latvia April 5 – 8, Riga

3. B.Berzina, V.Korsaks, L.Trinkler and J.Grigorjeva. *"Defect luminescence of III group element nitrides and hBN",* FM&NT Abstact book, p.45, Riga, 2011.
4. L.Trinkler, B.Berzina, Z.Jevsjutina, J.Grabis and I.Steins. *„Photoluminescence of Al2O3 nanopowders of different phases",* FM&NT Abstact book, p.103, Riga, 2011.

International Conference on New Diamond and Nano Carbons NDNC 2011, May 16 – 20, 2011, Matsue, Japan

5. V.Korsaks, B.Berzina and L.Trinkler. *„Defect luminescence of hBN: bulk powder and multiwall nanotubes",* NDNC 2011, Abstract book, p.100, Matsue, Japan, 2011.

9th International Conference on Nitride Semiconductors ICNS-9, 10 – 15 July 2011, Glasgow, UK

6. L.Trinkler, B.Berzina. *„Photo and thermoluminescence in AlN ceramics at low temperature"*, Abstract book, p. 67, Glasgow, UK, 2011.
7. B.Berzina, V.Korsaks and L.Trinkler. *„Native defect luminescence of III group element nitrides - AlN and hBN bulk and nanosize"*, Abstract book, p. 93, Glasgow, UK, 2011.

16th Conference on Nordic Society for Radiation protection, 22 – 25 August 2011, Reykjavik, Iceland

8. L.Trinkler and B.Berzina. *„UV radiation induced processes in AlN and its potential application for solid statne dosimetry",* Abstact book, p.76, Reykjavik, Iceland, 2011.

17th Internationas Symposium on Boron, Borides and Related Materials, 11 – 17 September 2011, Istanbul, Turkey

9. V.Korsaks, B.Berzina, L.Trinkler, R.Williams and B.Ucer. *„Spectral characterization of hBN powder and nanowall nanotubes",* Abstract book, p.134, Istanbul, Turkey, 2011.

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 2011

- 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

PhD Students

M.phys.G.Bakradze
M.phys. R.Zabels

Technical Staff

A.Petersons

Students

1. B.sc.R.Grants

Scientific visits abroad

1. R.Zabels, Nice, France (7 days).
2. Dr.J.Maniks, Nice, France (7 days)
3. Dr.I.Manika, St.Petersburg, Russia (7 days)
4. Dr.J.Maniks, Astana, Kazakhstan (14 days)

Visitors from Abroad

1. Prof.K.Schwartz, GSI, Darmstadt, Germany (6 days).
2. Dr.V.Sursajeva, ISSP Chernogolovka, Russia (19 days).

Cooperation

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

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

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

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

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

Main Results

SWIFT-ION-INDUCED NANOSTRUCTURING OF LiF CRYSTALS: COMPARISON BETWEEN HEAVY AND LIGHT PROJECTILES

J.Maniks[1], I.Manika[1], R.Zabels[1], R.Grants[1],E.Tamanis[2], K.Schwartz[3]
[1]ISSP, University of Latvia, 8 Kengaraga Str., LV 1063 Riga, Latvia
[2]University of Daugavpils, 1 Parades Str. LV5400 Daugavpils, Latvia
[3]GSI, Darmstadt, 1 Planckstrasse, D-64219 Darmstadt, Germany

Modifications of the structure of LiF crystals irradiated with swift heavy (^{238}U, ^{208}Au) and lighter (^{50}Ti, ^{12}C) ions of the specific energy of 11.1 MeV/u at fluences in the range of 10^{11} to 10^{13} cm^{-2} have been studied using the AFM, SEM, High-resolution XRD and nanoindentation methods. The structure was revealed by a chemical etching. The AFM and SEM studies on samples irradiated with heavy ions (^{238}U, ^{197}Au) showed a nanostructuring of the irradiated layer. The nanostructure consists of columnar grains with a width of about 50-100 nm. In the case of the lightest ions (^{12}C), the irradiation resulted in the formation of dislocation-reach structure. No bulk nanostructures were observed even at the highest fluence of 5×10^{12} cm^{-2}. For ions with an intermediate atomic mass (^{50}Ti), either a dislocation-reach structure or a nanostructure was formed in relation to the fluence and the energy loss.

In the nanostructured layer, the rocking curves obtained by a high-resolution X-ray diffraction expose the formation of a mosaic-type structure with low-angle boundaries between blocks.

Nanoindentation tests show a strong ion-induced increase of hardness (up to 150-200%) in the nanostructured zone confirming the high volume concentration of strong obstacles for dislocations, such as grain boundaries and defect aggregates. A marked hardening demonstrates also the dislocation-rich zone. The results show that swift-ion-induced structural fragmentation and nanostructuring in LiF can be reached at definite conditions of fluency and energy loss.

EFFECT OF NANO-POWDER MORPHOLOGY ON THE PROPERTIES OF ZnO SINTERED CERAMICS

R. Zabels, F. Muktepāvela, L. Grigorjeva, K. Kundziņš
Institute of Solid State Physics, University of Latvia, Latvia

In this work a simple method of Zn vapor condensation and oxidation in a tube furnace was utilized to obtain ZnO powders with grained (d=100-300 nm) and multipod-like (whiskers) (d=50-100 nm, l=3-10 μm) morphology. Powders were compacted at identical conditions and a following sintering performed at temperature of 1200 ^{o}C. Research included structural investigations using optical, AFM and SEM microscopies, a photoluminescence investigation for an evaluation of present defects and a nanoindentation to characterize a mechanical behavior and stability of obtained ceramics.

Ceramics sintered from the grained powder have large grains – in diameter ranging from 3 to 20 μm with an average size of about 10 μm. The surface of the ceramic is covered with large ZnO spheres which are a product of a rapid oxidation of an escaped excess Zn vapor. The porosity is high – polishing revealed that large voids with a size 10-80 μm are present throughout the volume of ceramics. Micropores are located not only at grain boundaries but inside grains as well. At 12 K besides an excitonic peak this ceramic exhibited a broad green luminescence band attributed to defect states (particularly oxygen vacancies or interstitial Zn) which is in an agreement with the SEM micrographs.

For the ceramic from the multipod-like powder grain sizes range from 1 to 10 μm with an average grain size of 4 μm. In this case micropores are present only in triple junctions of grain boundaries. No pores were detected inside the volume of grains. Luminescence at 12 K revealed a narrow excitonic band with a probable satellite peak and an almost non-existent green luminescent band which is an evidence of a high quality of ceramic sintered from whiskers powders. Mechanical properties (hardness is 3 GPa and Young's modulus 120 GPa.) of these ceramics are high and comparable to high pressure ceramics and a single crystal ZnO. Indentation tests have shown the specific role of the grain boundaries in the deformation behavior of ceramics. The effect of the powder morphology on the properties of sintered ceramics may be explained from the standpoint of contacts phenomena during the sintering.

Scientific publications

SCI publications

1. J. Maniks, I.Manika, R. Grants, R. Zabels, K.Schwartz, M.Sorokin, R.M.Papaleo, Nanostructuring and hardening of LiF crystals irradiated with 3-15 MeV Au ions**.** Applied Physics A: Materials Science and Processing 2011, vol.104, No.4, pp.1121-1128.
2. 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. Materials Science (MEDŽIAGOTYRA) 2011,vol. 17, No. 3, pp.223-228.
3. K. Kolev, T.Petkova, C.Popov, P.Petkov, F.Muktepavela, Surface development of $(As_2S_3)_{1-x}(AgI)_x$ thin films for gas sensor applications**.** NATO Science for Peace and Security, Series B: Physics and Biophysics**,** 2011, pp.203-209.

Other publications

4. V.Sursajeva, F.Muktepavela. Effect of the first order different edges on the motion of grain boundaries in Zn. Proc.9th Intern.Sci.and Tech. Conf. Advanced metal materials and technologies (AMMT'2011), June 22–24, 2011, St.Petersbugr, Russia. 400-401p.

5. E. Platacis. A Ziks, A Poznjak, F. Muktepavela, A. Shisko, S. Sarada. Corosion phenomena of FMS (P91) steel in Pb-Li flow in magnetic field. Proc. 8th PAMIR Int. Conf. Fundamental and Applied MHD. - September 5-9, Borgo, Corsica, France, 2011, p.587-592.
6. G.Bakradze**.** Initial oxidation of zirconium: oxide-film growth kinetics and mechanisms PhD thesis, Max-Planck Institute, Stuttgart University, Stuttgart 2011, p.111.
7.

Lectures on Conferences

International Conference on Functional materials and Nanotechnologies FM&NT 2011, April 5 –8, 2011, Riga, Latvia

1. R. Zabels, F. Muktepāvela, L. Grigorjeva, K. Kundziņš, Effect of nano-powder morphology on the properties of ZnO sintered ceramics. Book of Abstracts, PO-106, p.196..
2. J.Maniks, I.Manika, R.Zabels,R.Grants,E.Tamanis,K.Schwartz. Swift-ion-induced nanostructuring of LiF crystals: comparison between heavy and light projectiles. . Book of Abstracts, PO-107, p.197.
3. A.Dauletbekova, I. Manika, R. Zabels, R.Grants,. A.Akilbekov, M. Zdorovets. Aggregation processes and nanostructuring in LiF crystals irradiated with 150 MeV ^{84}Kr ions. Book of Abstracts, PO-108, p.198.

E-MRS 2011 Spring Meeting, May 9-13, 2011, Nice, France

4. J.Maniks, I.Manika, R.Zabels, R.Grants, E.Tamanis, K.Schwartz. Nanostructuring and strengthening of LiF crystals by swift heavy ions: AFM, XRD and nanoindentation study. Symposium B, Ion Beam Synthesis and Modification of Nanostructured Materials, Programm and Abstacts, PB1-12
5. A.Dauletbekova, J. Maniks, I. Manika, M. Zdorovets, A.Akilbekov, R.Zabels, R.Grants, Y. Bikhert, D.Akilbekova.. Ion-induced modification of LiF crystal properties: fluence and flux effects. Symposium B: Ion Beam Synthesis and Modification of Nanostructured Materials, Programm and Abstacts,PB2-31.
6. R. Zabels, F. Muktepavela, L. Grigorjeva, E. Tamanis, Deformation behavior and optical properties of nanostructured ZnO films on glass, Symposium D: Synthesis, Processing and Characterization of Nanoscale Multi Functional Oxide Films, Programm and Abstacts, P1-56.

3rd International Conference "Radiation Interaction with Materials and Its Use in Technologies, 20-23 September, 2011, Kaunas, Lithuania

7. 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, Wo-1, p.12.

International conference "Advanced Carbon Nanostructures" (ACN'2011), July 4-8, 2011, St.Petersburg, Russia

8. I.Manika, J. Maniks, R. Zabels, J. Gabrusenoks, M. Krause, M. Tomut, K. Schwartz, Nanoindentation and Raman spectroscopy study of graphite irradiated with swift ^{238}U ions. International conference "Advanced Carbon Nanostructures", St.Petersburg, Russia, 2011, July 4-8, Book of Abstracts, p.334.

9th Intern.Sci.and Tech. Conf. Advanced metal materials and technologies (AMMT'2011), June 22–24, 2011, St Petersburg

9. V.Sursajeva, F.Muktepavela. Effect of the first order different edges on the motion of grain boundaries in Zn., Russia Proc. 400-401p.(stenda)

27th Scientific conference of the ISSP, February 14-16, 2011, Riga, Latvia

10. R. Zabels, F.Muktepavela, L.Grigorjeva, K.Kundziņš, E.Tamanis. Obtaining of ZnO nanocrystallites via oxidation of Zn powder. Abstracts p.27.
11. R.Grants, R.Zabels, I.Manika AFM and nanoindentation study on LiF crystals irradiated with swift Kr ions. Abstracts p.28.

DEPARTMENT OF RADIATION PHYSICS

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

Research Area and Main Problems

The Department includes two research groups – the Laboratory of nuclear reactions and Laboratory of Transition Metals Compaunds 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 , FTIR, RAMAN and optical spectroscopies study of human blood after irradiation
- 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,γ), (d,p) and (d,t) nuclear reactions"** with Institute of Nuclear Physik (Rzez, Czech Republic), Technical University Munich, Institute Laue -Langevin (Grenoble, France).

Scientific Staff:

Dr.hab. J.Berzin
Dr.hab. M.Balodis
Dr.hab. V.Bondarenko
Dr.hab. N.Mironova - Ulmane
Dr. L.Simonova
Dr. T. Krasta
Dr. D.Riekstina
Dr. V.Skvortsova
Dr. O.Veveris
Dr.Ing.sc. A.Pavlenko
Mag. Sc. M.Polakovs
Dr. J. Proskurins

Technical Staff :

S.Afanasjeva

Students:

Mag. students K. Bavrins

Scientific visits abroad

Dr. hab. J. Berzins, European Commission Euratom, Brussels,Belgium (8 days), 2011.
Dr. hab. J. Berzins, Cyclotron Workshop, Ispra, Italy 28-29 November 2011.
Dr. hab. J. Berzins, Insitut Laue Lagevin, Grenoble, 2-5 February 2011.
Dr. hab. J. Berzins, Insitut Laue Lagevin, Grenoble, 5-13 December 2011.
N.Mironova-Ulmane, Institute of Physics Tartu Estonia (3 week)
N.Mironova-Ulmane Sweden (1week)
N.Mironova-Ulmane, Coimbra, Portugal (1week)
M..Polakovs Coimbra, Portugal (1week)
N.Mironova-Ulmane Minsk, Belarus (1week)
V. Skvortsova. , Minsk, Belarus(1week)
A.Pavlenko IAEA Wiena,Austria (10 mounth)

Cooperation

Latvia
1. Stradina university of Latvia (Dr. hab., Prof. M.Eglite, Dr.T.Zvagule).
2. Radiation Safety Center.
3. University of Latvia, Institute of Chemical Physics (Dr. G. Kizane)
4. Institute of Wood Chemistry (Dr. hab. G. Dobele, Dr.hab. G. Telesheva, Dr.hab.T.Dizbit)
5. Riga Technical University, Faculty of Material Science and Applied Chemistry (Dr.Berzina-Cimdina r).
6. Institute of Technical Physics, Rīga Technical University (Dr.J.Ruža).
7. Riga Technical University, Faculty of Material Science and Applied Chemistry (Prof. J.Dehtjar,).

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 (Dr. W. Urban, Dr. M. Jentchel).

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

Czech Republik
1. Nuclear Research Institute, Řež (Dr. J.Honzatko, Dr. I.Tomandl).

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

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 Metal Physics, Urals Division of Russian Academy of Sciences, 620219 Yekaterinburg, Russian Federation (Ac. Dr. Sc B.N.Goscickii, Dr. V.Voronin**).**

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

Main results

DEVELOPMENT OF THE ODD-ODD ^{188}Re NUCLEUS LEVEL SCHEME ABOVE 800 keV

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

Our previous study of the doubly odd transitional ^{188}Re nuclear structure [1] was based on γγ-coincidences measured following the ^{187}Re(n,γ)^{188}Re reaction with thermal neutrons at the nuclear reactor in Řež (Czech Republic). The level scheme of ^{188}Re was established up to 800 keV excitation energy, considerably extending and correcting the earlier level scheme of Shera et al. [2].

Due to extreme level density, characteristic to nuclei belonging to the transitional A~190 region, development of the ^{188}Re level scheme above 400 keV requires high precision data about γ-transition energies and intensities. Such data have been obtained via thermal neutron capture measurements with the same enriched ^{187}Re target at ILL (Grenoble, France), employing the high precision crystal-diffraction spectrometer GAMS5. Additional energy and angular γγ-coincidence measurements have been performed as well. Obtained spectra provided data about more than 800 γ-transitions in the energy range from 105 to 1860 keV. These data have essentially higher resolution above 350 keV energy than those of earlier crystal-diffraction measurements [2].

Analysis of obtained new and previous [1] spectroscopic information allowed establish confidently the depopulation data for 122 levels of ^{188}Re in the energy range from 800 to 1585 keV: 79 of these levels are populated by primary γ-rays. Five new levels have been established also in the energy range 600-800 keV. As a result, the level scheme of ^{188}Re now includes 190 levels: 115 levels of negative parity and 75 levels of positive parity. The level scheme is strongly supported by observed high-low and low-low γγ-coincidences.

In our earlier work [1], the most of ^{188}Re levels below 800 keV energy have been interpreted in terms of rotational bands based on Nilsson two-quasiparticle configurations. Now, in addition to already known 7 negative parity and 6 positive parity rotational bands, associated with proton orbits 5/2[402] and 9/2[514], and neutron orbits 1/2[510], 3/2[512], 7/2[503], 9/2[505] and 11/2[615], we propose three new tentative negative parity structures above 500 keV energy: the $K^{\pi}=0^-$ rotational band with 0^- level at 611.5 keV, 1^- level at 582.2 keV, and 2^- and 3^- members at 723.4 and 782.8 keV, respectively; the $K^{\pi}=1^-$ rotational band at 735.2 keV with 2^- level at 813.2 keV and 3^- level at 925.2 keV; and the $K^{\pi}=4^-$ band with 4^- member at 558.3 keV and 5^- member at 739.8 keV. These rotational bands are interpreted using two-quasiparticle configurations involving proton orbit 7/2[404]. The earlier proposed [1] $K^{\pi}=1^-$ rotational band with bandhead level 582.2 keV has been taken apart.

The Nilsson particle-plus-rotor model calculations, performed with program package described in [3], have shown that below 400 keV one can reproduce most of ^{188}Re levels assuming axially-symmetric core deformation with ε=0.18 and ε_4=0.05. However, the observed density of levels in the 400-1000 keV range, especially those with spins 3^+,4^+, is about three times greater than predicted by the particle-plus-rotor model calculations in the case of axially-symmetric deformation. Also, the calculated energies of two-quasiparticle bands with proton orbit 7/2[404] are about 200-300 keV lower than their proposed experimental positions. It can indicate a coexistence of states with different shapes at energies above 400 keV. A possibility of non-axial deformation for nuclear states including neutron orbits with high orbital moment j values, e.g., 11/2[615] and 9/2[505], in transitional region tungsten and osmium isotopes has been indicated also in [4].

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SYSTEMATIC STUDY OF PROTON-NEUTRON INTERACTION IN TRANSITIONAL ODD-ODD NUCLEI

T. Krasta, M. Balodis, J. Bērziņš

One of the outstanding and to date largely unresolved problems in nuclear spectroscopy is a proton-neutron coupling in nuclei. Proton-neutron interaction is believed to be a major force causing nuclear deformation. Proton-neutron levels can be studied experimentally by measuring properties of odd-odd nuclei. However, excitation patterns of these nuclei are far more complex than the structure of even-even or odd-A nuclei. In odd-odd nuclei, proton-neutron coupling results in many low-excitation levels, members of proton-neutron multiplets. A large number of low-energy transitions between these levels resulting in very complex spectra has for years limited effectively their studies. However, constant progress in experimental techniques permits nowadays to access with more confidence this difficult field.

In the case of nuclei belonging to transitional deformation region at A~190, there are still very few data about confidently established two-quasiparticle Gallagher-Moszkowski (GM) doublets and Newby shifts in K=0 bands [1]. Though the residual NN-interaction, and especially its tensor component, plays an essential role in the structure of low-lying levels of these γ-soft odd-odd nuclei due to considerably greater level density than in the stable deformation region, and also because the ΔK=0 mixing between two-quasiparticle states is most important due to large $\Delta\Omega$ values of involved proton and neutron orbits, the behaviour of residual NN-interaction matrix elements in the case when initial and final single-particle states belong to different deformation modes is yet unstudied problem.

Importance of correct accounting of all residual proton-neutron interaction terms both diagonal and non-diagonal, in order to reproduce the observed low-lying level scheme of transitional doubly odd nuclei, have been demonstrated by detailed particle-plus-rotor model calculations in the case of ^{188}Re. The values of corresponding V_{np} matrix elements have been calculated using expressions and parameter values given in [2]. It has been found that, in the case of ^{188}Re, it is especially important to include core polarization effects, i.e., the low-lying levels are best reproduced when one takes into account the central Gauss interaction potential with both short and long-range components, and includes spin polarization of central forces as well. The tensor interaction parameters: V_T=-32.5 MeV, V_{TM}=3.3 MeV, were chosen so as to

reproduce the empirical value E_{Newby}=-57.47 keV of levels in the $K^{\pi}=0^{+}$ (p:9/2[514]-n:9/2[505]) rotational band.

In order to study proton-neutron interaction in neighbouring transitional nuclei, the systematic of available experimental data about two-quasiparticle doublets and Newby shifts in odd-odd rhenium (Z=75) and iridium (Z=77) isotopes has been made. It has been found that for ^{190,192,194}Ir nuclei there are data about 18 GM-doublets (of which 6, mostly in ^{192}Ir, are questionable) and 7 Newby shifts. In the case of ^{186}Re, there are 5 complete GM-doublets (one questionable). Therefore, for thorough study of proton-neutron interaction in A~190 transitional deformation region nuclei, one must obtain additional experimental information about ^{186}Re and ^{192}Ir structure. Corresponding measurement project, employing the advantages of high precision crystal-diffraction spectrometer GAMS5, has been submitted to ILL, and first thermal neutron capture measurements of ^{186}Re nuclei have been performed.

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TRITIUM CONCENTRATION IN DRINKING AND GROUND WATER IN LATVIA

D.Riekstina, O.Veveris

The results of tritium content measurements in drinking and ground water are presented. The liquid scintillation counting (LSC) method has been used for determining tritium content in drinking water taken from 155 communal and 54 food manufacturer water sources in all regions of Latvia. Tritium concentration in all measured samples was < 10 Bq/L. Monitoring of tritium in the ground waters near the shutdown Salaspils nuclear reactor and the radioactive waste repository “Radon” has been carried out since 1997. During this period, the concentration of tritium has decreased from 8900 to 100 Bq/l in “Radon” and from 7200 to 29 Bq/L in Salaspils. Quality assurance of the obtained results has been ensured according to the EN ISO/IEC 17025 standard.

CONFORMITY ASSESSMENT IN RADIOACTIVITY MEASUREMENTS

Daina Riekstina, Janis Berzins, Olgerts Veveris

The role of conformity assessment in measurements of radioactivity is discussed. In our Laboratory of Radiation Physics there is carried out testing of natural as well as artificial radionuclides in different environmental samples (soil, precipitation, different types of water, needles, etc.), of various types of samples irradiated in the nuclear reactor and in the radioactive polluted objects. The credibility of obtained results is ensured by the quality assurance and control. The main requisitions involved in the quality assurance of the laboratory according to the requirements of ISO/IEC 17025:2005 /1/ are: 1) the use of calibrated equipment only; 2) the regular and long-time use of reference materials for the control of equipment; 3) the estimation of uncertainty sources and determination of uncertainties within the given interval of credibility; 4) the validation and verification. One of the most important requirements is a regular participation in the interlaboratory comparison exercises, which enables one to estimate and disclose possible sources of non-conformities as well as to carry out the corrective actions.

STRUCTURE AND PHASE CHANGES IN NATURAL AND SYNTHETIC MAGNESIUN ALUMINIUM SPINEL

V.Skvortsova, N.Mironova-Ulmane, D.Riekstiņa

Natural spinel crystals from Ural and Pamir deposits and synthetic magnesium aluminium spinel single crystals with different stoichiometry ($MgO \cdot nAl_2O_3$) grown by Verneuil method were used. The photoluminescence (PL), its excitation (PLE) and optical absorption of stoichiometric and nonstoichiometric magnesium aluminium spinel crystals containing the chromium and manganese ions and defects produced by fast neutron irradiation(fluence up to $10^{20}cm^{-2}$, E>0.1 MeV) are investigated. The broadening of R- and N-lines takes place in synthetic stoichiometric spinel. Structure of synthetic nonstoichiometric spinels (n>1) has to be more disordered, since in addition to the site exchange the so called stoichiometric vacancies are present in the structure. The R- and N-lines broadening takes place after spinel crystals irradiation by fast neutron too. The neutron irradiation causes increasing of the spinel inversion. Furthermore the great deviation from stoichiometry leads to the local structure of α-Al_2O_3 formation around Cr^{3+} ions. The orange emission band at 570 nm is belonging to complex center "Mn^{2+}-F^+ (or F centre)".

OPTICAL ABSORPTION AND LUMINESCENCE OF NEUTRON IRRADIATED MAGNESIUM OXIDE

V. Skvortsova, L. Trinkler

It is known that the absorption spectra of the neutron irradiated pure MgO consists of four bands with maxima 250, 357, 570 and 980 nm, associated with radiation defects [10-12]. In additional to above mentioned bands after irradiation by fast neutron at fluence $10^{18}cm^{-2}$ are observed two week bands at maxima ~ 485 and 746 nm. Figure 1 gives the absorption spectra of MgO crystal after fast neutron irradiation and annealed at different temperature. The addition band with maxima 485 and 745 nm disappear at temperature above 700 K. These bands position coincide with band position observed in irradiated and annealed $Mn_cMg_{1-c}O$ single solid solution [13], when band with maximum ~ 500 nm belongs to a complex Mn^{3+}-V_{Mg}. The lowest spin–allowed transition $^5E \rightarrow {}^5T_2$ of Mn^{3+} was observed in [14]. Jahn-Teller effects modify the energy level scheme from the Tanabe-Sugano description. The band 745 nm coming from Mn^{3+}. Appearance and disappearance take place in consequence the next reaction: $Mn^{2+} + h\nu \rightarrow Mn^{3+} + e^-$; $Mn^{3+} + Fe^{2+} \rightarrow Mn^{2+} + Fe^{3+}$. The absorption and luminescence spectra behaviour of magnesium oxide containing transition metal ions exposed to a fluence of fast neutrons up to $10^{18}cm^{-2}$ (E>0.1 MeV) and annealed are investigated. It is shown that the sharp lines after irradiation with fast neutrons in the 850-950 nm regions belong to exchange coupled Fe^{3+} - Fe^{3+} pairs. The absotption band 745 nm in irradiated MgO crystals coming from Mn^{3+}.

EPR AND FT-IR SPECTROSCOPIES STUDY OF HUMAN BLOOD AFTER IRRADIATION

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In the present work we report results of investigations of blood after irradiation by electron paramagnetic resonance (EPR) and infrared spectroscopies. The blood of Chernobyl clean-up workers was investigated using EPR tehnique and blood of patients after radioisotope Tc_{99m} diagnosis was investigated by EPR and FT-IR spectroscopy.

FT-IR absorption spectra of initial (control) and irradiated blood samples were recorded on a micro plate reader HTS-XT (Bruker) in 400-4000 cm^{-1} region. Data were processed by OPUS 6.5 using hierarchal cluster analysis (HCA), 2nd derivatives, and integration for sample discrimination and quantitative analysis.

The EPR spectra of blood were measured on a BRUKER EMX-6/1 spectrometer equipped with an Aspect 2000 data system. An ER 4102 ST Universal X-Band Resonator (TE102 mode) was used. The g-factors of EPR signals were determined by reference to the external magnetic field value measured by a Bruker ER 035 Gaussmeter and of the microwave frequency measured by a Systron Donner 6235A frequency counter.

HCA discriminated initial and irradiated samples confirming the radiation caused changes in blood. Main changes were detected in intensities and profiles of both amid bands. Irradiation caused the decrease of protein concentration. Evaluation of initial and irradiated sample IR spectra profiles clearly showed changes in proteins. The ratio of Amid I and Amid II band intensities was significantly higher in initial samples. FT-IR spectra analysis showed that blood proteins are influenced by radiation.

Compared the EPR spectra of human blood not participated in Chernobyl clean-up action and spectra of chernobyl clean-up workers we are confirmed in opinion that chernobyl clean-up workers meet methemoglobin (Fe^{3+} in high spin state) higher than normal people. The heightened level of transferrin was registered as well. The EPR spectra of people blood after radioisotope diagnosis show the Fe^{3+} (in high and low spin states) higher level compared to spectra of people before radioisotope diagnosis.

EPR and FT-IR spectroscopy could to be powerfull instrument for investigation of influance of radiation on human blood. EPR can detect the concentration of methaemoglobin and transferrin ions of more accurately than any other technique.

EXCITATION WAVELENGTH-DEPENDENT CHANGES IN RAMAN MICRO-SPECTROSCOPY OF HEMOGLOBIN

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In the present work we report the application of the Raman technique to study hemoglobin (Hb) in single erythrocyte using three different laser excitation lines: ultraviolet (441.6), visible (514.5 nm, 532 nm) and near-infrared (830 nm). The Raman spectra of the hemoglobin in single erythrocytes were recorded on ”Nanofinder-S” using the 441.6 nm and 532 nm excitation line and on a Renishaw Via instrument using 514.5 nm excitation radiation

from a argon laser system and 830 nm from diode laser. Raman excitation line used in 441.6 nm cause resonance enhancement with absorption band 415 nm (Soret band). The local coordinate of this band (pyrrole half ring stretching vibration) involves principally C–N stretching. We report the unusual enhancement of several bands in Raman scattering spectra of hemoglobin at excitation line 830 nm compared with the 441.6, 514.5 and 532 nm wavelengths investigated. The origin of unusual enhancement of Raman scattering bands of hemoglobin will be discussed.

Resonance Raman (RR) spectroscopy is a particularly sensitive probe for studying the electronic and structural properties of metalloporphyrin complexes including haemoglobin (Hb) and myoglobin. The interpretation of the intense spectra obtained from metalloporphyrin complexes has been based on vibronically induced scattering from the B (Soret) or Q states from the porphyrin macrocycle. Resonance Raman scattering from Hb occurs only at its surrounding ligands group because only this part of the molecule absorbs in the visible and near ultraviolet region. Thus it is possible to investigate exclusively vibrations of the four heme groups of Hb without interference by scattering of the surrounding globin or other parts of the red blood cell (RBC) or erythrocyte. In this technique, laser excitation within an electronic absorption band produces selective enhancement of Raman bands associated with vibrations of the protein. In the case of heme proteins, vibrations of the porphyrin ring are enhanced due to resonance with the π-π* transitions which dominate near ultraviolet absorption spectra. (the Soret band) and the visible (the α-β band). Different Raman scattering bands are brought out by excitation in the regions of the Soret absorption band or of the α-β absorption band.

NUCLEAR LEVELS OF ^{183}W STUDIED WITH *(n,γ)* AND *(*d, p*)* REACTIONS

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The level structure of ^{183}W has been studied using gamma–gamma coincidences from thermal neutron capture in 182W accompanied with the reaction *(*_d, p*)*. From these data and those of previous studies a total of 76 levels and about 490 connecting *γ* -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 numbe rof 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 *γ* -soft nuclei in the Os-Pt region.

Scientific Publications

1. V. Bondarenko [d], I. Tomandl [a,b], J. Honzátko [b], H.-F.Wirth,[e], T. von Egidy, „Nuclear levels of 183W studied with (n,γ) and (d, p) reactions" Nucl.Phys. A 856 (2011) p. 1-45.
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. D. Riekstina, O.Veveris. Tritium concentration in drinking and ground water in Latvia, LSC 2010, Advances in liquid scintillation spectrometry, Proc of the 2010 Int, LSC, Paris, France, Edit. P. Cassette, Tucson, Arizona, USA, 2011, pp. 95-98.
4. D. Riekstina, J. Berzins, O.Veveris. Conformity assessment in radioactivity measurement.Pros. of The 4th International Conference on Metrology, Jerusalem, Israel, 23-24 May 2011.
5. V Skvortsova, N. Mironova-Ulmane, D. Riekstina, Structute and phase changes in natural and synthetic magnesium aluminium spinel, Proc. of 8th Int. Scient and Pract. Conf. June 20-22, 2011, Rezekne, pp. 100-106.
6. J. Berzins, D. Riekstina, N. Mironova-Ulmane, in "50 years of Salaspils research reactor" (0n Latvian) Riga, Zinatne. 2011.
7. J Proskurins, "Study of Quantum chaos and phase transitions in nuclear models" Doctoral thesis, Riga, 2011.
8. N. Mironova-Ulmane, A. Kuzmin, , J. Grabis I. Sildos, V.I. Voronin, I.F. Berger and V.A. Kazantsev Structural and Magnetic Properties of Nickel Oxide Nanopowders. Solid State phenomena (2011) Vols.168-169. pp.341-344
9. N. Mironova-Ulmane, A. Kuzmin, I. Sildos, and M. Pars, Polarisation dependent Raman study of single-crystal nickel oxide, Centr. Eur. J. Phys. 9 (2011) 1096-1099.
10. N. Mironova-Ulmane, M. Polakovs, J. Grabis, V. Serga, L.Kulikova, D. Jakovlevs, I. Sildos, Mairov. Raman spectroscopy and magnetic properties nanosized of $CoFe_2O_4$. Proc. Int. Conf. "Actual problems of solid state physics-2011", 18-21 October 2011, Minsk, Belorus,.pp.101-103.
11. V. Skvortsova, L. Trinkler. Transition metal ions luminescence in neutron irradiated magnesium oxide. *IOP Conference Series: Materials Science and Engineering* , 2010, v. 15, p.012055(1-6).
12. V. Skvortsova, N. Mironova-Ulmane, D. Riekstiņa. Structure and phase changes in natural and synthetic magnesium aluminium spinel, "Environment. Technology. Resources", Proceedings of the 8th International Scientific and Practical Conference, Rēzeknes Augstskola, Rēzekne, RA Izdevniecība, 2011, vol. 2, pp. 100-106.
13. N. Mironova-Ulmane, Radiation-induced processes in oxides Proc. Int. Conf. "Actual problems of solid state physics-2011", 18-21 October 2011, Minsk, Belorus,.pp. 20-22.

Conference Presentations

1. J.Bērziņš, M. Balodis, T.Krasta Nuclear structure studies at Salaspils reactor, LU CFI 27. sci.. conf.. 2011 g. 14.-16. Febr. Abstracts, p.17.
2. J.Bērziņš, M. Balodis, T.Krasta, V. Bondarenko, Ļ.. Simonova Structure studies of A~190 transitional region odd-odd nuclei, LU CFI 27. sci. conf. 2011 g. 14.-16. Febr. Abstracts,p.18.
14. D.Riekstiņa. Neutron activation analysis in Salaspils nuclear reactor. LU CFI 27. sci.. conf.. 2011 g. 14.-16. Febr. Abstracts, p.19.

15. D.Riekstiņa, J. Berzins, O.Veveris. Conformity assessment in radioactivity measurement. The 4th International Conference on Metrology, Jerusalem, Israel, 23-24 May 2011.
16. M.Balodis, J.Bērziņš, V.Bondarenko, T.Krasta, L.Simonova M.Jentschel, W.Urban Tomandl, „Thermal neutron capture study of ^{188}Re levels", CGS-14 (The 14th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics)Guelph, Canada, August 28 – September 2, 2011.
17. D.Riekstiņa, J.Berzins, O.Veveris, Application of gamma spectrometry and LSC in control of environment. Programme quide & book of abstracts 14th International Congress of Radiation Research, Warsaw, Poland, 28.08 - 01.09, 2011, pp. 170-17.
18. N. Mironova-Ulmane Radiation-induced processes in solids Abstracts of the 27th Scientific Conference g. February 14.-16. febr.2011 p.20.
19. V. Skvortsova. Luminescence of chromium and iron ions in magnesium oxide crystals. Abstracts of the 27th Scientific Conference . February 14.-16. febr.2011 p. 84.
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23. M. Polakovs , N. Mironova-Ulmane, A. Pavlenko, T. Zvagule, N. Kurjane, N.Gabrusheva Study of iron proteins in blood of Chernobyl clean-up workers by EPR. . International Baltic Sea Region conference „Functional materials and nanotechnologies FM&NT-2011" 5-8 April, Riga, Latvia, p. 115.
24. N. Mironova-Ulmane, M. Polakovs, J. Grabis, V. Serga, L.Kulikova, D. Jakovlevs, I. Sildos.Raman spectroscopy of $CoFe_2O_4$. . International Baltic Sea Region conference „Functional materials and nanotechnologies FM&NT-2011" 5-8 April, Riga, Latvia, p.274.
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26. M.Polakovs, N. Mironova-Ulmane, I. Sildos excitation wavelength-dependent changes in Raman micro-spectroscopy of hemoglobin 14th European Congress on Spectroscopy of Biological molecules (ECSBM-11), Coimbra, Portugal, August 29t August - 3rd September 2011, p.4.
27. M.N. Palatnikov, A.N. Salak, K. Bormanis, O.B. Scherbina, V.V. Efremov, N.V. Sidorov, I.N. Efremov, and N. Mironova-Ulmane. Structure and Elastic Properties of Sodium Niobate Ceramics Prepared at High Pressure. 16th-semiconducting-and-insulating-materials-conference (SIMC-16) Tu3-31.
28. K. Bormanis, A. Kalvane, A.I. Burkhanov, I.E. Tumanov, and N. Mironova-Ulmane Dielectric properties of PMN+2%Li_2O at low and infra-low frequencies. 16th-semiconducting andinsulating-materials-conference (SIMC-16) Tu3-33.

29. M.N. Palatnikov, K. Bormanis, V.V. Efremov, N.V. Sidorov, I.N. Efremov, and N. Mironova-Ulmane. Dielectric Properties of Lithium-Sodium Tantalate-Niobate Solid Solutions. 16th-semiconducting-and-insulating-materials-conference (SIMC-16) Tu3-31.

Physics Doctor students:

1. Jevgenijs Proskurins – Study of quantum chaos and phase transitions in nuclear models. Supervised by Dr.T.Krasta. the thesis were preentedin June 2011.

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Lectures at Universities, Institutes …

During 2011, 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		**PhD students**
Inta Muzikante	Dr.habil.phys.	Elīna Laizāne
Lilita Gerca	Dr.chem.	Jānis Latvels
Egils Fonavs	Dr.phys.	Andrejs Tokmakovs
Mārtiņš Rutkis	Dr.phys.	Aivars Vembris
Oskars Vilītis	Dr.phys.	Edgars Nitišs
Andrejs Jurģis	Msc.phys.	Jurģis Sīpols

Students

Martins Porozovs	Martiņš Narels
Kaspars Pudžs	Santa Popova
Raitis Gržbovskis	Eduards Titavs
Igors Mihailovs	

Scientific projects of the Latvian Council of Sciences

09.1548	Physical Processes in Multilayer and Multicomponental 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

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

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

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

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

International projects

Projects of Mutual scientific co-operation fund of Republic of Lithuania and the Republic of Latvia with R.O.C. (Taiwan):	
ISSP LU Kaunas Technology University	Design, Synthesis and Studies of New Effective Materials for Organic (Opto)electronics (2008-2011)

Institute of Chemistry, Academia Sinica, R.O.C., Taiwan	

Main equipments:

1. 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).
2. 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.
3. Computer controlled corona poling systems.
4. Computer-controlled Kelvin probe setup with the temperature control up to +130ºC 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
5. Scanning Kelvin Probe SKP5050
6. Surface Profile Measuring System Dektak 150
7. Computer-controlled SHG setup (λ=1064 nm) allows us to measure SHG (λ=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 x 10^{-6} pm/V

Cooperations

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

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

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

Taiwan
1. Institute of Chemistry, Academia Sinica, (Prof. Chao-Ping Hsu)

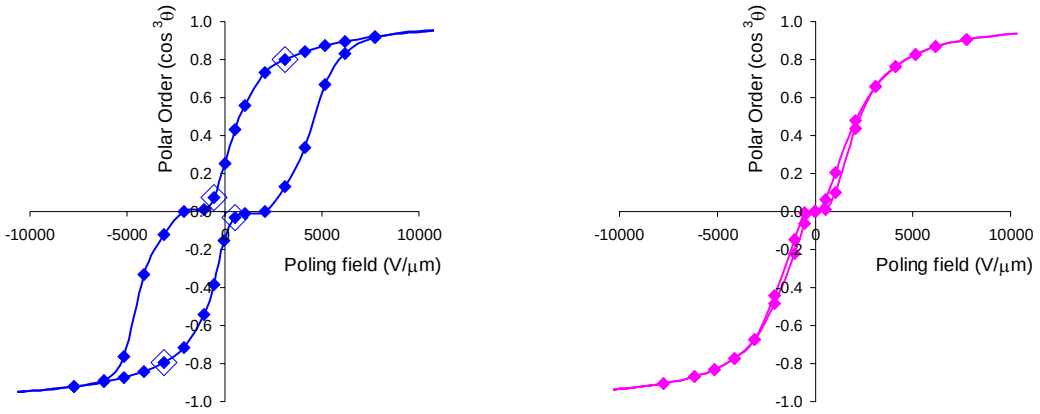
Main results

INSIGHT IN NLO POLYMER MATERIAL BEHAVIOR FROM LANGEVIN DYNAMIC MODELING OF CHROMOPHORE POLING

M. Rutkis, A. Jurgis

Calculation of chromophore polar order, i.e. polarization, of poled by external field nonlinear optically (**NLO**) active polymers is challenging. One of possible solutions is to reproduce the orientation polarization of chromophores under external field using Langevin dynamics (**LD**) molecular modeling.

a ***b***



DC poling hysteresis loops of model clusters built from 10 D dipoles with dipole density N = 10x10^{20} mol/cc: a) "Guest/ Host" system; b) and "Grafted" system

In spotlight of this investigation we would like to describe NLO polymer as a "coloid" mixture or "ferrofluid" were chromophores (in our case model dipolar molecules) take part in the role of active particles - electrets. According to our simulations of model systems at low dipolar densities such system behaves "paraelectric" like. For dipole densities within a range of practical interest polarization behavior of such "ferrofluid" profoundly depends on translation movement freedom of electrets and their dipole moment. In the model systems where translation movement of "electrets" is prohibited ("Grafted" models) an "antiferroelectric" behavior start to show up with increase of dipole density and moment value. In a case when "electrets" allowed moving freely ("Guest/Host") model systems behavior is different. Dipolar "chains" and "rings" are formed with dipole density rise in "Guest/Host" model systems. The dipolar "chains" could form "ferroelectric" like structure when oriented parallel or "antiferroelectric" like if in opposite orientation and "rings" definitely behaves "antiferroelectric" like. The shape of obtained polarization hysteresis loops allows us to suggest coexistence of both "antiferroelectric" and "ferroelectric" like structures in densely loaded "Guest/Host" model systems.

The outcome of these chromophore poling simulations of model systems by Langevin Dynamics convinced us, that method could be applicable for modeling of real chromophore/polymer composites. Results obtained within an investigated model systems give us some inspirations for practical **NLO** polymer design. First of all our model simulations confirm that at low (typically used for **NLO** polymers) poling fields high dipole moment chromophores are preferable and should yield a higher load factor and therefore

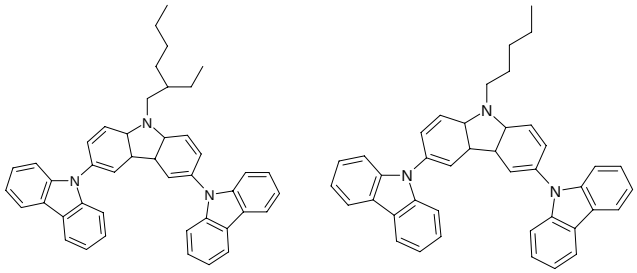
better **NLO** efficiency. In a case when one could achieve a higher poling field values low dipole moment chromophores should perform better and higher **NLO** efficiency achieved. Increased (above typically used nowadays) poling fields could be a key for breakthrough in **EO** polymer design. Possibility to achieve same (or even higher) NLO efficiency by using low $\boldsymbol{\mu}$ with high $\boldsymbol{E_p}$ scheme in contradiction to high $\boldsymbol{\mu}$ with low $\boldsymbol{E_p}$ could be recommended also due to eventually better ***PO*** stability.

*This research was granted by Latvian National Research Program in Materials Science, Project No.3 "Materials for photonics and nanoelectronics based on novel functional low molecular organic compounds and polymers" and Latvian Council of Science collaboration project 10.0032 „ Development of research and technology potential for elaboration of new and nanostructured materials and related applications." subproject 10.0032.14 "Supramolecular nanostructuring of photonic materials – theoretical modeling and experimental investigations"***.**

ENERGY STRUCTURE OF THIN FILMS OF CARBAZOLE DERIVATIVES WITH METAL ELECTRODES

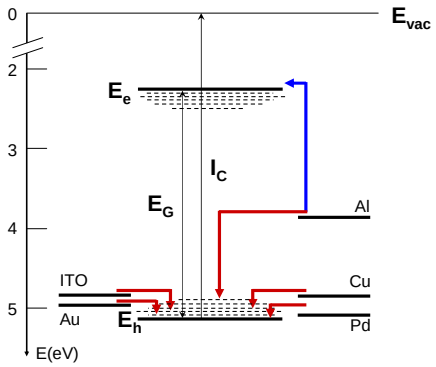
K.Pudzs, I.Muzikante, E.Fonavs**,**
J.Simokaitiene, S.Grigalevicius, J.V.Grazilevicius

Study of charge carrier transport in organic electroluminescent devices, organic photovoltaic devices, and organic field-effect transistors is one of the most important points. In order to realize comparable electron and hole transport in thin organic films with electrodes the energy structure of such devices are of great importance. In this work, we have studied electrical properties and energy structure of two carbazole derivatives.



1 **2**

*Chemical structure of carbazole derivatives **1** and **2** under study*



Energy diagram of electronic states in thin film of compound 1 and work functions of Al, Au, Ni, Cu and Pd electrodes.

The energy gap of two carbazole derivatives 1 and 2 in thin film is obtained. The energy gap characterisized by threshold energy of photoconductivity quantum efficiency is 2.90 eV and optical energy gap following from optical absorption spectrum is 3.3 eV for compound **1** in thin films. The values of the surface potential characterisizing ionization potential in solid state (hole conducting energy level) are 5.17 eV for compound **1** and 5.19 eV for compound **2**. The values of work function of ITO, Au, Cu and Pd electrodes are energetically close to conductivity level of holes (E_h) and holes injection dominates from electrodes. In these thin

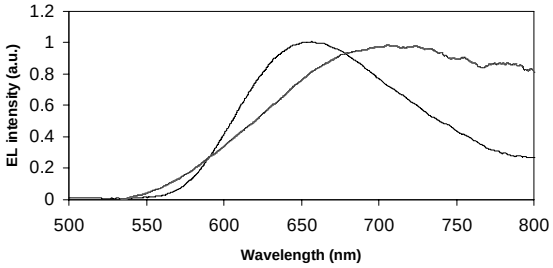
films local trapping states of holes are situated at holes conducting level. When electrode is Al layer the local shallow trapping states for electrons at $E_t = 0.10$ eV for compound 1 and at $E_t = 0.18$ eV for compound **2** are determined

This work is supported by ERAF Project Nr. 2DP/2.1.1.2.0/10/APIA/VIAA/010 and Latvian-Lithuanian-Taiwan joint project „Design, Synthesis and Studies of New Effective Materials for Organic Optoelectronics"

PYRANYLIDENE INDENE-1,3-DIONE DERIVATIVES AS AN AMORPHOUS RED ELECTROLUMINESCENCE MATERIAL

A.Vembris, M.Porozovs, I.Muzikante,
V.Kokars, E.Zarins

The organic light emitting diode (OLED) has a promising applications in flat panel displays and novel light sources. So far the OLED structures have mostly been made by thermal evaporation in vacuum. An alternative approach is to use small molecules which form amorphous (glassy) structure from solutions. Such compounds can be used in the ink-jet printing technologies and result in reducing the OLED prices. In this paper, we present an original red fluorescent organic compound 2-(2-(4-(bis(2-(trityloxy)ethyl)amino)styryl)-6-methyl-4H-pyran-4-ylidene)-1H-indene-1,3(2H)-dione (ZWK1) and it derivative 2-(2,6-bis(4-(bis(2-(trityloxy)ethyl) amino)styryl)-4H-pyran-4-ylidene)-1H-indene-1,3(2H)-dione (ZWK2) where methyl group replaced with 4-substituted-styryl group. This change could improve the formation of glassy structure.



Electroluminescence spectrum of ZWK1 (line) and ZWK2 (doted line)

The thickness of the electroluminescent layer in the device was optimized to the higher power efficiency and obtained: ITO/PEDOT:PSS(40nm)/ZWK1(95nm) /LiF(1nm)/Al(100nm) and ITO/PEDOT:PSS(40nm)/ZWK2(85nm)/LiF(1nm)/Al(100nm). The maximum of electroluminescence spectra for the device with ZWK1 compound was 667 nm wich correspond to the CIE coordinates x=0.65 and y=0.34. The power and luminance efficiency at the luminance of 100 cd/m^2 is 0.63 lm/W and 1.78 cd/A, respectively. Adding additional 4-substituted-styryl group to ZWK1 molecule shifted maximum of EL spectra to red region (705 nm) and decreased the efficiencies by one order.

This research was granted by Latvian National Research Program in Materials Science, Project No.3 "Materials for photonics and nanoelectronics based on novel functional low molecular organic compounds and polymers" and by the European Social Fund within the project «Support for Doctoral Studies at University of Latvia»

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Abstracts

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31. A.Vembris, I.Muzikante, R.Karpiz, V.Gulbinas, Red apmlified spontaneous emission in original; organic compounds, Book of Abstracts, p.89
32. M.Rutkis, I.Mihailovs, A.Tokmakovs, A.Ernstsons, Hyper-Rayleigh scattering measrements of molecular hyperpolarizability – comparison of internal and external standard methods, Book of Abstracts, p.90
33. E.Laizāne, D.Gustiņa, I.Muzikante, A.Vembris, Optical study of thin solid films with azobenzene molecules containing carboxyl groups, Book of Abstracts, p.60
34. E.Nitišs, E.Titavs, M.Rutkis, O.Vilītis, Current – voltage characteristics of corona triode setup for NLO polymer poling, Book of Abstracts, p.61

35. E.Nitišs, M.Rutkis, M.Svilans, Application of Abes matrix formalism for determination of thin organic film EO coefficients by Mach – Zehnder interferometer, Book of Abstracts, p.62

54th Scientific conference for young students of physics and natural science „Openreadings 2011", Vilnius, Lithuania, March 16-19,2011

1. K.Pudzs, A.Vembris, I.Muzikante, J.V.Grazulevicius, Energy structure of thin film determination in light emitting diode, Book of Abstracts,p.100
2. R.Grzibovskis, I.Muzikante, J.Latvels, M.Rutkis, Photoelectrical properties of DMABI derivatives in thin films, Book of Abstracts,p. 97

International Conference on Functional materials and Nanotechnologies FM&NT 2011, April 5 – 8, 2011, Riga, Latvia

1. S.Popova, A.Vembris, I.Muzikante, E.Kirilova, Optical properties of organic metal complex with Cr atoms, Book of Abstracts, p 106
2. A.Vembris, I.Muzikante, R.Karpicz, V.Gulbinas, Fluorescence characteristics of styryl-4H-pyran-4-ylidene fragment containing derivatives, Book of Abstracts, p 107
3. E.Laizane, D.Gustina, I.Muzikante, M.Narels, Optical study of thin solid films with azobenzene molecules containing carboxyl groups, Book of Abstracts, p 147
4. K.Traskovskis, I.Mihailovs, A.Tokmakovs, V.Kokars, M.Rutkis, Small Molecular Azobenzene and Indanedione Based Chromophores as Potential Non Linear Optics Materials, Book of Abstracts, p 148
5. K.Pudzs, I.Muzikante, Studies of energy structure of organic films with metal electrodes, Book of Abstracts, p 149
6. R.Grzibovskis, J.Latvels, I.Muzikante, M.Rutkis, "Photoelectrical Properties of Thin Films of DMABI Derivatives", Book of Abstracts, p 154
7. I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, M.Roze, G.Rozite, Open circuit voltage dependence on electrode material for P3HT based organic solar cells, Book of Abstracts, p 155

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1. K.Pudzs, I.Muzikante, A.Vembris, J.V.Grazulevicius, Determination of eenergy structure of carbazole derivatives thin films with metal electrode, Book of abstracts, p. 52
2. M.Narels, E.Laizane, I.Muzikante, Photoinduced optical properties of azobenzene-polymer films, Book of abstracts, p. 58
3. M. Rutkis, Design of organic materials for NLO applications: insights on theory based construction strategy, characterization and achievements, Book of abstracts, p. 20
4. E. Nitišs, M. Rutkis, M. Svilāns, Application of Abeles matrix formalism for determination of thin organic film EO coefficients by Mach – Zehnder interferometer, Book of abstracts, p. 24
5. R.Grzibovskis, J.Latvels, I.Muzikante, M.Rutkis, Energy Structure of Thin Films of DMABI Derivatives, Book of abstracts, p. 54

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1. I.Muzikante, J. Indrikova, J. Latvels, K. Pudzs, M. Rutkis, Determination of the energy structure of the sandwich-type organic thin films, Programme.

2. I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, P.Shipkovs, G.Kashkarova, M.Roze, J.Kalnachs, A.Murashov, J.Latvels, G.Rozite, Bi-layer GaOHPc:PCBM/3P3HT:PCBM solar cell, Programme.

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1. A.Vembris, I.Muzikante, R.Karpicz, V.Gulbinas, Stimulated emission from original glass forming organic compounds, Book of Abstracts, p.60
2. M.Rutkis, A.Jurgis, Inspirations for EO Polymer Design Gained from Modeling of Chromophore Poling by Langevin Dynamics, Book of Abstracts, p.51
3. I.Muzikante, E.Fonavs, R.Grzibovskis, J.Indrikova, J.Latvels, K.Pudzs, M.Rutkis, Determination of the energy structure of the organic molecules in thin films, Book of Abstracts, p.55
4. R.Grzibovskis, M.Indrikova, J.Latvels, I.Muzikante, B.Turovska, P.J.Pastors, V.Kampars, Photoelectrical properties of thin films of DMABI derivatives, Book of Abstracts, p.135.
5. A.Vembris, I.Muzikante, R.Karpicz, V.Gulbinas, S.Jursenas, A.Masojedovas, Luminescence properties of styryl-4H-pyran-4-ylidene fragment containing derivatives, Book of Abstracts, p.61
6. E. Nitišs, E. Titavs, M. Rutkis, O. Vilītis, Poling of EO polymers - corona disscharge process optimization, Book of Abstracts, p.126.
7. K.Pudzs, I.Muzikante, M.Rutkis, J.V.Grazulevicius, R.Reghu, Studies of charge carrier transport in organic films with carbazole derivative, Book of Abstracts, p.127.
8. J.Kreicberga, J.Sirotkina, V.Kampars, I.Mihailovs, M.Rutkis, A.Jurgis, Covalently coupled multi-DMABI hromophores: synthesis, linear and nonlinear optical properties, Book of Abstracts, p.148.
9. E.Laizane, D.Gustina, I.Muzikante, M.Narels, Temperature impact on photoisomerisation of carboxyl group containing azobenzene molecules in polymer films, Book of Abstracts, p.151.
10. I.Kaulachs, I Muzikante, L.Gerca, G.Shlihta, I.Tale, G.Rozīte, Electrodes for GaOHPc :PCBM/P3HT:PCBM Bulk Heterojunction Solar Cell, Book of Abstracts, p.112

European Conference on Organised Films ECOF-12, July 17-20, 2011, Sheffield, UK

1. I.Muzikante, E.Fonavs, J.Sipols, R.Grzibovskis, J. Latvels, M. Rutkis, V.Kampars, P.Pastors, B.Turovska, Determination of the energy structure of indandione chromophores in thin films, Abstracts, p.66,
2. E.Laizane, D.Gustina, I.Muzikante, M.Narels, Photoisomerisation kinetics of carboxyl group azobenzene derivatives at different temperature, Abstracts, p. 105
3. J.Teteris, J.Aleksejeva E.Laizane, Photo-induced mass transport in azobenzene containing organic polymers, Abstracts, p. 52
4. K.Pudzs, I.Muzikante, M.Rutkis, J.V.Grazulevicius, R.Reghu, Studies of charge carrier transport in organic films of perylene derivatives, Abstracts, p. 98
5. A.Vembris, I.Muzikante, R.Karpicz,V.Gulbinas, E.Zarins, V.Kokars, Red stimulated emission from glass forming organic compounds, Abstracts, p. 104

International Conference "Advanced optical materials and devices AOMD-7", August 28-31, 2011, Vilnius, Lithuania

1. E. Nitišs, M. Rutkis, M. Svilāns, Influence of multiple internal reflection and sample thickness change effects on determination of polymer film EO coefficients using MZI technique, Abstracts, p. 24

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1. I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, P.Shipkovs, G.Kashkarova, M.Roze, J.Kalnachs, A.Murashov, J.Latvels, G.Rozite, Electrode influence on bi-layer bulk heterojunction solar cell containing P3HT, CD

52th International Scientific Conference of Riga Technical Universit, October 13-15, 2011, Riga, Latvia

1. V.Kampars, P.Pastors, M.Rutkis, I.Muzikante, J.Sipols, B.Turovska, Evaluation of LUMO energies of DMABI analogues by voltammetry and quantum chemical calculation, Abstracts, p. 17
2. V.Kampars, J.Kreicberga, P.Pastors, M.Roze, S.Gaidukovs, K.Balodis, M.Plotniece, J.Sirotkina, L.Laipniece, N.Kiričenko, K.Pīterāne, L.Vesjolaja, G.Bērziņa, B.Turovska, I.Muzikante, M.Rutkis, Jaunu organisko hromoforu sintēze un to raksturojumi, Abstracts, p. 90
3. E.Zariņš, J.Jubels, V.Kokars, A.Vembris, I.Muzikante, Apjomīgotritilgrupu saturošo luminoforu sintēze un īpašības, Abstracts, p. 87

LABORATORY OF ELECTRONIC ENGINEERING

Head of Laboratory Dr. phys. A. Kristins

Main Problems

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

Scientifical Staff

1. Dr. A.Kristins
2. Mg. ing. D.Gusevs

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

The prospects of the instruments look at appendix.

2. Competence Centre ELIKO

Estonia

1. Tallinn University of Technology

Our Clients

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

etc.

Lectures on Conferences

27th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2011

1. I.Gvardina, A.Kristiņš, J.Melderis, J.Zvirgzds *Heat pump control unit.* Abstracts, p.38.
2. D.Gusevs. *Usage of automatic passenger counting system for public transport purposesr.* Abstracts, p.39.
3. P.Annus, M.Rist, J Ojarand, R.Land, A.Kristiņš. *Current source considerations for bio-impedance measurement.* Abstracts, p.40.
4. A.Kristiņš, J.Melderis. *Device for monitoring and charging of reserve accumulators.* Abstracts, p.71.
5. I.Gvardina, A.Kristiņš, J.Melderis. *Controlling device for jewelry showcase*. Abstracts, p.72.

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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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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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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^{TM} 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.

	SF-1	**KT-2FA**	**KT-2FB**
Delay times (minutes)	3, 5, 10, 15	3, 5, 10, 15	3, 5, 10, 15
Access times (s)	5, 10, 15, 20	5, 10, 15, 20	5, 10, 15, 20
Dimensions (mm)	400 x 370 x 140	300 x 300 x 300	300 x 300 x 200
Weight (kg)	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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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 25 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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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 ÷ 0,15 s).

The device can be used for testing of 10 types of breakers: ВВШ-110; ВВБ-110; ВВУ-110; ВВН-110/6; ВВ-330Б; ВВН-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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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:	$2{,}8 \bullet 10^{14}$
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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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:	$2{,}8 \bullet 10^{14}$
User keys:	≤ 56 pcs.
Dimensions:	83x55x35 mm

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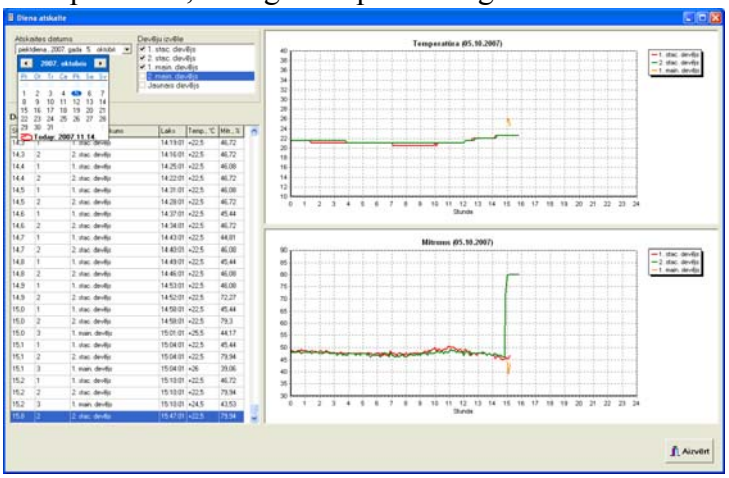
Monitoring of the environment temperature and relative humidity

The climate monitoring system has been developed for grain warehousing and drying. It performs a temperature registration in a range from -20°C up to +85°C with the step of 0.5°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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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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Device for Testing of Action of the Power Transformer's Step Switching Contacts "KODA-3-M"

This device for testing of the switching contacts of power transformers "KODA-3-M" is intended for fixing the moments of activation of the transformer's step switching contacts, and also for fixing the times of switching of transformer's contactor with the subsequent printing the results of testing as the table or the time diagram.

This testing device has two operational modes:

- *oscillograph mode* – for fixing the times of switching of transformer's contactor;
- *circle diagram mode* – for fixing all the moments of activation of the transformer's step switching contacts.

This device was designed on the base of Rabbit 3000 programmable microprocessor.

Processor program developed in Laboratory of Electronic Engineering, ISSP provides execution of the algorithm necessary for the activity of the device, accumulation in operative memory, processing and printing by the dot matrix printer of the measured data.

Device's structure and principles of its work are considered at a level of the block diagram.

Technical parameters of this testing device and real listings with the received results, both as diagrams and as the tables are given.

This testing device is intended for work in field conditions in a wide temperature range.

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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 (∅ 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°C to +85°C.

Touch Memories can accommodate over one million data changes.

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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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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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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:	$2{,}8 \bullet 10^{14}$
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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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:	$2{,}8 \bullet 10^{14}$
Maximal number of user keys:	56 (250) pcs.
Dimensions:	115x55x30 mm

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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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