

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



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2010

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INTRODUCTION

The research in solid state physics at the University of Latvia restarted after World War II. The **Institute of Solid State Physics (ISSP)** of the University of Latvia was established on the basis of Laboratory of *Semiconductor Research* and Laboratory of *Ferro- and Piezoelectric Research* in 1978. Since 1986 the ISSP has the status of an independent organization of the University and now is the main material science institute in Latvia.

Four laboratories from the Institute of Physics of the Latvian Academy of Sciences joined our Institute in 1995. Twenty scientists of the former Nuclear Research Centre joined the ISSP in 1999 and established Laboratory of Radiation Physics. In 2004 scientists from the Institute of Physical Energetics joined ISSP and established Laboratory of Organic Materials (Table 1).

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

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

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

The research of the ISSP includes:

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

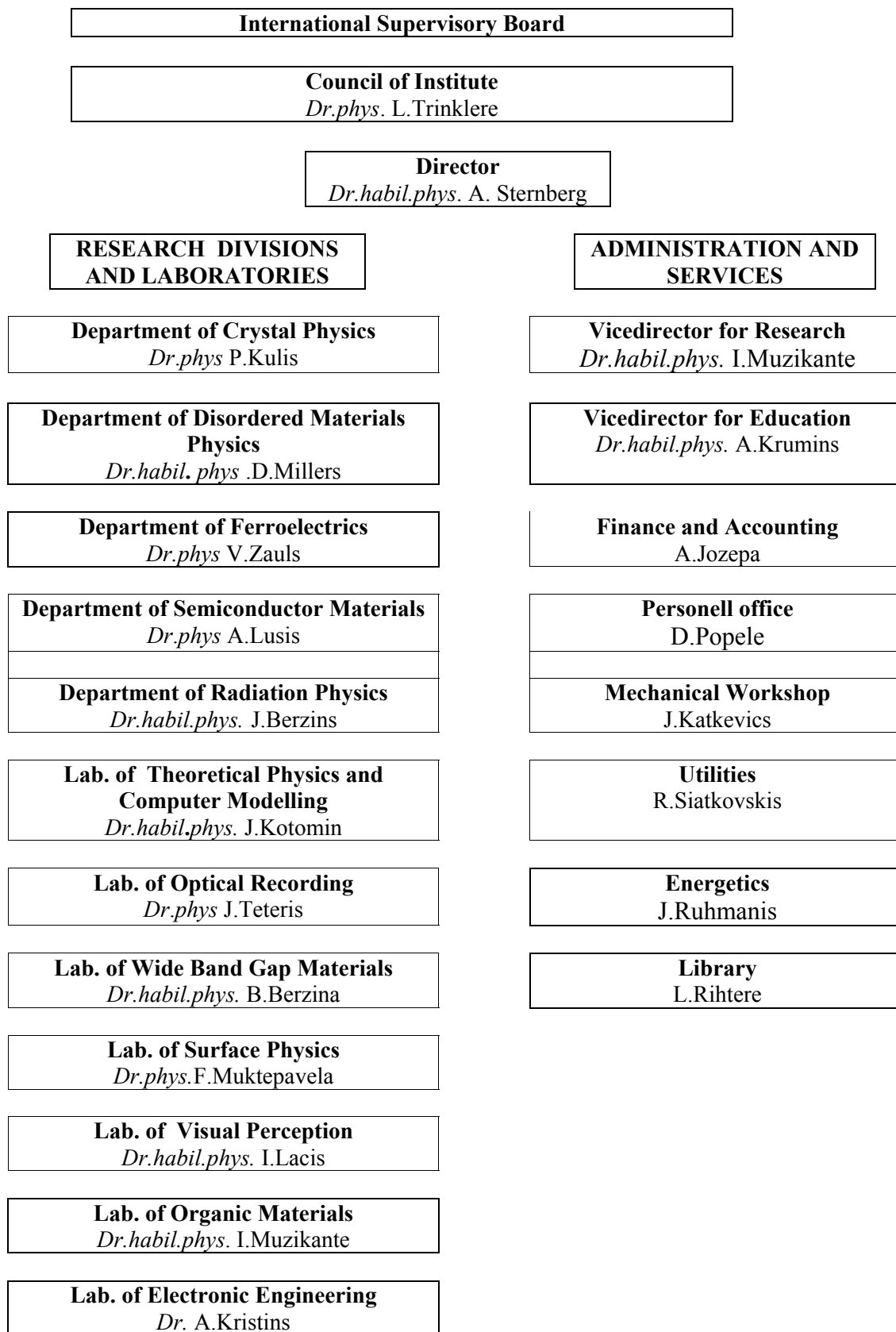
The highest decision-making body of the Institute is the **Scientific Council** of 21 members elected by the employees of the Institute (Table 2). Presently Dr. phys. L.Trinklere is the elected chairperson of the ISSP Council. The Council appoints director and its deputies.

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

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff**. At present there are 150 employees working at the Institute, 23 of 97 members of the research staff hold Dr.habil.degrees, 55 hold Dr. or PhD. At the end of 2009 there were 21 PhD students and 46 undergraduate and graduate students in physics and optometry programmes working at the ISSP.

Table 1

ORGANIZATIONAL STRUCTURE OF THE ISSP IN 2009



The Scientific Council of the Institute

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

International Advisory Board of the Institute

1. Prof. Dr.J.Banys, University of Vilnius, Lithuania
2. Prof. Dr. Gunnar Borstel, University of Osnabruck, Germany
3. Prof. Niels E.Christensen (chairman), University of Aarhus, Denmark
4. Prof. Dr.R.Evarestov, St.Petersburg University, Russia
5. Prof. Claes – Goran Granqvist, Uppsala University, Sweden
6. Prof. Dr.M.Kirm, University of Tartu, Estonia
7. Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia
8. Prof. Sergei Tuituinnikov, Joint Institute for Nuclear Research, Dubna, Russia
9. Prof. Juris Upatnieks, Applied Optics, USA
10. Prof. M. Van de Voorde, Max – Planck – Institute, Stuttgart, Germany
11. Prof. Harald W.Weber, Atomic Institute of Austrian Universities, Vienna, Austria

The annual report summarizes the research activities of the ISSP in 2008. The staff of the Institute has succeed in 11 **national science grants** and in **two national cooperation projects** (“Functional Materials and Technologies for Microelectronics and Photonics” and “Nanomaterials and Nanotechnologies”), with the total financing 190.8 thous. Ls (ca. 267.1 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 **materials science**. ISSP became coordinating institution for the Materials NRP and collaborates as well in the NRP “Energetics” attracting 440.9 thous. Ls budget in 2009. The infrastructure financing for ISSP in 2009 was 515.7 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 2009:

No	Author	Award
1.	Dr.phys. O.Dumbrajs	Member of Latvian Academy of Science
2.	Dr.habil.phys. J.Kotomins	The correspondent member of Latvian Academic of Science
3.	Dr.habil.phys. L.Grigorjeva	Dr.E.Silins award in physics
4.	B.sc. E.Nitiss	Award in physics young scientists
5.	Dr.phys. A.Kuzmins	Author of the best scientific achievement (from Latvian Academic of Science)

At the end of 2009, 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 2009 **three international conferences** have been organised at the Institute:

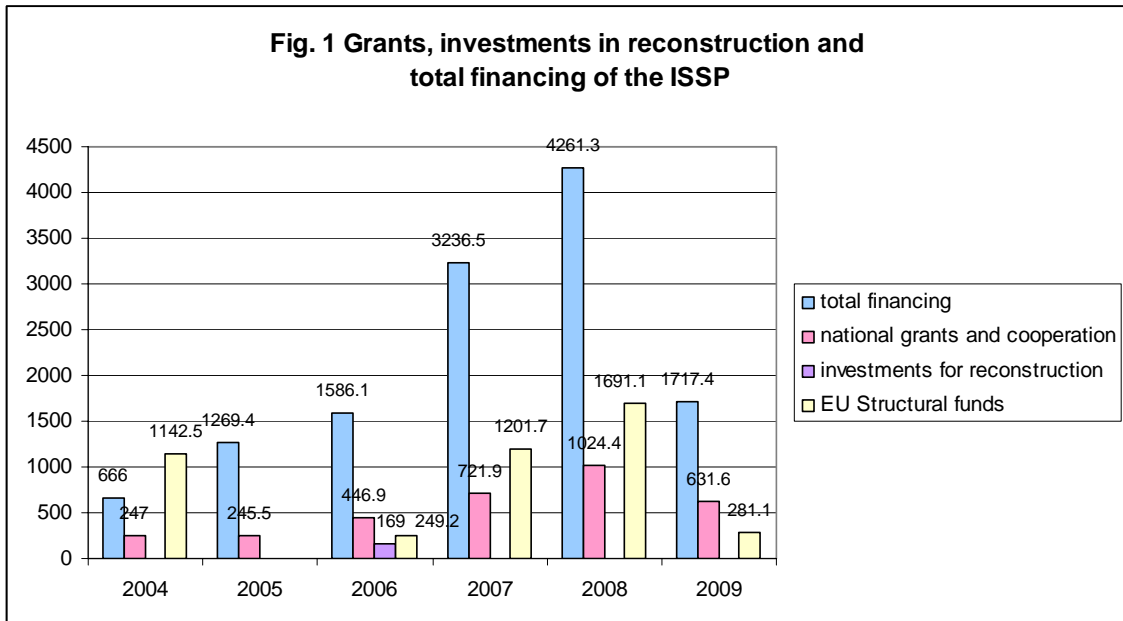
- Annual International conference “Functional materials and nanotechnologies”, March 31 - April 3, 2009, Riga, Latvia;
- International Student Conference “Developments in Optics and Communications 2009”, April 24 – 26, 2009, Riga, Latvia;
- 13th European Fusion Theory Conference, October 12 – 15, 2009, Riga, Latvia

Table 4

INCOME OF ISSP, THOUSAND Ls, FROM 2004 - 2009

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Structural funds from EU
2004	1 809	246.7	123.5	166.5	121.8	1142,5
2005	1 269,4	245,5	358,8 + 120)*	172,8	387,6	
2006	1586,1	466,9	403,4 + 169)*	152,4	135,6	249,2
2007	3 236,5	721,9	1110,2	98,7	92,6	1201,7
2008	4 261,3	1 024,4	1 088,8	155,9	291,8	1 691,1
2008	1717,4	631,6	578,1	64,2	162,4	281,1

*) – investment for building reconstruction



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

- F-Bridge – 8.7 thous. EUR
- Catherine – 54.3 thous.EUR
- 5 EURATOM project – 298.8 thous. EUR
- one INTAS project – 0.8 thous. EUR
- NASA-OTM project – 117.5 thous EUR
- Karlsruhe project – 13.6 thous. EUR

Main achievements in 2009

1. 96 SCI papers published by the staff of Institute.
2. 3 patent applications
- 3 10 B.sc. thesis and 6 M.Sc. thesis in physics were defended under the supervision of our scientists
4. J.Butikova were acquired degree of doctoe of physics (PhD) University of Latvia

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 nanocomposite materials prospective for the light emitters, detectors and visualization systems with enhanced quantum efficiency. Oxyfluoride compounds activated with lanthanide ions may exhibit emission of photons of greater energy than those absorbed during the excitation (up-conversion of energy). The glass and glassceramics samples were synthesized using conventional methods. Several chemical methods were tried for the synthesis of oxyfluoride nanostructures. The energy relaxation mechanisms were studied during up-conversion processes by means of spectral and time-resolved luminescence measurements both in glass and glass ceramics containing $\text{NaYF}_4:\text{Er}$, $\text{LaF}_3:\text{Er}$ and in chemically synthesized oxyfluorides.
3. Technology of Al-Ga nitride semiconductor heterostructures for light-emitting and laser diodes for violet and ultraviolet spectral regions - the goal of the project is the development of light-emitting diodes and laser diodes for violet and ultraviolet spectral region. The project involves installation of new MOCVD equipment AIXTRON AIX200 RF, synthesis and design of corresponding new materials on the basis of the third group nitrides, elaboration of the thin film heterostructures and further development of production of multifunctional photonic devices in joint stock company "Alfa".
4. Investigation and characterization of the impurity content in fusion plasmas and reactor hot wall are the main goals of EURATOM project. The objectives of this project require study of the influence of the liquid metal limiter on the main plasma parameters, including concentration of evaporated metal atoms in plasma. Laser spectroscopy techniques are proposed for development of procedures for research of impurities in plasma and plasma facing materials. According to the objectives emission of Ga metal vapours in plasmas during the evaporation of the metal gush has been considered. Density of metal vapours in plasma can be obtained using two spectroscopic methods: the steady state emission of the multiple ionised metal ions and the charge exchange emission during ionization of evaporated metal ions.
5. Laser-induced ablation for analysis of the impurities in plasma facing components as the method for the detection of any chemical element is used for the remote analysis. The major tasks of the present investigation are setting up and testing the equipment for laser ablation spectroscopy and developing the methodology for impurity depth profiling. The investigation is carried out using the plasma facing materials of ASDEX Upgrade tokamak by means of laser-induced ablation spectroscopy and profilometry of the corresponding ablation craters. The experimental set-up for the laser-induced ablation spectroscopy was developed and manufactured. The optimal conditions of the laser-induced ablation of the samples of ASDEX Upgrade divertor plates were found. Plasma emission spectra of these plasma facing components showing a substantial number of impurities were recorded. The impurity elements were determined, and the possible sources of the impurities suggested. The depth of the accumulation of basic impurities (hydrogen, boron) in the surface of the ASDEX Upgrade divertor plates (carbon R6710 tiles) is estimated using plasma emission spectra. Obtained results allows considering the method of the laser-induced ablation spectroscopy to be feasible for

rapid analysis of plasma facing materials. With minor modifications, this method can be suggested as an *in situ* technique for determination the state of the plasma facing components inside the chamber of a thermonuclear fusion reactor.

Scientific Staff

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

PhD Students

1. A. Gulans
2. A. Sarakovskis
3. G. Marcins
4. A. Voitkans
5. Dz. Berzins

Students

1. J. Aizezers
2. M. Cubarovs
3. G. Doke
4. J. Grube
5. A. Petruhins

Scientific visits abroad

1. A. Sarakovskis, International meeting „Principles and Applications of Time- Resolved Fluorescence Spectroscopy”, November 8 -12, 2009, Berlin, Germany
2. J. Grube, 11-th International Conference-School, Advanced Materials and Technologies, August 27 - 31, 2009, Palanga, Lithuania.
3. A. Voitkans, Italy, 26.10.-28.10.2009.
4. A. Voitkans, Germany, 04.06.-19.06.2009.
5. I. Tale, Italy, 26.10.-28.10.2009.
6. I. Tale, Lithuania, 26.08.-28.08.2009.
7. I. Tale, Poland, 03.11.-06.11.2009.
8. I. Tale, Germany, 18.03.-21.03.2009.
9. I. Tale, Germany, 17.06.-19.06.2009.
10. I. Tale, Germany, 05.10.-15.10.2009.

Cooperation

Latvia

Joint stock company “Alfa”

Germany

1. University of Paderborn, Germany (Prof. Dr. R. Wehrspohn, Prof. Emeritus, J.-M. Spaeth, Dr. hab. S. Schweizer, Dr. hab. S. Greulich-Weber).
2. University of Rostock, Germany (Prof. H.-J. Fitting).
3. "Aixtron" Aachen, Germany
4. Max Plank Institute of Plasma Physics, Garching, Germany

Portugal

Instituto Superior Tecnico (IST), Lisbon Portugal (Prof. Varandas).

THE MAIN RESULTS

LUMINESCENCE-DETECTED EPR OF OXYGEN-VACANCY COMPLEXES IN CaF_2

U. Rogulis, R.C. Baetzold*, J.-M. Spaeth**

*14204 Allan Road, Albion, NY 14411, USA

**Fakultät Naturwissenschaften, Department Physik, Universität Paderborn, 33098 Paderborn, Germany

In several CaF_2 single crystals grown by the Bridgman method and doped with CaO or in addition with SrF_2 or NaF a luminescence band between 470 and 600 nm could be excited at 212 nm, its peak wavelength depending on the doping. With photo-luminescence (PL) – detected EPR 5 spin triplet centres were identified. Their axial fine structure constants D varied from 87 to 690 mT whereby the most intense spectra had the smallest D value. Theoretical calculations of the fine structure tensors and superhyperfine interactions show that the most intense and probable triplet centre consists of a pair of an O_F^- on a F^- site next to a nearest neighbour F^- vacancy which, compared to the well-known F centre, is occupied by an excited electron in a shallow orbital and coupled to the 2p hole at the oxygen to form a $S=1$ excited state. This centre can be excited optically at low temperature to a metastable new configuration where the F centre jumps into a $\langle 111 \rangle$ position opposite the O_F^- . The other triplet centres have probably also an O⁻-F centre nearest neighbour configuration but have in addition a cation impurity or vacancy nearby.

PATTERNED LASER CRYSTALLIZATION OF a-Si

B. Polyakov, G. Marcins, M. Chubarov, A. Kuzmin, V. Klykov*, I. Tale

*Sidrabe Inc

Thin films of amorphous Si on glass were crystallized by pulsed nano- and picosecond lasers. Two methods for creating the desired patterns of crystallized regions were used. In the former, the pattern is produced by a focused laser beam, and in the latter it is made using a prefabricated mask. The electric conductivity of crystallized films increases by more than 4 orders of magnitude in comparison with untreated amorphous films.

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 spectrochemical 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.

OPTICAL SPECTROSCOPY OF Er DOPED TELLURITE GLASSES

J.Grube, G.Doke, I.Aulika, J.Gabrusenoks,
A.Sarakovskis, M.Springis

Tellurite glasses doped with rare-earth ions are intensively investigated because they have a wide IR transmission region, small phonon energy, large refractive index, desirable for radiative transitions of rare-earth ions. This makes the tellurite glasses an attractive media for optical devices including IR lasers, IR-to-VIS up-converters, fiber and waveguide amplifiers.

The present paper reports newly synthesized oxyfluorotellurite glass system $78\text{TeO}_2 - x\text{Na}_2\text{O} - (20-x)\text{BaF}_2 - 2\text{ErF}_3$, ($x = 20, 10, 0$). Differential thermal analysis, structural analysis by Raman scattering spectra, wide region absorption spectra from UV to IR, traditional and up-conversion luminescence spectra and kinetics are presented and influence of fluorine on these properties is studied. Increase of fluorine content in the glass changes the glass network of TeO_n entities by substitution of some oxygen by fluorine and increasing the $\text{Te}(\text{O},\text{F})_3/\text{Te}(\text{O},\text{F})_4$ ratio. Additionally, IR absorption of OH^- is significantly reduced when the fluorine concentration is increased, leading to the prolongation of the lifetimes of the emitting Er^{3+} levels. Possible mechanisms of the up-conversion processes are suggested and structural organization of the tellurite glasses is argued.

ENERGY TRANSFER IN Er^{3+} AND Yb^{3+} DOPED SILICATE GLASS AND GLASS CERAMICS

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

The aim of the current research was to study the energy relaxation mechanisms during up-conversion processes by means of spectral and time-resolved luminescence measurements both in glass and glass ceramics containing $\text{LaF}_3:\text{Er}^{3+}$, Yb^{3+} . For this purpose the transparent oxyfluoride silicate glass was synthesized. After the thermal treatment of the precursor glass oxyfluoride ceramics containing $\text{LaF}_3:\text{Er}^{3+}$, Yb^{3+} crystallites was obtained. Up-conversion and traditional luminescence spectra, excitation spectra, their temperature dependence as well as up-conversion luminescence intensity dependence on excitation power are presented for the glass and glass ceramics. Based on the experimental results, peculiarities of the energy transfer mechanisms in the glass and glass ceramics are discussed.

SYNTHESIS AND „UP-CONVERSION” LUMINESCENCE PROPERTIES OF NaLaF₄:Er³⁺

A.Sarakovskis, J. Grube, M. Springis

In the recent years much attention has been paid to the studies of up-conversion luminescence processes in rare-earth elements doped fluorides (LaF₃, PbF₂, SrF₂, CaF₂, BaF₂, NaYF₄ etc.), in which the photons of smaller energies (usually IR) are transformed into photons of higher energies (VIS or even UV). This interest is explained partly due to relatively high chemical stability of the fluorides and also small effective phonon energy of the materials, which suppresses the rate of nonradiative transitions, enhancing the efficiency of the up-conversion processes.

The aim of the current research was to synthesize NaLaF₄:Er³⁺ material by wet-chemistry method and to study the up-conversion properties of the phosphor. In the presentation the synthesis route will be described and the main spectroscopic parameters of the material will be evaluated.

Based on the obtained results the possible application of the synthesized material in the field of efficient up-conversion phosphors will be discussed.

Scientific publication

1. U. Rogulis, R.C. Baetzold, J.-M. Spaeth, Luminescence-detected EPR of oxygen-vacancy complexes in CaF₂, - *physica status solidi (b)*, 2009, vol. 246, No. 5, pp. 1099-1104. (SCI, impact. factor 1.166)
2. B. Polyakov, A. Petruhin, L. Grigorjeva, P. Kulis, I. Tale, Rapid annealing of black ZnO thin film prepared by Pulsed Laser Deposition, - *Latvian Journal of Physics and Technical Science*, 46, 1, 44-48, 2009.
3. B. Polyakov, G. Marcins, M. Chubarov, A. Kuzmin, V. Klykov, I. Tale, Patterned laser crystallization of a-Si, - *Latvian Journal of Physics and Technical Sciences* Vol.46;N3, p50-54, 2009.
4. B. Polyakov, A. Petruhins, J. Butikova, A. Kuzmin, I. Tale, Some aspects of pulsed laser deposition of Si nanocrystalline films, - *Eur. Phys. J. Appl. Phys.*, 48, 20502, 2009.
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6. A.N. Trukhin, J. Teteris, A. Fedotov, D.L. Griscom, G. Buscarino, Photosensitivity of SiO₂-Al and SiO₂-Na glasses under ArF (193 nm) laser, - *J. Non-Cryst. Solids* 355, 1066, 2009.
7. A. Sarakovskis, J. Grube, G. Doke, M. Springis, Excited state absorption and energy transfer mechanisms of up-conversion luminescence in Er³⁺ doped oxyfluoride glass ceramics at different temperatures, - *J. Luminescence* (accepted)
8. A. Fedotovs, U. Rogulis, A. Sarakovskis, L. Dimitrocenko, EPR of radiation defects in Lithium-oxyfluoride glass-ceramics, - *Radiation Effects and Defects in Solids*, (accepted).
9. B. Polyakov, R. Krutokhvostov, A. Kuzmin, E. Tamanis, I. Muzikante, I. Tale, Probing contact potential difference by macroscopic and scanning Kelvin probe methods, - Submitted to *Eur. Phys. J. Appl. Phys.*
10. J. Butikova, A. Sarakovskis, I. Tale: Laser-induced breakdown spectroscopy for determining impurity content and depth profile in plasma facing materials, submitted to *Optics and Lasers in Engineering*

Lectures on Conferences

25th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 11-13, 2009

1. J. Jansons, Ludvigs Jansons (1909-1958), - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 4-12.
2. G. Doke, A. Sarakovskis, J. Grube, I. Aulika, R. Zabelis, J. Gabrusenoks, M. Springis, Up-conversion processes in erbium doped tellurite glasses, - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 32.
3. A. Fedotovs, U. Rogulis, EPR spectra of oxyfluoride glasses and glass-ceramics, - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 36.
4. Dz. Berzins, U. Rogulis, Investigation of recombination luminescence by EPR optical detection, - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 37.
5. G. Kizane, A. Vitins, E. Pajuste, S. Kaleja, I. Dusenkova, M. Halitovs, J. Jansons, Behavior of tritium in plasma-facing materials of the joint European Torus (JET), - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 69.
6. , A. Sarakovskis, J. Grube, A. Misnovs, G. Doke, M. Springis, Energy transfer in Er³⁺ and Yb³⁺ doped silicate glass and glass ceramics, - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 80.
7. J. Grube, A. Sarakovskis, A. Misnovs, A. Veispals, G. Cikvaidze, M. Springis, Up-conversion processes in NaLaF₄:Er, - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 81.
8. E. Elsts, U. Rogulis, Magnetic resonance investigations of defect centres in luminescent detectors - Abstracts of the 25th Scientific Conference ISSP LU, 2009, p. 92.

International Baltic Sea Region conference "Functional materials and nanotechnologies", Riga, 2009, 31. march - 3. april

1. A. Sarakovskis, J. Grube, M. Springis, Synthesis and „up-conversion” luminescence properties of NaLaF₄:Er³⁺, - International Baltic Sea Region conference „Functional materials and nanotechnologies 2009 Book of abstracts, ISSP LU, Riga, 31. march-3. april, p. 38.
2. A. Petruhins, B. Polyakov, E. Tamanis, I. Tale, Fabrication of nanocrystalline sulphide (PbS) thin films using pulsed laser deposition, - International Baltic Sea Region conference „Functional materials and nanotechnologies 2009 Book of abstracts, ISSP LU, Riga, 31. march-3. april, p. 81.
3. B. Polyakov, J. Sipols, A. Kuzmin, I. Muzikante, I. Tale, Kelvin probe AFM for investigations of nonstructures, - International Baltic Sea Region conference „Functional materials and nanotechnologies 2009 Book of abstracts, ISSP LU, Riga, 31. march-3. april, p. 91
4. J. Grube, G. Doke, I. Aulika, J. Gabrusenoks, A. Sarakovskis, M. Springis, Optical spectroscopy of Er doped tellurite glasses, - International Baltic Sea Region conference „Functional materials and nanotechnologies 2009 Book of abstracts, ISSP LU, Riga, 31. march-3. april, p. 110.
5. G. Marcins, B. Polyakov, I. Tale, M. Chubarov, Laser crystallization of a-Si thin films, - International Baltic Sea Region conference „Functional materials and nanotechnologies 2009 Book of abstracts, ISSP LU, Riga, 31. march-3. april, p. 135.

E-MRS 2009 Fall Meeting, Warsaw, Poland, 14-18 sept. 2009

M. Chubarov, G. Marcins, I. Tale, L. Dimitroenco. Thermally stimulated electron-hole processes in GaN and AlGaIn thin films, - E-MRS 2009 Fall Meeting, Warsaw, Poland, 14-18 sept. 2009, Book of abstracts p.237.

11-th International Conference-School, Advanced Materials and Technologies, August 27 - 31, 2009, Palanga, Lithuania

J.Grube, A.Sarakovskis, G.Doke, M.Springis, Different energy transfer mechanisms between $\text{Yb}^{3+}/\text{Er}^{3+}$ ions in oxyfluoride glass and glass ceramics, - Advanced Materials and Technologies, August 27 - 31, 2009, Palanga, Lithuania, p. 72.

Popular Science Articles (in Latvian)

1. J. Jansons, Fizikas autodidakts Roberts Krastiņš, – „Zvaigžņotā Debess”, 2009. gada pavasaris (203), 28. – 36. lpp.
2. J. Jansons, LU fizikas docents Ludvigs Jansons (29.10.1909.–12.05.1958.) – 100, – „Zvaigžņotā Debess”, 2009. gada rudens(205), 25. – 28. lpp. un 2009./10. gada ziema (206), 31. – 42. lpp.

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
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Research area and Main Problems

Main problems. Studies of electronic excitations, energy transfer, defect states and doping effects in simple and complex oxides: single crystals, nanocrystals, nanostructured ceramics, thin films, glasses, optical fibers. The main materials under studies: ZnO, ZrO₂, YAG and YAP, ZnWO₄ and other tungstates, materials for persistent luminescence applications, materials for transparent conductive oxides (TCO); pure and doped SiO₂ – based glasses for high transparency optics or optical fibers, SiO₂ particles, crystalline SiO₂ polymorphs.

Experimental methods. The time-resolved luminescence and transient absorption spectroscopy in nanosecond time region are used and developed. The excitation sources: pulse electron beam accelerator (10 ns, 270 keV, 10¹² electrons/pulse), YAG:Nd and nitrogen lasers (266 nm, 337 nm, 532 nm), excimer lasers (248, 193 and 157 nm). Optical signals were detected by photomultipliers (Hamamatsu H8259 and H8259-02) and FastComTec card P7888-1E with minimal time channel 250 ps as well as oscilloscope Tektronix TDS 5052B with time resolution 10 ns. The measurements can be performed in temperature region 10-450K.

FTIR absorption spectroscopy: EQUINOX 55 (10000-400 cm⁻¹ and 22000-7000 cm⁻¹ spectral regions).

Vacuum ultraviolet spectroscopy: McPherson 234/302 200mm monochromator with D₂ lamp with MgF₂-window serving as light source (120-250 nm).

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

Energy-dispersive X-ray fluorescence microanalysis (EDAX-Eagle III spectrometer, elements from Na to U, spatial resolution 50 μm).

Laboratory of solid state radiation physics Dr.habil.phys.S.Chernov Dr.habil.phys. L.Grigorjeva Dr.habil.phys. D.Millers Dr.phys. V.Pankratov Technical staff Eng. A.Sitdikov Eng. E.Arhipova Ph.D students K.Smits M.Shorokhov Students L.Bukonte; J.Rikveilis L.Shirmane; Z.Bukonte; V.Liepina	Defect studies Group Dr.habil.phys. A.Silins Dr.habil. L.Skuja Students L.Tiluga	Laboratory of Solid state optics Dr.habil.phys.A.Trukhin Dr.phys.K.Trukhins
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Scientific Visits Abroad

1. Dr.habil.phys.L.Grigorjeva, Estonia (14 days)
2. Dr.habil.phys. D.Millers, Poland (4 days)
3. Dr.phys. V.Pankratov (10 months)
4. K.Smits, Germany, (7 days)
5. K.Smits, Poland (4 days)
6. K.Smits, Poland (5 days)
7. Dr.habil.phys.L.Grigorjeva, Spain (5 days)
8. Dr.habil.phys.L.Grigorjeva, Poland (5 days)
9. Dr.habil.phys. D.Millers, Poland (5 days)
10. Dr.habil. L.Skuja , Japan (2 months)
11. L.Shirmane, Poland (5 days)
12. Dr.habil. L. Skuja , Austria (5 days)
13. Dr.habil. A. Trukhin , France (6 days)

Cooperation

Latvia

SIA "Baltic BRUKER" (Dr.V.Gostilo)

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

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

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

USA

Wake Forest University (Prof.R.T.Williams)

ImpactGlass research international, 3938 E. Tucson, AZ 85712, USA (Ph.D. D.L. Griscom)

Solid State Division, Oak Ridge National Laboratory. Oak-Ridge, TN. 37831 (Ph.D. Lynn A.Boatner)

University of Central Florida, CREOL (Professor, Dr.L.B.Glebov)

Estonia

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

Russia

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

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

State University of Irkutsk, Institute of Geochemistry (Professors E.A. Radzhabov, A.I. Nepomnyaschihk)

L.F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia (Dr. T. Dyuzheva)

Fiber Optics Research Center of the Russian Academy of Sciences, 119333, Moscow, Russia (Prof. K. M. Golant)

Estonia

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

Poland

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

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).

Université Paris Sud, Orsay, Lab. Labo. Physico-Chimie des Solides UMR8648, (Dr.B. Poumellec)
Laboratoire de Physique des Lasers, Université des Sciences et Technologies de Lille, France (Prof. B.Capoen)

Germany

Institute of Inorganic Chemistry University of Karlsruhe (TH), (Prof.C.Feldman)
University of Rostock, Germany (Professor, Dr. H.-J. Fitting)

Denmark

Interdisciplinary Nanoscience Center (iNANO), University of Aarhus, Aarhus (Prof.B.Bech Nielsen)

Italy

University of Palermo (Prof. R. Boscaino, Dr. M. Cannas, Dr. S. Agnello)
University of Palermo, Prof. Roberto Boscaino, Inst. Nazionale di Fisica della Mat.and Dipartimento di Scienze Fisiche ed Astronomiche dell 'Università, via Archirafi, 36, I-90123 Palermo, Italy

Japan

Tokyo Institute of Technology (Prof. H.Hosono, M.Hirano)
Tokyo Metropolitan University (Dr. K. Kajihara)

Scientific publications

1. L.Grigorjeva, D.Millers, A.Kalinko, V.Pankratov, K.Smits. Time-resolved cathodoluminescence and photoluminescence of nanoscale oxides. J.of the European Ceramic Soc. v.29, 2009, p.255-259.
2. Grigorjeva, L., Millers, D., Smits, K., Pankratov, V., Łojkowski, W., Fidelus, J., Chudoba, T, Monty, C. Excitonic luminescence in ZnO nanopowders and ceramics. Optical Materials, 2009, 31, pp.1825-1827.
3. Andrew Wall, R., Lipke, K.C., Ucer, K.B., Williams, R.T., Millers, D., Smits, K., Grigorjeva, L. Time-resolved absorption and luminescence following electron-hole pair creation in ZnO Physica Status Solidi (C) Current Topics in Solid State Physics, 2009, 6 (1), pp. 323-326.
4. F.Muktepavela, G.Bakradze, L.Grigorjeva, R.Zabels, E.Tamanis. Properties of ZnO coatings obtained by mechanoactivated oxidation. Thin Solid Films, vol.518. 2009, pp.1263-1266.
5. Shorohov, M., Muktepavela, F., Grigorjeva, L., Maniks, J., Millers, D. Surface processing of TlBr single crystals used for radiation detectors. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2009, 607 (1), pp. 120-122.
6. M. Shorohov, F. Muktepavela, J. Maniks. Surface processing of TlBr crystals for x- and γ -ray detectors. Latvian J.of Phys.Techn.Sci.N3, 2008,p.1-19.
7. ^{60}Co gamma-ray-induced intrinsic defect processes in fluorine-doped synthetic SiO_2 glasses of different fluorine concentrations. Materials Science and Engineering: B v.161 p.96-99 (2009)
8. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono, Oxygen exchange at the internal surface of amorphous SiO_2 studied by photoluminescence of isotopically labeled oxygen molecules. Phys. Rev. Letters v.102, 175502(2009).

9. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono, Isotope Effect on the Infrared Photoluminescence Decay of Interstitial Oxygen Molecules in Amorphous SiO₂. *Applied Physics Express* vol.2, p. 056502 (2009).
10. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono, Photoluminescence study of diffusion and reactions of ¹⁸O-labeled interstitial oxygen molecules in amorphous SiO₂. *Electrochemical Society Transactions* v.25 (9) p.277-285 (2009).
11. A.N. Trukhin, K.M. Golant, peculiarities of photoluminescence excited by 157 nm wavelength F₂ excimer laser in fused and unfused silicon dioxide, *Journal of Non-Crystalline Solids* 355 (2009) p. 1719-1725.
12. Anatoly N. Trukhin luminescence of polymorph crystalline and glassy SiO₂, GeO₂ :A short review, *Journal of Non-Crystalline Solids* 355 (2009) 1013-1019.
13. A.N.Trukhin , J.Teteris , A.Fedotov , D.L.Griscom ,G.Buscarino, Photosensitivity of SiO Al and SiO Na glasses under ArF (193nm) laser, *Journal of Non-Crystalline Solids* 355 (2009) 1066-1074.

Lectures in Conferences

International Baltic Sea Region Conference "Functional materials and nanotechnologies 2009 (FM&NT)" 31. March-3.April, Riga, Latvia.

1. W.Lojkowski, T.Chudoba, S.Gierlotka, P.Gluchowski, D.Hreniak. W.Strek, V.Pankratov, D.Millers, L.Grigorjeva. Transparent nanocrystalline YAG ceramics and their optical properties. *Book of Abstracts*, p.35.
2. J.Fidelus, W.Lojkowski, D.Millers, L.Grigorjeva, K.Smits. Prospective memory oxygen pressure sensors based on nanocrystalline zirconia. *Ibid*, p.36.
3. K.Smits, L.Grigorjeva, D.Millers, A.Sarakovskis, A.Opalinska, J.Fidelus, W.Lojkowski. Europium doped zirconia luminescence. *Ibid*, p.37.
4. R.Zabels, F.Muktepavela, L.Grigorjeva, E.Tamanis, M.Mishes-Piesins. Nanoindentation and photoluminescence characterization of ZnO thin films and single crystals. *Ibid*, p.60.
5. V.Pankratov, A.I.Popov, A.Kotlov, S.A.Chernov, A.Zharkouskaya, C.Feldmann. Luminescence and energy transfer processes In LaPO₄:Ce, Tb nanocrystals. *Ibid*, p.111.
6. A.I.Popov, V.Pankratov, A.Kotlov, I.Karbovnyk, I.Bolesta. Time-resolved luminescence of CdI₂ single crystal under the excitation of synchrotron radiation. *Ibid*, p.112.
7. L.Shirmane, V.Pankratov, L.Grigorjeva, T.Chudoba, W.Lojkowski. Peculiarities of cerium related luminescence in YAG nanoceramics. *Ibid*, p.115.
8. K.Smits, L.Grigorjeva, D.Millers, A.Sarakovskis, D.Jakoviča, J.Grabis. Cerium stabilized nanocrystalline zirconia luminescence. *Ibid*, p.116.
9. L.Grigorjeva, D.Millers, K.Smits. Luminescence properties of zinc, indium and titanium oxides. *Ibid*. p.117.
10. A.N.Trukhin, K.M.Golant, Peculiarities of photoluminescence excited by 157 nm wavelength F₂ excimer laser in fused and unfused silicon dioxide. *Ibid.*, p. 119.

LU CFI 25th Scientific Conference, Feb.11-13 Riga

1. M.Shorohov. The properties of TlBr radiation detectors. *Tēzes*, p.54.
2. K.Smits. Luminescence of rare-earth ions doped ZrO₂ nanopowders. *Ibid*, p.35.
3. L.Shirmane. Cerium luminescence in YAG nanopowders and ceramics. *Ibid*, p.33.
4. L. Tiļuga, L. Skuja Elemental analysis of solids by X-ray fluorescence microanalyser EDAX Eagle III.
5. Trukhin A., Polimorfo kristālisko un stiklveidīgo SiO₂, GeO₂ luminiscence, p.79.

5th International Student Conference "Developments in Optics and Communications 2009" (DOC-5), Riga, April 24-26, 2009

L. Tiluga, L. Skuja "Energy-dispersive X-ray fluorescence microanalysis of chlorine in SiO₂ optical fiber preforms", Abstracts, p.73-74

7th International Conference on Luminescent Detectors and transformers of Ionizing Radiation. LUMDETR2009, 12-17July 2009, Krakow, Poland

1. L.Shirmane, L.Grigorjeva, T.Chudoba, W.Lojkowski, V.Pankratov. Peculiarities of luminescence properties of cerium doped YAG transparent nanoceramic. Book of Abstracts, p.174.
2. K.Smits, L.Grigorjeva, D.Millers, J.D.Fidelus, W.Lojkowski. Energy transfer in ZrO₂. Ibid, p.175.
3. L.Grigorjeva, D.Millers, K.Smits, J.Grabis, J.Fidelus, W.Lojkowski, T.Chudoba, K.Bienkowski. The luminescence of ZnO ceramics. Ibid, p.197.

3rd International Symposium on Science and Technology of Advanced Ceramics (STAC-3) (Yokohama, Japan, June 16-18),

1. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono, Quantitative measurement of ¹⁸O-labeled oxygen molecules to probe intrinsic reactivity of oxygen in amorphous SiO₂; Abstract 17aHsO-01, (2009).

216th Electrochemical Society Meeting, Vienna, Austria, Oct. 4-9, 2009

2. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono, Photoluminescence study of diffusion and reactions of ¹⁸O-labeled interstitial oxygen molecules in amorphous SiO₂, Abstract # 3237 (CD-ROM and online).

Bachelor thesis

Laura Bukonte. Cinka oksīdu saturoši nanokompozīti un to optiskās īpašības.

SOLID STATE OPTICS LABORATORY

Head of Laboratory, Professor, Dr. hab. Phys., Anatoly Trukhin

Research area and Main Problems

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

Scientific stuff:

1. Professor, Dr. hab. Phys. A. Trukhin
2. Dr. Phil., Dr. Phys. K. Truhins

Cooperation

Russia

State University of Irkutsk, Institute of Geochemistry (Professors E.A. Radzhabov, A.I. Nepomnyaschikh)

L.F. Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia (Dr. T. Dyuzheva)

Fiber Optics Research Center of the Russian Academy of Sciences, 119333, Moscow, Russia (Prof. K. M. Golant)

Germany

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

USA

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

France

Universite Paris Sud, Orsay, Lab. Labo. Physico-Chimie des Solides UMR8648, (Dr.B. Poumellec)
Laboratoire de Physique des Lasers, Université des Sciences et Technologies de Lille, France (Prof. B.Capoen)

Italy

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

Estonia

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

THE MAIN RESULTS

PECULIARITIES OF PHOTOLUMINESCENCE EXCITED BY 157 nm WAVELENGTH F₂ EXCIMER LASER IN FUSED AND UNFUSED SILICON DIOXIDE

A.N. Trukhin¹, K.M. Golant²,

¹*University of Latvia, Solid State Physics Institute, LV-1063, Riga, Latvia*

²*Institute of Radio-engineering and Electronics of RAS, 125009 Moscow, Russia*

Photoluminescence (PL) spectra and kinetics of high purity amorphous silicon dioxide with ultra low hydroxyl content is studied under the excitation by F₂ excimer laser (157 nm wavelength) pulses. Materials synthesized in the SPCVD plasma chemical process are studied before and after fusion. Two bands are found in the PL spectra: one centered at 2.6-2.9 eV (a blue band) and the other at 4.4 eV (a UV band). Luminescence intensity of unfused material is found to increase significantly with exposure time starting from a very small level, whereas in fused counterpart it does not depend on irradiation time. Both bands show complicated decay kinetics, to which add exponential and hyperbolic functions. The UV band of the unfused material is characterized by decay with exponential time constant $\tau \sim 4.5$ ns and hyperbolic function t^{-n} , where $n=1.5 \pm 0.4$. For the blue band the hyperbolic decay kinetics with $n \sim 1.5$ extends to several milliseconds, gradually transforming to the exponential one with $\tau = 11 \pm 0.5$ ms. In fused glass relative contribution of the fast component to the UV band is small whereas for the blue one it is great, that allows one to more accurately determine the hyperbolic law factor $n=1.1 \pm 0.1$ typical for tunneling recombination. Simultaneous intracenter and recombination luminescence, the later occurring with the participation of laser radiation induced defects, add particular features to the decay kinetics. Spectra of the above luminescence processes are different. A less sharp position of bands is associated with the recombination luminescence. The origin of the observed PL features we attribute to the presence of oxygen deficient centers in glass network in the form of twofold coordinated silicon. Such centers being affected by network irregularities can be responsible for the recombination PL component. A great variety of network irregularities is responsible for centers' structural inequivalence, which causes a non-uniform broadening of PL spectral and kinetic parameters.

PHOTOSENSITIVITY OF SiO₂-AL AND SiO₂-NA GLASSES UNDER ArF (193 NM) LASER

A.N. Trukhin*, J.Teteris*, A.Fedotov*, D.L.Griscom**, G. Buscarino***

**Solid State Physics Institute, University of Latvia, Kengaraga, 8, LV-1063 Riga, Latvia*

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

****Istituto Nazionale per la Fisica della Materia and Dipartimento di Scienze Fisiche ed Astronomiche dell'Università, via Archirafi, 36, I-90123 Palermo, Italy*

Photosensitivity of SiO₂-Al and SiO₂-Na glass samples was probed by means of the induced optical absorption and luminescence as well as by electron spin-resonance (ESR) after irradiation with excimer-laser photons (ArF, 193 nm). Permanent visible darkening in the case of SiO₂-Al and transient, life time about one hour, visible darkening in the case of SiO₂-Na was found under irradiation at 290 K. No darkening was observed at 80 K for either kind of material. This investigation is dedicated to revealing the electronic processes responsible for photosensitivity at 290 and 80 K. The photosensitivity of both materials is related to impurity defects excited directly in the case of SiO₂-Na

and/or by recapture of self-trapped holes, which become mobile at high temperature in the case of SiO₂-Al. Electrons remain trapped on the localized states formed by oxygen deficient defects.

LUMINESCENCE OF POLYMORPH CRYSTALLINE AND GLASSY SiO₂, GeO₂

Anatoly N. Trukhin

University of Latvia, Solid State Physics Institute, LV-1063, Riga, Latvia

Studies of SiO₂, GeO₂ crystals with α -quartz and rutile structures were performed during last two decades. The goal of study was comparison of properties with glassy modifications of these crystals. Luminescence of an oxygen deficient center in these glassy materials resembles luminescence of rutile-type modification rather than α -quartz modification. In the last similar luminescence centers appears only after damaging irradiation with electron beam at low temperatures (<60 K) and at ambient temperatures after gamma or neutron irradiation.

Presentation at conferences

1. Trukhin A., Polimorfo kristālisko un stiklveidīgo SiO₂, GeO₂ luminiscence, 25. CFI LU Zinātniskās konferences referātu tēzes, Rīga, Latvija, 11.-13. Februāris 2009, 79.lpp.
2. A.N. Trukhin, K.M. Golant Peculiarities of photoluminescence excited by 157 nm wavelength F₂ excimer laser in fused and unfused silicon dioxide, International conference „Functional materials and nanotechnology” Riga, Latvia March 31-April 3. 2009 Po-21, p. 119.

Scientific publications

3. Anatoly N. Trukhin luminescence of polymorph crystalline and glassy SiO₂, GeO₂ :A short review, Journal of Non-Crystalline Solids 355 (2009) 1013-1019.
4. A.N. Trukhin , J. Teteris , A. Fedotov , D.L. Griscom , G. Buscarino, Photosensitivity of SiO₂-Al and SiO₂-Na glasses under ArF (193nm) laser, Journal of Non-Crystalline Solids 355 (2009) 1066-1074.
5. A.N. Trukhin, K.M. Golant, Peculiarities of photoluminescence excited by 157 nm wavelength F₂ excimer laser in fused and unfused silicon dioxide, Journal of Non-Crystalline Solids 355 (2009), pp. 1719-1725

DEPARTMENT OF FERROELECTRICS

Head of Department Dr. phys. V. Zauls

Research area and Main Problems

The Department of Ferroelectric Physics is involved in the basic and applied research and education in the field of functional oxide materials for dielectric applications including various aspects of theoretical modelling, studies of structure-property relationships for ferroelectric, piezoelectric and pyroelectric ceramics, including nanocrystalline materials and thin film multilayers. Synthesis and processing of ceramics is based on chemical coprecipitation and two stage hot pressing technologies. Characterization methods include x-ray diffraction, atomic force microscopy and piezo response force microscopy, electron scanning microscopy with EDX option, full range of dielectric impedance and hysteresis measurement tools, optical studies with emphasis on ellipsometry and reflectometry. Recently more possible applications of functional oxide materials are considered both for research and innovation including environment-friendly lead-free materials based on alkaline and earth-alkaline niobates and tantalates with ferroelectric, relaxor or anti-ferroelectric compositions, and conducting materials based on complex perovskites.

Scientific staff

1. Dr. phys. Ilze Aulika
2. Dr. phys. Eriks Birks
3. Dr. phys. emeritus Karlis Bormanis
4. Dr. sc. ing. emeritus Maruta Dambekalne
5. Dr. habil. phys. Vilnis Dimza
6. Dr. phys. Eriks Klotins
7. Dr. habil. phys. Andris Krumins
8. Dr. phys. Maris Kundzins
9. Dr. phys. Anatoly Mishnev
10. Dr. habil. phys. Maris Ozolins
11. Dr. habil. phys. Andris Sternberg
12. Dr. phys. Vismants Zauls
13. Dr. habil. phys. Juris Zvirgzds
14. Mg. chem. Maija Antonova
15. Mg. chem. Anna Kalvane
16. Mg. phys. Karlis Kundzins

Technical staff

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

Doctorants

1. Mg. phys. Roman Krutohvastov
2. Mg. ing. Ilze Smeltere
3. Mg. phys. Sergejs Fomins
4. Mg. phys. Varis Karitans

Graduate Students

1. B. sc. Marija Duncce
2. B. sc. Eriks Klotins (junior)
3. B. sc. Ainars Kuznecovs
4. B. sc. Reinis Taukulis

Visitors from Abroad

Prof. J. Banys, Vilnius University, Vilnius, Lithuania.

Prof. N. Iroshnikov, Adaptive Optics Laboratory, Moscow State University, Russia.

Dr. B. Garbarz-Glos, **Prof. J. Suchanich**, Institute of Physics, Krakow Pedagogical University, Krakow, Poland.

Scientific Visits Abroad

Dr. phys. **Ilze Aulika**

1. 15th Semiconducting and Insulating Materials Conference (SIMC XV), June 15-19, 2009, Vilnius, Lithuania (6 days);
2. FIAT research Centre (CRF), January 21-26, Turin, Italy (7 days);
3. Institute of Physics, Academy of Sciences of the Czech Republic, April 26 – May 25, Prague, Czech Republic (30 days);
4. October 20-21, Warsaw, Poland (3 days);
5. Faculty of Physics, University of Vienna, November 5-12, Vienna, Austria (7 days);
6. Institute of Physics, Academy of Sciences of the Czech Republic, November 16 – December 12, Prague, Czech Republic (28 days).

Dr. phys. **Karlis Bormanis**

1. 15th Semiconducting and Insulating Materials Conference (SIMC-XV), June 15-19, 2009, Vilnius, Lithuania (6 days);
2. International Conference „Phase Transitions, Critical and Nonlinear Phenomena in Condensed Matter”, September, 2009, Makhachkala, Russia (12 days);
3. 6th International Seminar on Ferroelastics Physics ISFP-6(11), September 22-25, 2009, Voronezh, Russia (7 days).

Dr. phys. **Eriks Klotins**

1. Williamsburg Workshop on Fundamental Physics of Ferroelectrics, February 8-11, 2009, Williamsburg, Wirginia (6 days);
2. Conference „Localized Excitations in Nonlinear Complex Systems”, July 14-17, Sevilla, Spain (6 days).

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

1. 20th Symposium of the International Colour Vision Society ICSV-2009, July 24-28, 2009, University of Minho, Braga, Portugal (6 days).
2. European Conference on Visual Perception, ECVP-2009, August 24-28, 2009, Regensburg, Germany (6 days).
3. The 14th Applied Vision Association Christmas Meeting AVA-2009, December 18, 2009, University of Bristol, Bristol, England (3 days).

M.Sc.ing. **Ilze Smeltere** (PhD)

1. Scientific exchange to Ceramics Laboratory at Ecole Polytechnique Federale de Lausanne, Switzerland, January 18 – February 14, 2009 (28 days);
2. Electroceramics for End Users “Piezo 2009”, February 28 – March 4, 2009, Zakopane, Poland (5 days);
3. International Conference and Exhibition of the European Ceramic Society (ECERS), June 21 – 25, 2009, Cracow, Poland (5 days);
4. The 11th International Conference-School Advanced Materials and Technologies August 27 – 31, 2009. Palanga, Lithuania (5 days).

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

1. Meetings of the Consultative Committee For the Euratom Specific Research and Training Programme in the Field of Nuclear Energy, Brussels, 2 times (4 days).
2. Meeting of the EFDA Steering Committee, 3 times: in Prague (2 days), Barcelona (2 days) and Brussels (2 days).
3. The European Joint Undertaking for ITER and the Development of Fusion Energy, Barcelona, 3 times (9 days).

4. COST Domain Committee Materials, Physics and Nanosciences, Meetings in Brussels, 2-3 March (2 days), Istanbul, 16-18 September (4 days).
5. MATERA: WP4 + WP1&WP2 Meetings, Board and Working Group Meetings in Rome (3 days), Luxembourg (3 days) and Istanbul (3 days).
6. Meetings of the High Level Group of EU Member States and FP7 Associated States on Nanoscience and Nanotechnologies, Prague (2 days) and Brussels (2 days).
7. 12th International Meeting on Ferroelectricity and 18th IEEE International Symposium on Applications of Ferroelectrics, Xi'an, China, August 23-27, 2009 (1 week).

Dr. phys. Vismants Zauls

1. MIND Project Review Meeting, April 16-17, 2009, Ferroperm Piezoceramics A/S, Copenhagen, Denmark (2 days).
2. MIND Project Meeting at IEEE Ultrasonics Conference, September 19-21, 2009, Roma, Italy (3 days)
3. Micro & Nano- Engineering (MNE-2009) Conference, September 28- October 2, 2009, Ghent, Belgium (5 days).
4. Institute of Fundamental Technological Research, PAN, October 20-22, Warszawa, Poland (3 days).

Cooperation

Latvia

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3. University of Latvia, Institute of Chemical Physics (Dr. D. Erts).
4. Company "GroGlass SIA".

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2. Volgograd State Architectural and Engineering Academy, Volgograd (Dr. phys. A. Burkhanov).
3. Joint Institute for Nuclear Research, Dubna (Dr. S. Tiutiunnikov, Dr. V.V. Jefimov).
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 (A.Larichev, N.Iroshnikov).

Slovenia

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THE MAIN RESULTS

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

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

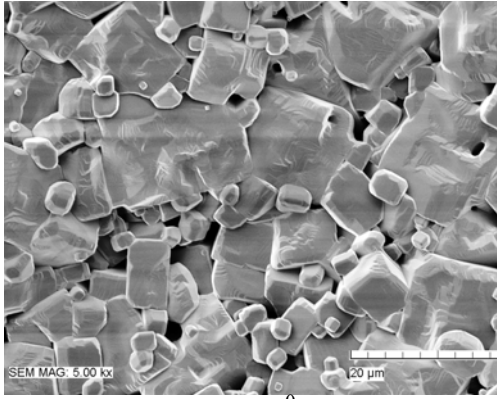
In the present work modified lead-free piezoelectric ceramics $(K_{0.5}Na_{0.5})NbO_3$ (KNN) were prepared by addition of 1wt.% CdO, ZnO, MnO_2 , V_2O_5 , and WO_3 . For further modification 0.5 mol% MnO_2 was added as a sintering aid, and effect of Sb^{5+} and Ta^{5+} substitution for Nb^{5+} on the Curie temperature, structure, dielectric and piezoelectric properties was studied.

Oxide addition promoted the densification of KNN ceramic body and increased the dielectric permittivity of the samples. The best ferroelectric and piezoelectric properties had samples doped with MnO_2 ; therefore it has been taken as sintering aid in substituted KNN ceramics. $KNNSb_x+0.5MnO_2$ ($x = 0, 0.02, 0.04, 0.05, 0.06, 0.07$ and 0.10) $KNNTa_x+0.5MnO_2$ ($x = 0, 0.02, 0.04, 0.05$) ceramics were sintered from 1050° to $1170^\circ C$ for 4 h. 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, and the highest values of dielectric permittivity. The optimal sintering temperature for Sb and Ta-substituted KNN ceramics occurs within $1110^\circ - 1140^\circ C$ and $1140^\circ - 1170^\circ C$, respectively. Density reached $4.40g/cm^3$ (97.6% of TD).

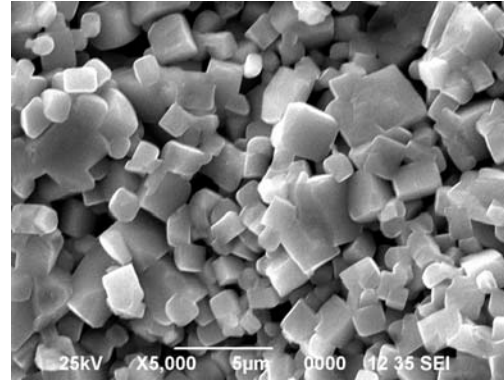
Microstructure of KNN based solid solution is considerably affected by doping elements as well as substitution level and sintering temperature.

The co-effects of MnO_2 doping and substitution for Nb^{5+} lead to significant improvements in dielectric and piezoelectric properties of KNN.

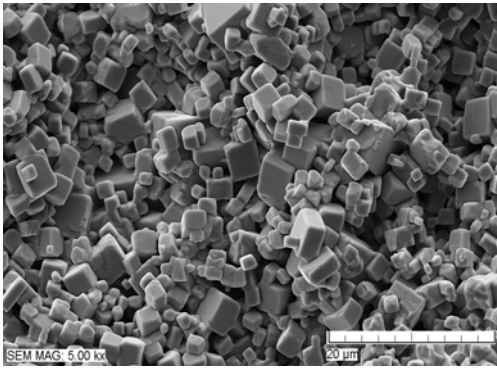
Sb^{5+} substituted ceramics reached high values in dielectric and piezoelectric properties: ϵ at the T_c increased from 6000 (KNN) to 12400 ($x=0.04$), $d_{33} = 92 \div 192 \text{pC/N}$, $k_p = 0.32 \div 0.46$, $k_t = 0.34 \div 0.48$. Ta^{5+} substitution increased the properties of KNN samples however not so noticeably.



SEM of KNN at 1160°C .



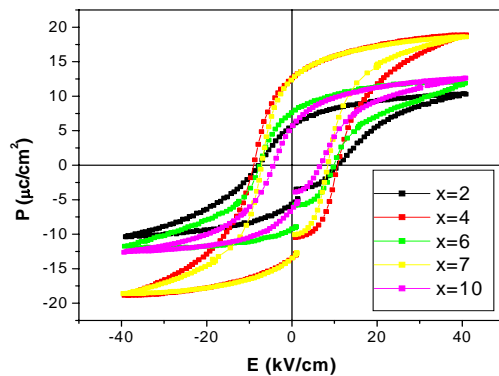
SEM of $\text{KNN}+0.5\text{MnO}_2$ ($x = 0$) at 1100°C .



SEM of $\text{KNNSb}_x+0.5\text{MnO}_2$ ($x = 0.06$).



SEM of $\text{KNNTa}_x+0.5\text{MnO}_2$ ($x = 0.05$).



INTRINSIC SPATIALLY LOCALIZED AND TIME PERIODIC EXCITATIONS IN COMPLEX OXIDES

E. Klotins

Solutions providing a guideline for the dynamical effects in complex oxides are found within the framework of localized excitations and ionic relaxation approaches.

Transition metal complex oxides categorized as ferroelectric relaxors attract considerable attention due their impressive structural variety and rich spectrum of functionalities. Central issue in understanding the novel behavior of these oxides is to discover the nature of short-range polar correlations presumably initiated by somewhat artificial metastable configurations as a challenge for theory. We have advanced to a resemblance between the metastable configurations on one hand and possible accumulation of energy in localized excitations supported by lattice nonlinearity on other. In these terms the effective Hamiltonians for ferroelectric relaxors comprising anharmonic insite and harmonic intersite potentials falls into category of systems specified by effective mass, optical modes, dynamical instability and chemical disorder, and the technicalities based on discrete nonlinear Schrödinger equations. The output is slow macroscopic kinetics determined by a balance between the energy and entropy (Fig). Necessary condition for associate symmetry breaking to arise is the presence of defects. For more complex ferroelectric relaxors evidencing local deviations from the randomness the first principles theory predicts local stoichiometric polar nanoregions, supercells, and relaxation of the constituting ions with respect to ideal lattice positions so supporting low symmetry local structures. The corresponding empirically modified Hamiltonian with first principles parameters yields statistical analysis within the mean field approach with temperature response of individual supercells as well as its correlation and pair distribution functions with dipole-dipole interaction as the external control parameter. Due the presence of polar nanoregions the corresponding metastable configurations emerge in natural way with a potential for slow kinetics as a part of the next generation modeling of complex oxides.

- (1) E. Klotins, Intrinsic localized excitations in nonlinear lattices: Heuristic explanation for the nature of polar nanoregions, *Physica E* (in press)
- (2) Klotins, A. Kuznetsov, A. Bely, Polarization response explored by joint Hamiltonian and stochastic approach, *Appl. Phys. A* (2009) 96:549-555
- (3) E. Klotins and A. Kuznetsov, Mesoscopic Scale Structural Instability in Ferroelectrics, *Ferroelectrics*, 378:111-120, 2009

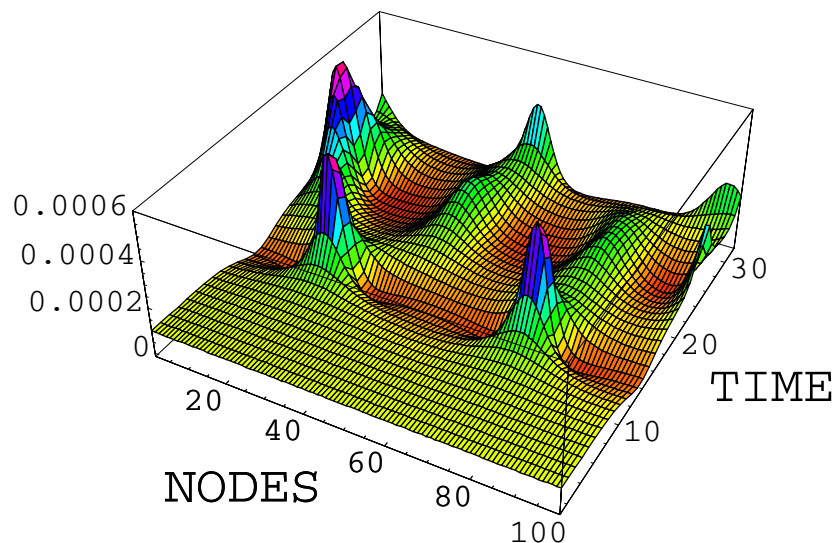


Figure. Emergence of localized excitations specified by squared modulus of complex mode amplitudes as function of the lattice node and the time. Reducing the plane wave amplitude due the exchange of energy with excitations is evident.

PHASE TRANSITIONS IN $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3\text{-PbTiO}_3$ SOLID SOLUTIONS

Marija Duce, Eriks Birks, Maija Antonova, Maris Kundzinsh,
Anatolijs Mishnovs, Maris Livinsh, and Andris Sternberg

Wide research of $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ (NBT) solid solutions is mainly connected with a possibility to obtain lead-free compositions, which would be perspective for practical applications. At the same time, the nature of phase transitions is not completely understood even in pure $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$. In the present work a new family of solid solutions $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3\text{-PbTiO}_3$ (NBT-ST-PT) was synthesized. For the first time there were done studies of structure and dielectric properties in NBT-ST-PT solid solutions and the transfer of nature of the phase transition was established in dependence of ratio of components in the solid solution. Addition of PbTiO_3 (PT) to $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3$ (NBT-ST) solid solutions causes the change of crystallographic lattice symmetry from cubic to tetragonal. In addition, the tetragonality increases if concentration of PT is increased. Phase transitions in these compositions were studied using measurements of temperature and frequency dependences of dielectric permittivity and polarization hysteresis loops. There were also done studies of electrocaloric effect, x-ray diffraction and microstructure (SEM).

The results show that gradual substitution of Sr or ($\text{Na}_{1/2}\text{Bi}_{1/2}$) by Pb in the initial composition 0.4NBT-0.6ST represents all sequential steps of the transfer from relaxor to normal ferroelectric phase transition. The initial composition 0.4NBT-0.6ST and compositions with low PT concentrations are characterized by relaxor behaviour without phase transition to ferroelectric state, even if electric field is applied. If concentration of PT increases, there are obtained compositions with relaxor behaviour with a possibility to induce ferroelectric state, only if electric field is applied, at temperatures below the maximum of the relaxing dielectric permittivity. Furthermore, the induced ferroelectric state is destroyed at temperature T_t during heating without applying electric field. Further increase of content of PT stabilizes ferroelectric state. The characteristic relaxor behaviour remains only in temperature range between T_t and T_m (temperature of maximum of dielectric permittivity). The phase transition to ferroelectric state at temperature T_t occurs spontaneously, without electric field applied. If concentration of PT increases, difference $T_m - T_t$ decreases. At higher PT concentrations sharp phase transition between macroscopically non-polar and ferroelectric state is obtained. Temperatures T_m and T_t as functions of PT concentration for the family of solid solutions, where Sr is gradually replaced by Pb, are showed in Figure 1.

For compositions in PT concentration range, where relaxor behaviour is observed, temperature dependence of dielectric permittivity is described by power law, and frequency dependence of temperature of dielectric permittivity maximum

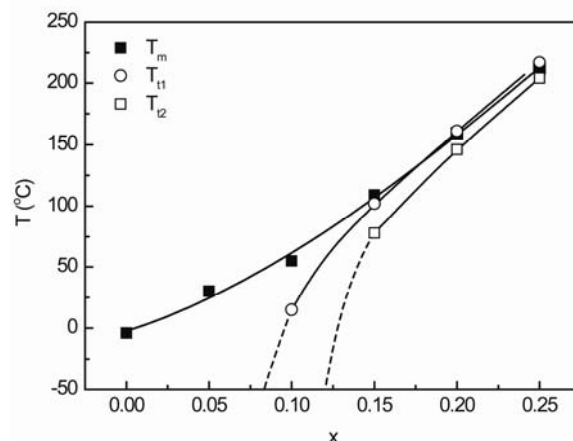


Fig. 1. Temperature T_m (at 1 kHz), which was obtained during cooling measurements, and temperatures T_{t1} and T_{t2} , which were obtained during heating and cooling measurements accordingly and at which the phase transition between relaxor and ferroelectric state occurs, as functions of PT concentration for solid solution family 0.4NBT-(0.6-x)ST-xPT. *In the concentration range where T_{t2} does not exist, T_{t1} was obtained after cooling under applied electric field.*

T_m – by Vogel-Fulcher relationship. The presence of the first order phase transition between relaxor and ferroelectric phases at temperatures below the maximum of dielectric permittivity is established both by double hysteresis loops of polarization and by behaviour of the electrocaloric effect. Furthermore, there was observed rather high electrocaloric effect in some compositions. For examples, in 0.4NBT-0.4ST-0.2PT it reaches approximately -1 °C.

X-ray diffraction measurements revealed 100% perovskite structure for all compositions. At low PT concentrations cubic or pseudocubic structure is observed. However at a definite PT concentration tetragonality, which is larger than 1, appears and grows with increasing PT content (in composition 0.4NBT-0.35ST-0.25PT it reaches approximately 1.015). Microstructure studies showed that, despite the observed porosity, all samples are qualitative, dense ceramics with well developed grain form.

The above mentioned properties allow us to include the serie of the investigated solid solutions in the group of such compounds as $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ - PbTiO_3 , $\text{Pb}_{1-x}\text{La}_x(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$, where similar transformation from relaxor to normal ferroelectric state if ratio of the components is changed.

It is also shown in the work that addition of NaNbO_3 to NBT-ST-PT solid solutions acts contrary to PT, stabilizing the relaxor state.

FERROELECTRIC LIQUID CRYSTAL GOGGLES FOR AMBLYOPIA RESEARCH

S. Fomins, M. Ozolinsh, G. Krumina, and V. Karitans

Institute of Solid State Physics

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Ferroelectric Liquid Crystal (FLC) filters offer the speed of electronic light shutters and the vibration free operation. These characteristics make them ideal for applications requiring short exposure times and minimal blur, offering switching faster than 1/5000 of a second. FLC filters can be used as the optical shutter for machine vision purposes, also in vision research. On the basis of FLC filters we have developed ferroelectric glasses, allowing temporally differentiate optical information for both eyes. In the case of amblyopia („lazy eye”) the only way to oblige the „lazy” eye to work is to close the other better-seeing eye. We advice a system for dynamic visual system training to retain the functionality of the worse-seeing eye. For fast switching the filters are powered by bipolar minus to plus control voltage power supply separate for two left and right channels, with optical isolation for higher safety reasons. The duration of the glasses open state for each of the filters is controlled through the PC parallel port. The main application of the system is use for amblyopia research and training. Fast switching speed allows its use in stereo vision temporal characteristics studies.

ELECTRICAL PROPERTIES OF LEAD FERROTANTALATE CERAMICS

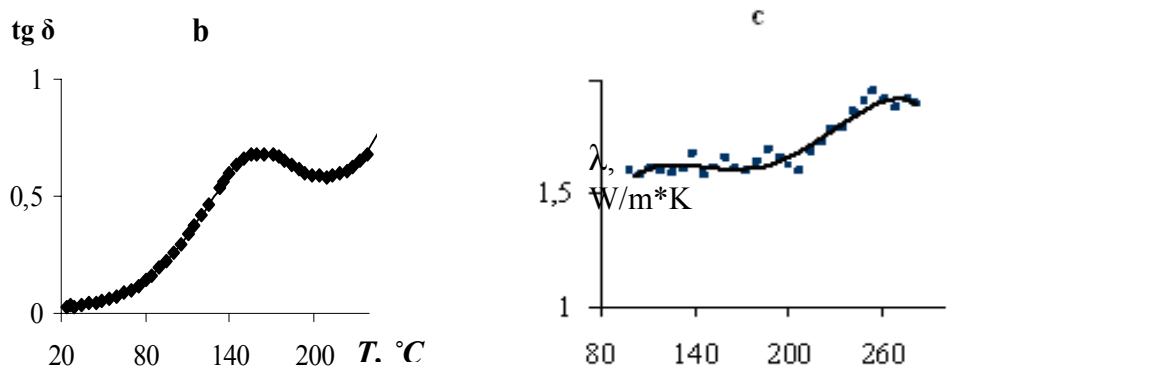
K. Bormanis, A.I. Burkhanov*, A.I.Waingolts*, and A. Kalvane

Lead ferrotantalate ($\text{PbFe}_{1/2}\text{Ta}_{1/2}\text{O}_3$), a member of the perovskite family, is known to belong to the group of so called ferroelectric-magnetic compounds [1] the Neel temperature of which is $T_N \sim -140$ °C and the Curie temperature $T_C \sim -40$ °C. Because of such unusual properties the material is of current interest for both fundamental studies and application.

Powders of lead ferrotantalate were synthesized from the corresponding oxides by solid state reaction. Ceramic samples were produced by conventional ceramics technology. An excess amount of PbO was added to the mixture to compensate evaporation of PbO at sintering. The synthesis and sintering phase constitution were examined by differential thermal analysis and X-ray diffraction.

Results of the study of dielectric dispersion of ϵ' in the range of low and infra-low frequencies and behaviour of heat conductivity λ at $T > T_c$ are reported.

Fig. a illustrates a monotonous pattern of the $\epsilon'(v)$ curves in the $\text{PbFe}_{1/2}\text{Ta}_{1/2}\text{O}_3$ ceramics at $T > T_c$. The growth of ϵ' at heating and frequencies below 10 Hz starts immediately while a decrease with the temperature is observed at higher frequencies. Studies within the range of higher temperatures revealed a relaxation maximum of dielectric loss ($\text{tg}\delta$) at 1000 Hz (Fig. b). Further growth of $\text{tg}\delta$ (T) is related to a considerable contribution from bulk conductivity being in agreement with the behaviour of λ (T) (Fig. c) showing a noticeable increase around 220 °C. As observed in a study of λ (T) in $\alpha\text{-LiIO}_3$ [2], that might be due to a growing contribution to heat conductivity by charge carriers in the material.



* Cooperation with Volgograd State Architectural and Engineering University, Volgograd, Russia

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QUANTITATIVE EVALUATION OF PSEUDOISOTHERMATIC ISHIHARA AND RABKIN COLOUR DEFICIENCY TESTS USING MULTISPECTRAL COLOUR ANALYSIS

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We have applied a multispectral colour analysis spectrally scanning Ishihara and Rabkin colour deficiency test book images by use of tunable liquid crystal LC filters (Nuance II, Cri) for quantitative characterization of printed tests. Comparing to reflectance spectroscopy with excellent spectral resolution (Lee&Honson, 2003 Color Research and Application 28 267-276) multispectral analysis keeps information regarding spatial content of the tests. Images were taken in the range of 420 to 720nm with a 10nm step under halogen incandescent lamp illumination. 10nm steps allow to obtain at least 10 independent spectral inputs within the spectrum range of any L, M and S cone colour sensitivity range. Inputs of L, M and S cone systems were estimated and processed according to colour opponency models using cone functions. For all tests we obtain satisfactory alignment of colour pigments along the protan and deutan confusion lines in CIE xyz colour gamut. Cross-correlation was performed between the test image M (protan), M(deutan), and L-cM inputs and reference image containing only the pseudoisochromatic plate high contrast

latent object. Thus the signal-to-noise value – a ratio of the cross-correlation peak value (at position when the latent object in reference image spatially coincides with the related object in the cone input chart) to the mean valley value (at position where objects on both images are distant each from other) characterizes the subject ability to recognise the corresponding latent object in the test plate. That allows to find the recognition task „signal-to-noise” ratio of pseudoisochromatic test plates for subjects with different types and degrees of colour deficiency. Thus for an annulus in the 17th test plate (Rabkin) the ratio of signal/noise equals to 2.2 for L-cone input (deutans) , and 1.3 for M-cone input (protans).

LINEAR PROFILE SENSOR FOR DETECTING POSITION OF AN EYE

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A method for stabilizing gaze of an eye is developed. The basis of the method is use of a linear profile sensor that determines coordinates of a moving light spot. The sensor has 1 x 1024 pixel array. Each pixel outputs an analog video signal sequentially. This signal is converted into digital format by 10-bit ADC. By reading all pixels intensity of all adjacent pixels is compared. The order number of the most intense pixel is stored. After all the array has been scanned, it is known which is the most intense pixel. After the angle at which the ray hits the sensor is calculated. By means of a translation stage a position of a mirror is found when the light illuminates an optoswitch. The optoswitch signalizes to stop the movement because the direction of gaze coincides with the optical axis. This method would be useful to prevent the disturbing effects of eye movements on correcting optical aberrations.

FRACTAL STRUCTURES IN SINGLE CRYSTALS OF FERROELECTRIC LITHIUM NIOBATE GROWN UNDER STRONGLY UNSTABLE CONDITIONS

M. Palatnikov^{*}, O. Shcherbina^{*}, N. Sidorov^{*}, K. Bormanis, and A. Sternberg

Different from crystallography the fractal geometry allows to study disordered structures under conditions of reproducibility of elements. Formation of fractal structures under conditions far from thermodynamic equilibrium being a general feature qualifies them as dissipative structures emerging at powerful energy flows. Due to such flows a system becomes active acquiring the ability of creating autonomous structures. Single crystals of lithium niobate containing lanthanide admixtures were grown under substantially alternating thermal conditions introducing defects presenting regular heterogeneous distribution of the admixture and, consequently, a regular domain structure (RDS) the period of which was determined by the ratio of the speed of draw to the speed of rotation of the crystal. The synergetic approach enables applying fractal analysis to the obtained microstructures considering the periodic RDS as regularly repeated similar fractal structures being the product of self-organisation in an open system.

By atomic force microscopy nano-size fractal structures of period from 10 to 100 nm were revealed in the region of the periodic RDS of the lithium niobate single crystals containing lanthanide admixtures. The periodic division is observed taking place along the polar axis of the crystal as well as in the direction perpendicular to it the periodic structural formations extending to the volume of some hundreds of elementary cells. The width of the weak “additional” Raman bands revealed in lithium niobate crystals containing lanthanide admixtures anomalously decrease with the disordering of the cation sublattice as the composition of the single crystal is changed. This may be some evidence featuring ordering of structural units of the cation sublattice in lithium niobate

single crystals of a congruent composition containing lanthanide admixture emerging due to self-organisation at an overall disordering of it. Such behaviour of bandwidths may be assumed related to a structure of cluster defects in the cation sublattice of the crystal. Calculations show that clusters in the structure of lithium niobate are formed at intrinsic defects Nb_{Li} generating ordered sublattices of the size of a few periods of translations, it is, the span of 1 – 2 nm. Such periodic fractal structures of the size of 1 nm – 100 μ m are formed in single crystals of lithium niobate containing lanthanide admixtures grown under strongly non-stationary conditions.

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

DIELECTRIC PROPERTIES OF $SrBi_2Ta_2O_9$ CERAMICS AT INFRA-LOW FREQUENCIES

K. Bormanis, A. Sternberg, A.I. Burkhanov*,
Yu.V. Kochergin*, and A. Kalvane

Presently attention is paid to $SrBi_2Ta_2O_9$ as a ferroelectric composition used in devices of autonomous memory. Deterioration processes under conditions of numerous switching of polarisation in this material are much less pronounced compared with other ferroelectrics. A study of the features of relaxation of polarisation in $SrBi_2Ta_2O_9$ ceramics at low- and infra-low frequencies is reported.

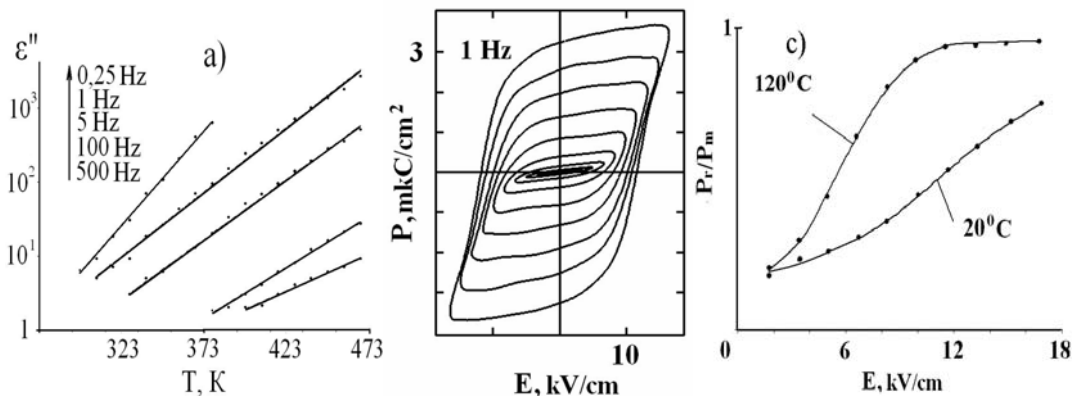
The ceramic samples of $SrBi_2Ta_2O_9$ were produced by conventional ceramic technology from high purity grade oxides: SrO, Bi_2O_3 , and Ta_2O_5 .

Contribution to dielectric loss from conductivity of $SrBi_2Ta_2O_9$ grows at decreasing the frequency (Fig. a). The thermal dependence of $\varepsilon''(T)$ is well described by $\varepsilon''(T) = A \cdot e^{aT}$ where a depends on the frequency. The estimates of conductivity from $\gamma = 2\pi\nu\varepsilon''\varepsilon_0$ in AC field at relatively low temperatures, it is, well below T_c showed dependence on frequency described by power function $\gamma \approx \omega^\alpha$ suggesting a jumping mechanism of conductivity. At rising the temperature γ becomes partly independent on frequency pointing to a gradual increase of the contribution from bulk conductivity.

In a series of polarization loops at frequencies 1 and 10 Hz recorded on a Sawyer-Tower bridge the hysteresis of polarization at switching is well pronounced by gradual evolution of the shape of polarization curves from Rayleigh biangle into quasi-saturated strongly rectangular loops (Fig. b). The shape of the loops is characteristic to the ferroelectric phase when domains provide the main contribution to polarization at strong measuring fields.

Curves of the ratio of the value of remnant polarization to the corresponding maximum value of polarization P_r/P_m obtained from the polarization loops at different temperature and frequency of 1 Hz are shown in Fig. c.

A qualitative estimate of thermal behaviour of the coercive field (E_c) shows that the temperature at which $E_c = 0$ is close to 320 °C being in good enough agreement with data on the Curie temperature of $SrBi_2Ta_2O_9$.



* Cooperation with Volgograd State Architectural and Engineering University, Volgograd, Russia

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Lectures in Conferences

Workshop on the Fundamental Physics of Ferroelectrics 2009, University of Pennsylvania, February 8-11, 2009, Colonial Williamsburg, VA.

1. E. Klotins. Intrinsic Localized Excitations in Nonlinear Lattices: Clues to Relaxor State in Ferroelectrics? Abstracts, 2 p.

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1. I. Smeltere, M. Dambekalne, M. Antonova, M. Livinsh, A. Kalvane, V. Zauls. Processing and properties of doped $(\text{K}_{0.5}\text{Na}_{0.5})\text{NbO}_3$ ceramics. Book of abstracts, p. 63.

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1. G. Pikurs, J. Zvirgzds. Ģeotermālo siltumsūkņu vadības algoritmu optimizācija. Optimisation of Ground Source Heat Pump Control Algorithms. Tēzes 24. lpp.
2. G. Muižnieks, Ē. Geriņš. Šķidrums plūsmas rotorsūkņu rotoru virsmas fizikāli mehānisko īpašību uzlabošanas metožu analīze. Process Analysis of Surface Fiscal Mechanical Properties Improving for Oil Flooded Rotary Pump Rotor. Tēzes 25. lpp.
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5. V. Karitāns, M. Ozoliņš, S. Fomins. Adaptīvā optika redzes zinātnē – hiperasuma pētījumi acī ar koriģētām augstāko kārtu aberācijām. Adaptive Optics in Vision Science – Research of hyperacuity in an Eye with Corrected Higher Order Aberrations. Tēzes 48. lpp.
6. R. Krutohvostovs, K. Kundziņš, V. Zauls. Domēnu inženierijas vispārīgie principi nelineāros kristālos. General Principles of Domain Engineering in Nonlinear Optical Crystals. Tēzes 56. lpp.
7. I. Aulika, V. Zauls, M. Kundziņš. Segnetoelektrisko kristālu un plāno kārtiņu termooptiskie pētījumi: sasniegumi un problēmas. Thermo-Optical Investigations of Ferroelectric Crystals and Thin Films: Achievements and Problems. Tēzes 57. lpp.
8. E. Birks, M. Dunce, M. Kundziņš, M. Antonova, A. Mišņovs. $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3 - \text{SrTiO}_3 - \text{PbTiO}_3$ cieto šķīdumu dielektriskās īpašības. Dielectric Properties of $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3 - \text{SrTiO}_3 - \text{PbTiO}_3$ Solid Solutions. Tēzes 58. lpp.
9. R. Taukulis, V. Zauls. Uzlabots interferences joslu mērīšanas paņēmieni diferenciālajam interferometram. Improved Fringe Subdivision Technique for Differential Interferometer. Tēzes 59. lpp.
10. A. Šternbergs. Pētnieciskie projekti un nepieciešamās ierīču izstrādes ITER attīstībai no 2009. gada skatpunkta. R&D Missions and Associated Milestones Contributing ITER Programme: Outlook Henceforth. Tēzes 67. lpp.
11. A. Šarakovskis, J. Grūbe, A. Mišņovs, G. Doķe, M. Sprinģis. Enerģijas pārnese īpatnības ar Er^{3+} un Yb^{3+} aktivētos sīkātstiklā un keramikā. Energy Transfer in Er^{3+} and Yb^{3+} Doped Silicate Glas and Glass Ceramics. Tēzes 80. lpp.
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13. E. Laizāne, K. Kundziņš, I. Muzikante, J. Teteris. Hologrāfiskais ieraksts azobenzolu atvasinājumu plānās kārtiņās. Holography Recording in Azobenzene Containing Polymer Films. Tēzes 88. lpp.

Functional Materials and Nanotechnologies 2009. International Baltic Sea Region Conference, March 31–April 3, Riga, Latvia.

1. Marija Dunce, Maija Antonova, Eriks Birks, Maris Kundzinsh, and Andris Sternberg. Phase Transitions in Modified $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3 - \text{SrTiO}_3$ Solid Solutions. Book of Abstracts p. 51.
2. E. Klotins. Localization Transition and Emergence of Polar Nanoregions in Relaxor Ferroelectrics. Book of Abstracts p. 59.
3. A. Kuznetsov. Localization in Klein-Gordon Lattices and Its Relevance Polar Nanoregions. Book of Abstracts p. 108.
4. Jurgis Grube, Guna Doke, Ilze Aulika, Jevgenijs Gabrusenoks, Anatolijs Sarakovskis, and Maris Springis. Optocal Spectroscopy of Er^{3+} Doped Tellurite Glasses. Book of Abstracts p. 110.
5. E. Laizane, D. Gustina, K. Kundzins, I. Muzikante, and J. Teteris. Optical Induced Patterning of Polymer Films Doped with Azobenzen Molecules. Book of Abstracts p. 125.
6. Ilze Aulika, Alexandr Dejneka, Anna Lynnyk, Armin Fuith, Vismants Zauls, and Maris Kundzins. Multilayer BST/PZT Thin Films Studied by Spectroscopic Ellipsometry. Book of Abstracts p. 144.
7. K. Bormanis, A.I. Burkhanov, A.I. Waingolts, and A. Kalvane. Electrical Properties of Lead Ferrotantalate Ceramics. Book of Abstracts p. 155.

8. M. Palatnikov, O. Shcherbina, A. Frolov, O. Makarova, P. Chufyrev, and K. Bormanis. Formation of Fractal Micro- and Nano-Structures in Ceramic Tantalum Pentoxide Under Concentrated Flux of Light Affecting Thermal Expansion. Book of Abstracts p. 156.
9. N.V. Sidorov, P.G. Chufyrev, A.A. Janichev, B.N. Mavrin, M.N. Palatnikov, and K. Bormanis. Manifestation of Micro- and Nano- Structures in Raman Scattering of Photorefractive Lithium Niobate Single Crystals. Book of Abstracts p. 157.
10. B. Garbarz-Glos, R. Bujakiewicz-Koronska, D. Majda, M. Antonova, and A. Kalvane. DSC Investigation of Polycrystalline $\text{BaTi}_{1-X}\text{Zr}_X\text{O}_3$ for $0 \leq X \leq 0.125$. Book of Abstracts p. 160.
11. W. Smiga, B. Garbarz-Glos, A. Kalvane, M. Antonova. Strontium Concentration Dependence of Selected Structural and Mechanical Properties of Polycrystalline $\text{Ba}_{1-X}\text{Sr}_X\text{TiO}_3$ for $0 \leq X \leq 0.4$. Book of Abstracts p. 161.
12. Ilze Smeltere, Maruta Dambekalne, Maris Livinsh, and Marija Duncce. Sintering of Lead-Free $(\text{K}_{0.5}\text{Na}_{0.5})\text{NbO}_3$ Based Solid Solutions. Book of Abstracts p. 162.
13. B. Garbarz-Glos, W. Smiga, R. Bujakiewicz-Koronska, W. Suchanicz, M. Dambekalne, M. Livinsh, A. Sternberg. Influence of Zirconium on Structural, Microstructural and Ferroelectric Properties of $\text{BaZr}_{0.20}\text{Ti}_{0.80}\text{O}_3$ Ceramic. Book of Abstracts p. 163.
14. J. Suchanicz, T. Glos, G. Stopa, T. Kruzina, I. Jankowska-Sumara, D. Wcislo, K. Konieczny, R. Rosiek, A. Finder, M. Dambekalne, and A. Sternberg. Lead-Free $(\text{Na}_{0.5}\text{Bi}_{0.5})_{1-X}\text{Ba}_X\text{TiO}_3$ Single Crystals ($0 \leq X \leq 0.05$) and its Dielectric and Pyroelectric Properties. Book of Abstracts p. 164.
15. Sergejs Fomins, and Maris Ozolinsh. Multispectral Analysis of Colour Deficiency Tests and Modelling of Cones Influence on Perception of Colour. Book of Abstracts p. 203.

Developments in Optics and Communications (DOC-5), April 24–26, 2009, University of Latvia, Riga, Latvia.

1. S. Fomins. Masking Study of Instant Stimuli Texture Segmentation. Abstract Book, p. 20-21.
2. G. Ikaunieks, M. Ozolinsh, A. Stepanovs, V. Lejiete, and N. Reva. Effect of Optical and Physiological Factors on Light Scattering in the Eye. Abstract Book, p. 40.

Second International Meeting on Materials for Electronic Applications IMMEA, May 7-9, 2009, Hammamet, Tunisia.

1. M. Palatnikov*, V. Efremov*, O. Makarova*, N. Sidorov*, And K. Bormanis** Effects of Concentration on Electric and Elastic Properties of Ferroelectric $\text{Li}_x\text{Na}_{1-x}\text{Ta}_{0.1}\text{Nb}_{0.9}\text{O}_3$ Solid Solution Ceramics
2. I. Smeltere, M. Dambekalne, M. Livins, A. Mishnov, R. Krutokhvostov, M. Antonova, A. Kalvane, And K. Bormanis. Processing and Properties of Potassium-Sodium Niobates Modified by Oxides
3. K. Bormanis, Yu.V. Kochergin, A.I. Burkhanov, and A. Kalvane. Dielectric Properties of Layered Ferroelectric $\text{SrBi}_2\text{Ta}_2\text{O}_9$.

15th Semiconducting and Insulating Materials Conference (SIMC-XV), June 15-19, 2009, Vilnius, Lithuania.

1. R. Grigalaitis, J. Banys, Š. Bagdzevičius, K. Bormanis, A. Sternberg. Dielectric Investigation of Lead-Free Perovskite Strontium Titanate with 25% Bismuth Ceramics. Programme & Abstracts, p. 112.
2. Aulika, A. Dejneka, A. Lynnyk, V. Zauls, K. Kundzins, A. Fuith. Thermo-Optical Investigations of Ferroelectric Thin Films in the Wide Temperature Range of 4-820 K. Programme & Abstracts, p. 115.
3. K. Bormanis, A.I. Burkhanov, Yu.V. Kochergin, and A. Kalvane. Polarization of $\text{SrBi}_2\text{Ta}_2\text{O}_9$ Ceramics at Infra-Low Frequencies. Programme & Abstracts, p. 116.

4. M. Palatnikov, V. Efremov, O. Makarova, K. Bormanis. Semiconductor Posistors on the Basis of $\text{Li}_{0.12}\text{Na}_{0.88}\text{Ta}_y\text{Nb}_{1-y}\text{O}_3$ Solid Solutions. Programme & Abstracts, p. 117.
5. M. Dunce, M. Antonova, E. Birks, A. Sternberg. Phase Transitions in Modified $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3$ Solid Solutions. Programme & Abstracts, p. 118.

11th International Conference and Exhibition of the European Ceramic Society (ECERS), June 21-25, 2009, Krakow, Poland.

1. Palatnikov M., Shcherbina O., Makarova O., Chufyrev P., Sidorov N., Bormanis K. Studies of Formation of Fractal Micro- and Nano-Structures in Niobium and Tantalum Pentoxide Ceramics and Related Effects on Thermal Expansion. Programme and Book of Abstracts, pp. 72-73.
2. Bormanis K., Burkhanov A., Kalvane A., Antonova M. Dielectric Dispersion In Lead Ferro-Niobate And Lead Cobalt-Tantalate Ceramics. Programme and Book of Abstracts, p. 103.
3. Grigalaitis R., Banyys J., Brilingas A., Bormanis K., Sternberg A., Zauls V. Broadband Dielectric Studies of (1-x)PMN-(x)PT Relaxor Ceramics. Programme and Book of Abstracts, p. 103.
4. Dambekalne M., Antonova M., Livins M., Kalvane A., Smeltere I., Mishnov A., Krutohvastov R., and Bormanis K. Production and Dielectric Properties of Modified Potassium-Sodium Niobate Solid Solutions. Programme and Book of Abstracts, p. 104.

Localized Excitations in Nonlinear Complex Systems (LENCOS), July 14-17, Sevilla Spain.

1. E. Klotins. Localized Excitations in Complex Oxides: Polar Nanoregions. Book of Abstracts, p.32

20th Symposium of the International Colour Vision Society ICSV-2009, July 24-28, 2009, University of Minho, Braga, Portugal.

1. M. Ozolinsh, I. Martín, and M.C. Puell. Colour and Luminance Contrast in Depth Perception. Abstracts, p.103.
2. I. Martín, S. Fomins, and M. Ozolinsh. Multispectral Analysis of Colour Deficiency Tests and Modelling of Cones Influence on Test Perception.” Abstracts, p.145.

12th International Meeting on Ferroelectricity and 18th IEEE International Symposium on Applications of Ferroelectrics, (IMF-ISAF-2009), August 23-27, 2009, Xi'an, China.

1. K. Bormanis, A. Sternberg, A.I. Burkhanov, Yu.V. Kochergin, and A. Kalvane. Dielectric Properties of $\text{SrBi}_2\text{Ta}_2\text{O}_9$ Ceramics at Infra-Low Frequencies. Program book, Abstract CD: DP-029.
2. M. Palatnikov, O. Shcherbina, N. Sidorov, K. Bormanis, and A. Sternberg. Fractal Structures in Single Crystals of Ferroelectric Lithium Niobate Grown Under Strongly Unstable Conditions. Program book, Abstract CD: CP-025.
3. I. Smeltere, M. Dambekalne, M. Antonova, A. Kalvane, M. Livinsh, A. Mishnov, A. Sternberg. Effect of Mn- and W- Doping on the Sintering and Properties of KNN Based Lead-Free Ceramics. Program book, Abstract CD: DP-040.
4. M. Dunce, M. Antonova, E. Birks, and A. Sternberg. Phase Transitions in $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3\text{-SrTiO}_3\text{-PbTiO}_3$ Solid Solutions. Program book, Abstract CD: EP-001.

European Conference on Visual Perception, ECVP-2009, August 24-28, 2009, Regensburg, Germany.

1. V. Karitans, M. Ozolinsh, and S. Fomins. Dependence of Vernier Acuity on the Presence/Absence of Aberrations of a Human Eye. Perception 38, p.128.
2. U. Atvars, and S. Fomins. Chaser Illusion and Opponent Color Aftereffects. Perception 38, p.135.

3. M. Ozolinsh, and S. Fomins. Multispectral Analysis of the Color Deficiency Tests and Modelling of Cones Influence on Test Perception. Perception 38, p. 37.
4. D. Lauva, M. Ozolinsh, and S. Fomins. Modelling of RGB Colour Contribution to Visual Acuity in Conditions of Fog Evoked Decrease of Luminance and Contrast. Perception 38, p. 35.
5. S. Fomins, and L. Zarina. Segmentation of Instant Isoluminant Chromatic Textures. Perception 38, p. 54.

**«Фазовые переходы, критические и нелинейные явления в конденсированных средах»,
Сент. 7-10, Махачкала, Россия.**

1. С.Н. Каллаев, З.М. Омаров, А.Р. Билалов, Х. Алилов, С.А. Садыков, К. Борманис. Особенности тепловых свойств керамики на основе ЦТС с нанополярной структурой. Сборник трудов, Махачкала, 2009, с. 30-33.
2. М.Н. Палатников, В.В. Ефремов, И.П. Раевский, О.В. Макарова, Н.В. Сидоров, К. Борманис. Позисторные материалы на основе ТР $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$ для работы в средах с низким парциальным давлением кислорода. Сборник трудов, Махачкала, 2009, с. 140-143.
3. А.И. Бурханов, А.И. Вайнгольц, К. Борманис, А. Калване. Низко- и инфранизкочастотные диэлектрические свойства керамики $PbFe_{1/2}Ta_{1/2}O_3$. Сборник трудов, Махачкала, 2009, с. 147-150.
4. С.Н. Каллаев, Р.М. Митаров, З.М. Омаров, Х. Алилов, К. Борманис. Теплоемкость сегнетокерамики ЦТСЛ в области размытого фазового перехода. Сборник трудов, Махачкала, 2009, с. 159-162.

6th Int. Seminar on Ferroelastics Physics ISFP-6(11), September 22-25, 2009, Voronezh, Russia.

1. Dmitry Kiselev, Igor Bdikin, Andrei Kholkin, Karlis Bormanis, and Marija Kosec. Local Ferroelectric Properties, Domain Evolution and Fractal Analysis of PLZT Ceramics via Scanning Probe Microscopy. Abstract book, p. 68.
2. А.И. Бурханов, Ю.В. Кочергин, К. Борманис, А. Калване. Поляризационные процессы в керамиках $BaBi_2Nb_2O_9$ и $SrBi_2Ta_2O_9$ в полях инфранизкой частоты. Abstract book, p. 187.
3. М.Н. Палатников, О.Б. Щербина, Н.В. Сидоров, К. Борманис. Фрактальные микро- и наноструктуры в легированных лантаноидами монокристаллах ниобата лития. Abstract book, p. 189.

Baltic Polymer Symposium, September 22-25, 2009, Ventspils, Latvia.

1. A. Sternberg, I. Muzikante. Research of Functional Materials and Composites in Latvian Research Programme in Materials Sciences. Programme and Proceedings, p. 18.

«Актуальные проблемы физики твердого тела» (ФТТ-2009), Октябрь 20-23, Минск, Беларусь.

1. К. Борманис, А.И. Бурханов, А.И. Вайнгольц, А. Калване. Низкочастотные диэлектрические свойства керамики $PbFe_{1/2}Ta_{1/2}O_3$. Сборник докладов, 2, 278-280.
2. (М.Н. Палатников,) В.В. Ефремов, Н.В. Сидоров, К. Борманис. Упругие характеристики сегнетоэлектрических керамических твердых растворов $Li_xNa_{1-x}Ta_{0.1}Nb_{0.9}O_3$. Сборник докладов, 2, 264-266.
3. I. Smeltere, M. Dambekalne, M. Antonova, M. Livinsh, A. Kalvane, M. Dunce, A. Sternberg. Synthesis and Characterization of Substituted $(K_{0.5}Na_{0.5})NbO_3$ Lead-Free Ceramics. Сборник докладов, 2, 272-274.

4. М.Н. Палатников, О.Б. Щербина, А.А. Фролов, В.Н. Павликов, К.Я. Борманис. Микро- и наноструктуры фрактального типа и механизмы теплового расширения в керамическом пентаоксиде тантала. Сборник докладов, 3, 239-241.

The 14th Applied Vision Association Christmas Meeting AVA-2009, December 18, 2009, University of Bristol, Bristol, England.

1. M. Ozolinsh, S.Fomins, and M. Colomb. Quantitative Evaluation of Ishihara and Rabkin Colour Deficiency Tests Using Multispectral Colour Analysis.” Abstract Book, p. 29-30.

PATENTS

1. I. Kalviņš, A. Birmans, M. Vēveris, A. Ļebedevs, A. Mišņovs. Gamma-Butyrobetaine Succinate and Method of Preparing Thereof. LR Patenta Pieteikums Nr P-09-113 no 25.06.2009.
2. I. Kalviņš, A. Birmans, M. Vēveris, A. Ļebedevs, A. Mišņovs. A Combination Medicinal Product for the Treatment and/or Prevention of Metabolic-Related Disorders. LR Patenta Pieteikums Nr P-09-116 no 25.06.2009.
3. I. Kalviņš, A. Birmans, M. Vēveris, A. Ļebedevs, A. Mišņovs. Medicinal Products Comprising Meldonium Succinate. LR Patenta Pieteikums Nr P-09-114 no 25.06.2009.
4. I. Kalviņš, A. Birmans, M. Vēveris, A. Ļebedevs, A. Mišņovs. Combination Medicinal Product Comprising Meldonium. LR Patenta Pieteikums Nr P-09-115 no 25.06.2009.

**SEMICONDUCTOR MATERIALS
AND SOLID STATE IONICS**
SEMICONDUCTOR MATERIALS DIVISION
Head of Division Dr.phys. A.Lusis

Research areas and expertise

- Resource science – resource physics and chemistry
- Electrophysics and electrochemistry of specific semiconductor materials, mixed conductors, ion conductors (transition metal oxides, bronzes, metal hydrates, solid electrolytes, nanostructured and porous materials, composites etc.)
- Material preparation methods: thin and thick film technologies, sol-gel process, leaching, sonochemical processes
- Material characterization by spectroscopic methods (Raman scattering, optical and X-ray absorption, EXAFS), electrical and electrochemical impedances, AFM, TGA/DTA, etc
- Solid state ionics:
 - electro-, photo-, thermo-, chemo- or gaso-chromic phenomena in transition metal oxides
 - structural changes due to ion intercalation
 - lattice dynamics and structural and electronic phase transitions
 - solid state reactions at interfaces electrode – solid electrolyte
 - gases and ions sensing phenomena and detection technologies
- Functional coatings and multi layer electrochemical systems
- Hydrogen absorption phenomena in metals, semiconductors and insulators
- Development of hydrogen generation equipment and new nano structured materials for hydrogen storage
- New measurement technologies and instruments with artificial intellect (encl., eNose)
- Development methods and techniques for quality and reliability testing for lead -free joints of PCB

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 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.
- Hydrogen technologies: production through electrolysis, biofermentation, storage in metal hydrides and composites, usage for electricity production (fuel cells) and as additional fuel for internal combustion vehicles, heat production.
- Hydrogen – Solar and Hydrogen – Wind technologies.
- High capacity energy storage units, nickel hydride and lithium batteries.
- Nano size and structured materials for Hydrogen and Solar technologies, for thin film batteries.
- 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.

Scientific staff:

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

Technical staff:

1. J. Balodis
2. L. Jēkabsons
3. A. Kalinko
4. A. Kursitis
5. V. Nēmcovs

Postgraduate students:

1. J. Hodakovska
2. L.Pētersone
3. M.Vanags
4. Ģ.Vēveris

Students:

1. J. Blūms
2. I. Dirba
3. A. Gruduls
4. L. Kazule
5. I. Klepere
6. G. Kucinskis
7. Z. Lapina
8. P. Nazarow
9. E. Rancans
10. J. Timošenko
11. J. Smits
12. A. Zīle

LABORATORIES OF SEMICONDUCTOR MATERIAL DIVISION

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

1. University of Latvia - Department of Chemistry (Dr. G. Kizane, Dr. A.Vīksna, Dr.J.Kviesis)
2. University of Latvia – Institute of Chemical Physics, Laboratory of Radiation Chemistry of Solids (Dr. G. Kizane).
3. University of Latvia, Faculty of Chemistry (Prof. A.Vīksna); Faculty of Biology (Prof. I.Muiznieks); Faculty of Economics and Management (Prof. B.Sloka)
4. Riga Technical University (RTU) – Institute of Biomaterials and Biomechanics (Dr. I.Lasenko)
5. Riga Technical University - Institute of Inorganic Chemistry (Dr. J. Grabis, Dr. E.Palcevskis, Dr. A. Dindune).
6. Latvian Academy of Science - Institute of Physical Energetics
7. Latvian Electroindustry Business Innovation Centre (LEBIC).
8. Riga City Council - Environmental Department.
9. Riga Technical University, Institute of Industrial Electronics and Energetic (Prof. L. Ribickis).

Denmark

RISOE Centre, Denmark Technical University (Dr. F.W.Poulsen)

Estonia

Tartu University - Department of Chemistry (Prof. E.Lust);

France

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

China

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

Czech Republic

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

Germany

1. Max-Planck-Institut für Festkörperforschung (Stuttgart, Germany) –

Prof. J. Maier.

2. Kassel University (Prof. Jürgen Zick)

Italy

1. University of Trento (Trento, Italy) - Prof. G.Dalba, Prof. P.Fornasini
2. IFN-CNR CeFSA (Trento, Italy) - Dr. F. Rocca.
3. Università della Calabria (Arcavacata di Rende, Italy) - Prof. E.Cazzanelli.
4. Laboratori Nazionali di Frascati, INFN, Frascati (National Lab. of Synchrotron Radiation) – Dr. A. Marcelli

Lithuania

University of Vilnius - Department of Physics (Prof. A.Orliukas)

Poland

University of Warsaw, Department of Chemistry (Prof. A.Czerwinski)

Russia

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

South Africa

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

Sweden

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

Participation in Research Projects:

Latvian:

1. Functional Materials and technologies for Microelectronics, Nanoelectronics, Photonics, Biomedicine and Composites. **State Research Program No. PP-05-15 (2005-2009)** – *A.Lusis, J.Purans, J.Kleperis*
2. **State Research Program in Energetics, Project No.3 “Development and integration of materials and devices for hydrogen energy” (2006-2009)** – *J.Kleperis*;
3. Functional materials and technologies for microelectronics and photonics- **Cooperation project of Latvian Science Council SP 05.0005 (2005-2009)** – *A.Lusis*
4. “Modification physiochemical properties of nanostructured surface of glass fibers for development of new products” - **Cooperation project of Latvian Science Council SP 06.0029.2.10 (2006-2009)** – *A.Lusis*.
5. "X-Ray Absorption Spectroscopy with Picometer Accuracy", **Latvian Government Grant, 2005-2008** - *J. Purans*.
6. "Advanced Spectroscopic Approach to the Study of Nanomaterials Structure", **Latvian Government Grant, 2005-2008** - *A. Kuzmin*.
7. “Research of hydrogen adsorption and absorption in new nanomaterials and composites with aim to optimize the surface and bulk hydrogen in solid material storage devices”, **Grant from Latvian Science Council No. 09.1192 (2009)** – *L.Grinberga*.

8. "Research and development of proton conducting PEEK polymer and composite membranes and catalysts for use in direct methanol and hydrogen fuel cells" **Grant from Latvian Science Council No. 09.1195 (2009)** – *J. Kleperis*.
9. "Integration of Humidity and temperature sensors in grain drying places" **Research Project from Ministry of Education and Science (2006-2008), In collaboration with Latvian Agricultural University** – *J.Kleperis*;

International:

1. 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” (Dr. G. Kizane, Dr.A.Vitins).
2. EFDA JET Fusion Technology task JW8-FT-1.12 „Determination of tritium and analysis of carbon-based plasma-facing components before and after their detritiation with different methods” (Dr. G. Kizane, Dr.A.Vitins).
3. EFDA JET Fusion Technology task JW9-FT-3.46 „ Analysis of tritium distribution in plasma facing components” (Dr. G. Kizane, Dr.A.Vitins).

Didactic work at the University of Latvia

1. Master degree course "Solid State Ionics" – 4 credit points (A.Lusis)
2. New course "Structure and Description of Nanomaterials" (A.Kuzmin)
3. Dr.chem. G. Bajārs together with:
 - 1) Dr.phys. J.Kleperis, Dr.Phys. L.Grīnberga and Mg.phys. M.Vanags elaborated and delivered two credit point study course “Energy sources and its environmental impact”,.
 - 2) Dr.phys. U.Rogulis, Dr.phys. J.Klaviņš (LLU) et.al. elaborated and delivered two credit point study course “New materials and technologies”.
3. Practical work and educational lectures and excursions about hydrogen technologies;

THE MAIN RESULTS

SOLID STATE IONICS

DEVELOPMENT OF NANOSTRUCTURED AND FUNCTIONAL MATERIALS BASED ON GLASS FIBERS

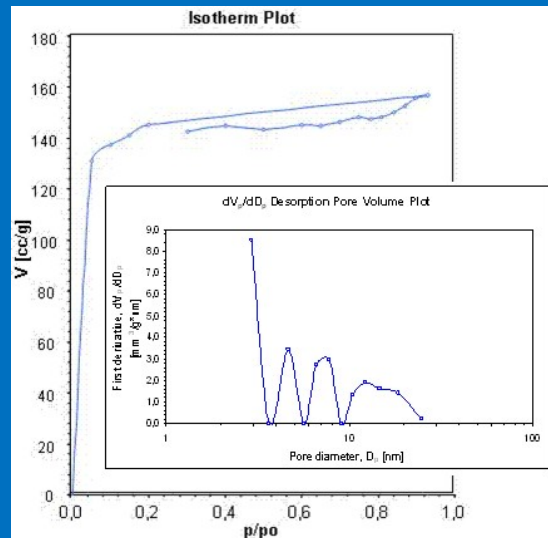
V. Eglitis, J.Gabrusenoks, A,Vitiņš, A. Lusis, E.Pentjušs, J.Balodis, L.Pētersone*

* *MS Student Physics&Matematics faculty of UL*

The leaching technology and sonochemistry have been used for nanostructuring and funtionalization of technical silicate glass fibers. The materials for functionalization are used technical silicate glass fibers from A/S VŠŠ: **E** and **K** glasses fibers. **E** glass is based on calcium alumoborosilicates and **K** glass is based on sodium alumosilicates. The metal vacuum coatings for functionalization of leached glass fabrics are used.

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

Pores structure and ion exchange of glass fibers



The influences of ultrasound on leaching process versus temperature and time have been studied. The pore size 2-15 nm with specific 0,1-300 m²/g for leached fibers have been obtained. The shrinking of glass fibers leached at 80 °C with and without ultrasound are 13% and 11% accordingly. The pore area of leached glass fibers is 10-100 m²/g and can absorb 10-15 wt% water. The ultrasound shifted pores distribution to micropores direction and reduced volume of mesopore.

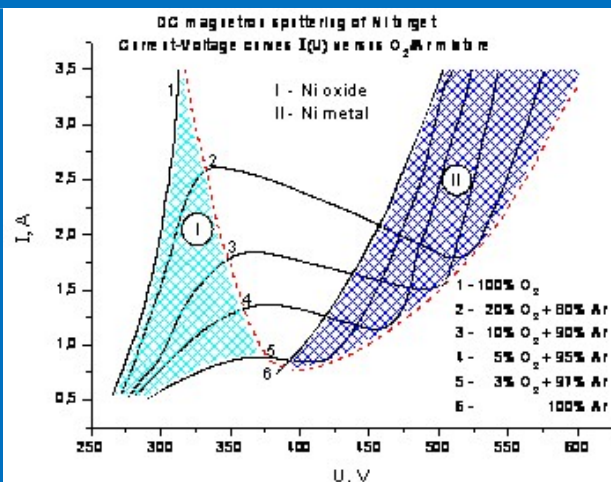
The functionalization of technical glass fibers and fabrics with metal coatings have practical interest. The plasma treatment and thin film coatings in combination with sonochemical processes are used for nanostructuring and functionalization of fibers and fabrics. The leached K-glass fiber fabric (GFF)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

Thin film vacuum coatings

Vacuum coating machine



Reactive coating process control diagram



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

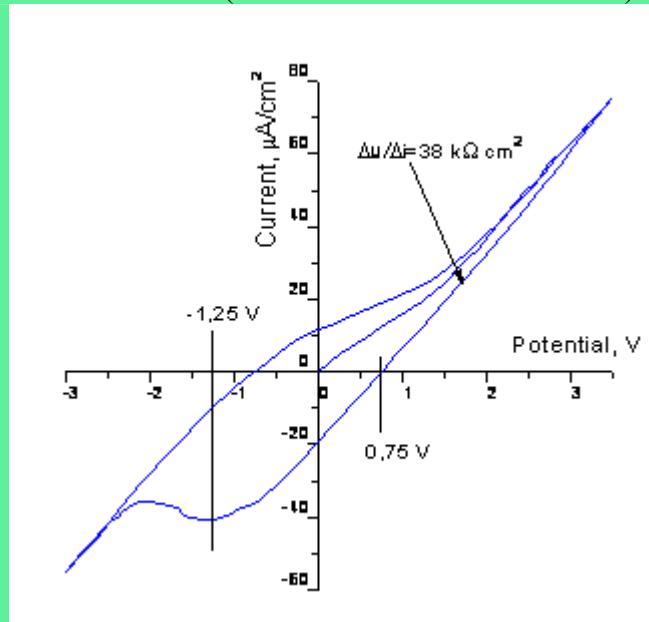
Dielectric permittivity ϵ and electrical conductivity S of the GFF coated with metal are depended of absorbed water content and metal properties. The measured values of ϵ and S at 100 kHz are:

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

Cyclic voltamperometry and impedance spectroscopy

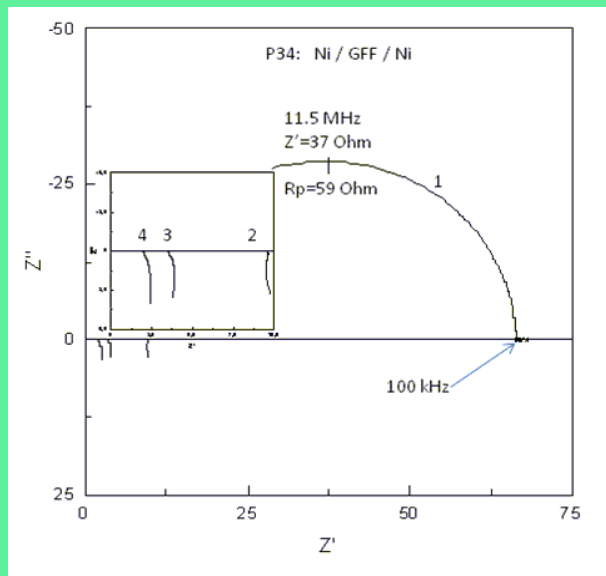
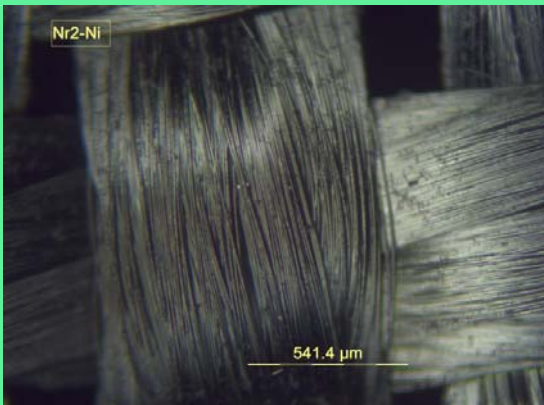
Solartron Instruments
Electrochemical Analyser

Voltammetry graph of the glass fiber fabric coated with Ni (sheet resistance $38 \text{ k}\Omega \text{ cm}^2$)



The glass fiber fabric coated with Ni

Impadance Nyquist plots

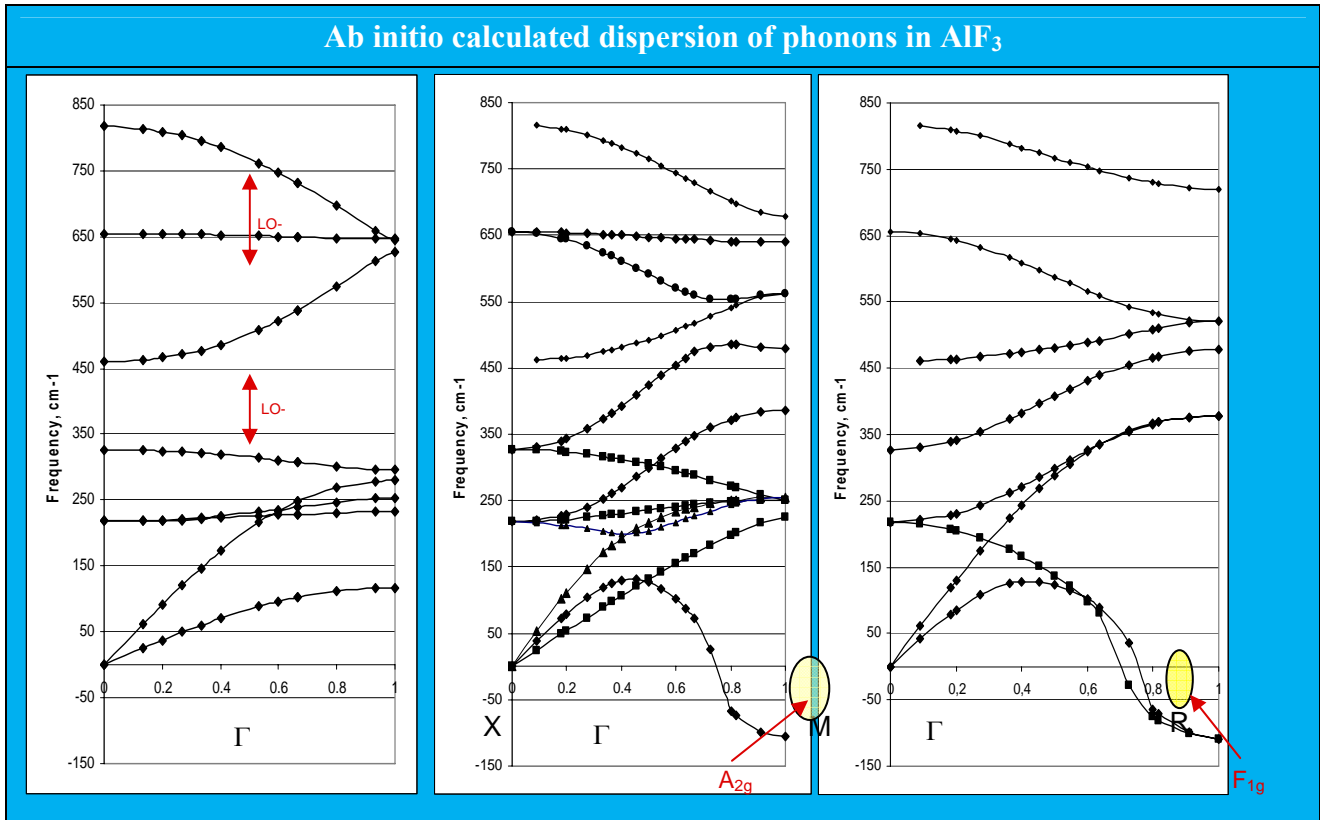


LATTICE DYNAMICS AND STRUCTURAL PHASE TRANSITIONS

J.Gabrusenoks

Symmetry Properties of Lattice Dynamics of W-O Network. The tungsten-oxygen compounds have crystalline lattices with different topology. It determines dynamic behaviour of lattice. WOCl_4 , WO_2Cl_2 and WO_3 form crystals lattices with one-, two- and three-dimensional network of W-O bonds respectively. In case of WOCl_4 octahedron are linked by oxygen and form one dimensional chains $-\text{W}-\text{O}-\text{W}-\text{O}-$. In the two and three dimensional lattice $-\text{W}-\text{O}-\text{W}-\text{O}-\text{W}-\text{O}-$ chains are placed in two or tree directions and are mutually perpendicular.

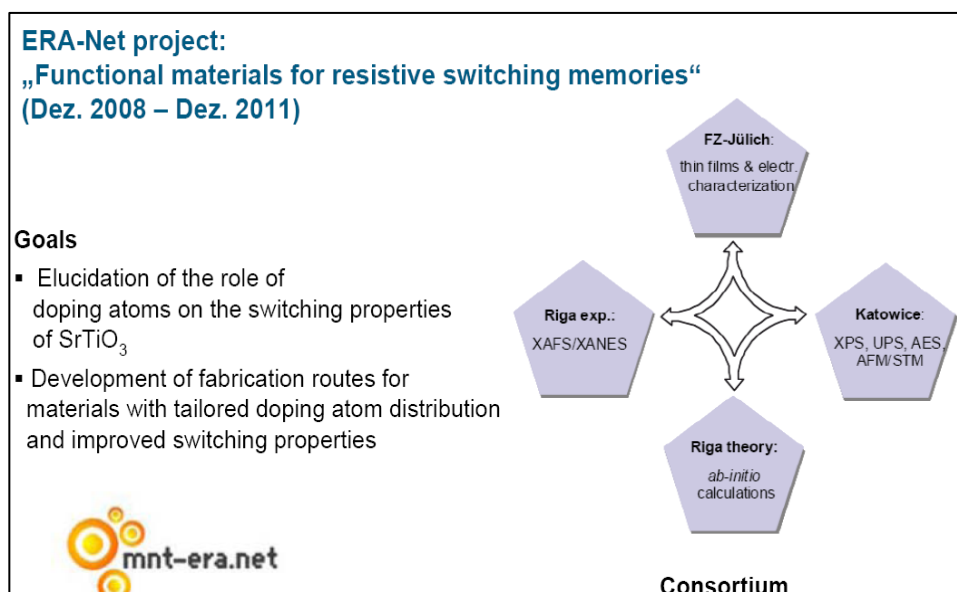
Dynamical properties of AlF_3 . The vibrational modes of cubic and rhombohedral AlF_3 phases have been investigated. Calculations have been performed by using hybrid exchange density functional theory as implemented within the CRYSYAL06 program to determine the equilibrium geometries and phonon frequencies in high symmetry directions of the Brillouin zone. The calculated phonon frequencies are used to adjust the parameters of a rigid ion model. The longitudinal-transverse splitting of optical modes at $k=0$ has been determined directly by ab initio in the directions Γ -X, Γ -M and Γ -R calculated phonon dispersions. The phonon dispersion curves show large instability region around the M-R direction.



**LOCAL STRUCTURE STUDIES BY EXAFS WITH
FEMTOMETER ACCURACY**

1. MNT ERA-NET Matra Project "Functional materials for resistive switching memories" (FMRS), XAS studies -contribution of ISSP

J. Purans, A. Kuzmin, R. Kalendarev and A. Kalinko



The main aim of the X-ray absorption studies with synchrotron radiation is to clarify the role of doping atoms in resistive switching SrTiO₃ thin films. Therefore the valence state and local distortion (Jahn-Teller effect for Fe⁴⁺ and position of vacancies near Fe³⁺) would be studied in great detail to clarify the resistive switching SrTiO₃ thin films.

To make this challenging task feasible, the best in the world Synchrotron Radiation analytical tools, like HASYLAB (Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY) and ESRF (Grenoble) European Synchrotron Radiation Facility (www.esrf.eu) have been employed. Two experimental proposals have been approved and realized in the first year of the MATERA project:

- ESRF (European Synchrotron Radiation Facilities, Grenoble) project MA923 (www.esrf.eu) „XAFS studies of functional materials for terabit resistive memories”.
- HASYLAB project I-20090034 EC „XAFS studies of functional materials for terabit resistive memories” (www.door.de)

The proposed experiments were performed in fluorescence step-by-step scanning mode at the EXAFS beamlines BM29 and A1 providing a focused, high intensity photon beam in the energy range of the Ti K-edge and Fe K-edge. Here, we have focus our attention on local structure of thin films and compared it to the corresponding ceramic PLD target material. The valence state and local distortion (Jahn-Teller effect for Fe⁴⁺ and position of vacancies near Fe³⁺) will be studied in great detail in thin films.

2. Near field X-ray spectromicroscopies: new tools for nanoscience

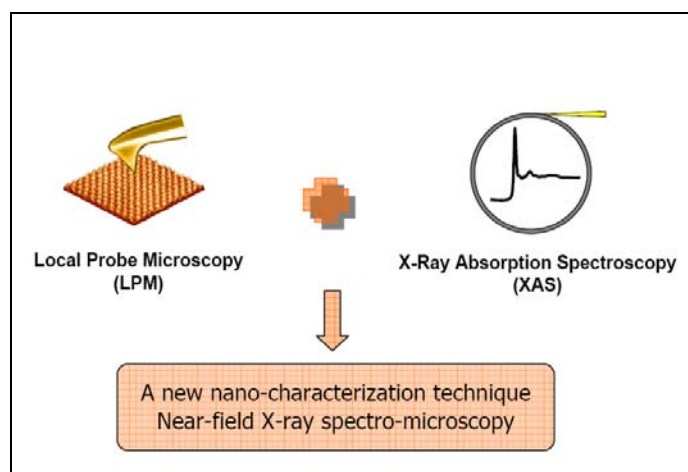
Juris Purans, A.Kuzmin, R. Kalendarev (ISSP)

S. Larcher², F. Rocca², D. Pailharey³, F. Jandard³, R. Graziola⁴

²CNR-IFN, Unita` FBK-CeFSA di Trento, Via alla Cascata 56/C, Trento 38100, Italy

³CRMC-N and Universite` de la Me`diterrane`e, Campus de Luminy, Marseille 13009, France

⁴Dipartimento di Fisica, Universita` di Trento, Via Sommarive 14, Trento 38100, Italy



Near Field (NF) X-ray Spectromicroscopy (FF illumination and NF detection) is a fully new approach for the detailed investigation of nanostructures down to the nanometer level. The extremely high lateral resolution of Local Probe Microscopies (LPM, AFM, STM) makes them among the most largely used in nanoscience. However, these tools suffer of a lack in chemical sensitivity. On the other hand, *far field X-ray spectroscopy* probes the chemical and structural properties of materials. A combination of X-ray spectroscopies and LPM is the ideal answer to many problems in nanosciences. **This report highlights the most important contributions which were held in the combination of X-ray spectroscopies and LPM techniques.**

The first observations of core-level photoelectrons generated by X-ray irradiation of the tip-surface region of STM have been published by Tsuji. Ishii has measured the capacitance XAS signal with a metal tiny electrode. The combination of XAS and scanning near-field optical microscopy (SNOM) as a local detector was proposed by Purans, while a combination of XRF technique and LPM with a cantilever, having a hole of 100 nm, as a *collimator* of X-ray beam was proposed by Nagamura. First STM and SNOM experiments under *focused* synchrotron-radiation (SR) were performed at ESRF on the microbeam line ID-3. Detailed STM study using soft SR X-rays was performed by Matsushima et al. [9]. A STM dedicated to in situ experiments under the irradiation of highly brilliant hard-X-rays of synchrotron radiation has been developed by Saito et al. [10] and a current modification was detected at the absorption edge with a spatial resolution of the order of 10 nm. Finally, Ishii and Hamilton et al. have combined electrostatic force microscopy (EFM) with tunable synchrotron x-ray source excitation.

Further progress we have achieved in the framework of the European X-TIP project by the focusing SR beam to increase the density of the incident photons. X-ray optics at third generation Synchrotron Radiation facilities have lead to the stable production of X-ray microbeams with extremely high photon densities making this approach feasible. We have started with three types of experiments: (i) XAS-AFM: X-ray excited secondary electrons detection by conductive tip in AFM mode; (ii) XAS-SNOM: X-ray excited optical luminescence (XEOL) detection by SNOM in AFM mode; (iii) XAS-SCM/AFM: X-ray excited capacitance or/and photoconductivity of sample detection by conductive tip in SCM, KFM or AFM mode.

The new instrumentation developed within this project offers the possibility to carry out a selective structural analysis of the sample surface with the subwavelength spatial resolution determined by the SNOM probe aperture. In addition, the apex of the optical fibre plays the role of a topographic probe, and chemical and topographic mappings can be simultaneously recorded.

3. Quantum mechanics–molecular dynamics approach to the interpretation of XAFS

A. Kuzmin (ISSP) and R A Evarestov (Dep. Quant. Chem., St Petersburg)

The quantum mechanics–molecular dynamics approach to the simulation of configuration-averaged EXAFS spectra is proposed, and its application is discussed for the example of the Ti K-edge EXAFS spectrum in cubic perovskite SrTiO₃. Proper use of *ab initio* quantum mechanics allows a number of empirical parameters, used in the molecular dynamics simulation, to be reduced, whereas the molecular dynamics allows us to account for temperature effects. All together, the approach provides a way of accounting for static and dynamic disorder in EXAFS signals from the coordination shells above the first one, where many-atom (multiple-scattering) effects are often important.

4. Ab initio study of the electronic and atomic structure of the wolframite-type ZnWO₄

A. Kalinko (ISSP), A. Kuzmin (ISSP),
R.A. Evarestov (Dep. Quant. Chem., St Petersburg)

Ab initio quantum chemistry calculations of the structural and electronic properties of monoclinic wolframite-type ZnWO₄ crystal have been performed within the periodic linear combination of atomic orbitals (LCAO) method using six different Hamiltonians, based on density functional theory (DFT) and hybrid Hartree-Fock-DFT theory. The obtained results for optimized structural parameters, band gap and partial density of states are compared with available experimental data, and the best agreement is observed for hybrid Hamiltonians. The calculations show that zinc tungstate is a wide band gap material, with the direct gap about 4.6 eV, whose valence band has largely O 2p character, whereas the bottom of conduction band is dominated by W 5d states.

5. Characterization of rhenium oxide films and their application to liquid crystal cells

J. Purans, A. Kuzmin and R. Kalendarev (ISSP); E. Cazzanelli, M. Castriota, S. Marino, N. Scaramuzza, Dep. Phys.University of Calabria (Italy); G. Mariotto and G. Das, Dep. Comp. Sci. University of Verona (Italy).

Rhenium trioxide exhibits high electronic conductivity, while its open cubic crystal structure allows an appreciable hydrogen intercalation, generating disordered solid phases, with protonic conductivity. Rhenium oxide thin films have been obtained by thermal evaporation of ReO_3 powders on different substrates, maintained at different temperatures, and also by reactive magnetron sputtering of a Re metallic target. A comparative investigation has been carried out on these films, by using micro-Raman spectroscopy and x-ray diffraction. Two basic types of solid phases appear to grow in the films: a red metallic H_xReO_3 compound, with distorted perovskite structures, like in the bulk material, and ordered HReO_4 crystals based on tetrahedral perhenate ions. Because of its conduction properties, the electrical and electro-optical behaviors of ReO_3 films deposited on standard indium tin oxide/glass substrate have been tested inside asymmetric nematic liquid crystal cells, showing an appreciable capability of rectification of their electro-optical response, in similar way to tungsten trioxide.

RESEARCH AND DEVELOPMENT OF MATERIALS AND DEVICES FOR HYDROGEN ENERGY TECHNOLOGIES

J.Kleperis, G.Vaivars, L.Grīnberga, G.Chikvaidze, M.Vanags, I.Klepere, V.Ļemcovs, L. Jēkabsons

Hydrogen absorption/desorption in modified SiO_2 glass and alumina. An efficient storage media for hydrogen is desirable for the common applications of fuel cells and the adoption of hydrogen as an energy source. Nanostructuring of materials and enhancement of surface absorption capability are two main factors to increase the amount of sorbed hydrogen. One way to combine the effectiveness of hydrogen absorption in metal hydrides and the desirable weight/volume proportion is to make composite material from alloy forming hydride and appropriate support material. In a regular circumstances SiO_2 glass are not absorbing notable amount of hydrogen, however doping small quantities of palladium in these materials can provide a capturing of significant amount of this gas. We studied hydrogen sorption properties in composites made of palladium nano-particles coated on the surface of porous nano-powder of SiO_2 by using extractive-pyrolytic method. To investigate an interaction of hydrogen with Pd/oxide composites the volumetric method was used. Phase composition of materials was determined by XRD method. Alumina granules (obtained from Al_2O_3 nanoparticles by E. Palcevskis) with platinum and palladium nanoparticles (coated by extractive-pyrolytic method) were tested for hydrogen absorption-desorption, and only small activity was found.

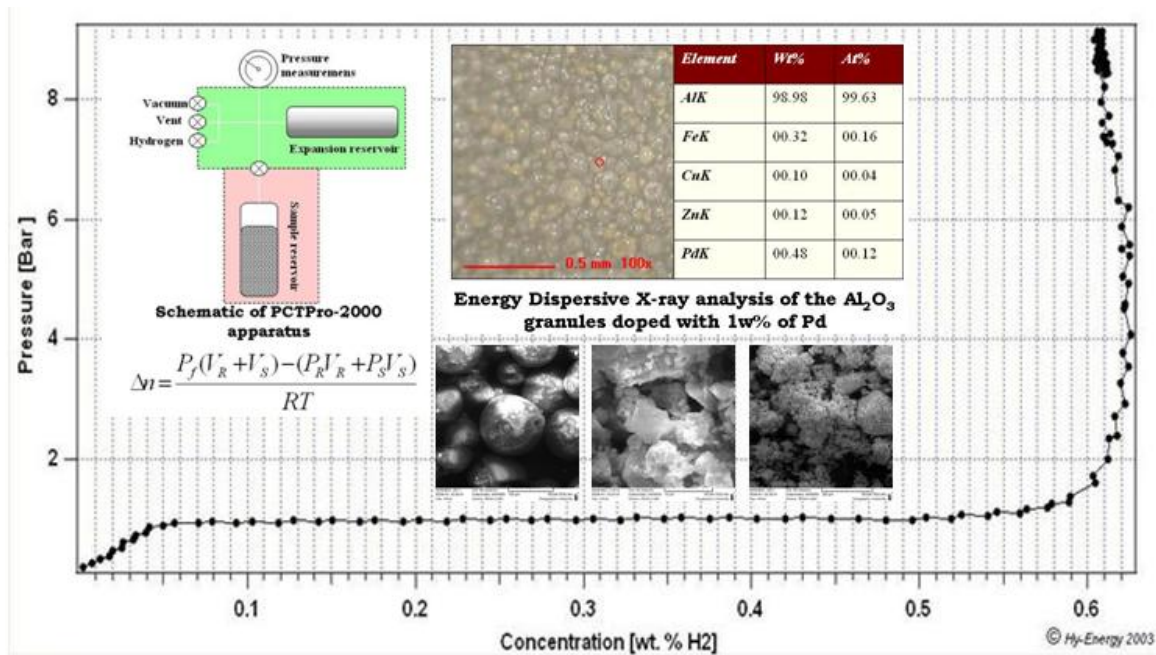


Figure 1. Hydrogen absorption/desorption curve of Pd-activated SiO_2 glass sample, measured with PCT Pro-2000 instrument.

Water electrolysis using AC power formed from short pulses. Inductive kick-back voltage (IKV) pulses were used to investigate the electrolysis phenomena on platinum and tungsten electrodes in alkali solution. Firstly microelectrode was used to investigate the changes of liberated and dissolved hydrogen in initial stages of electrolysis. The delay of hydrogen evolution on platinum electrode in comparison with tungsten electrode was observed from voltage and current oscillograms as well as from measurements of dissolved hydrogen concentrations close to the electrode surface. Following mechanism of the hydrogen evolution during electrolysis with IKV pulse is proposed – some amount of pulse energy is consumed for the formation of hydrogen adsorption/absorption layer on platinum electrode, limiting the formation of hydrogen molecules. There is no hydrogen adsorption/absorption peak for tungsten electrode, and during very short IKV pulse the electrons from metal directly discharge hydrogen ions and H_2 molecules are formed intensively.

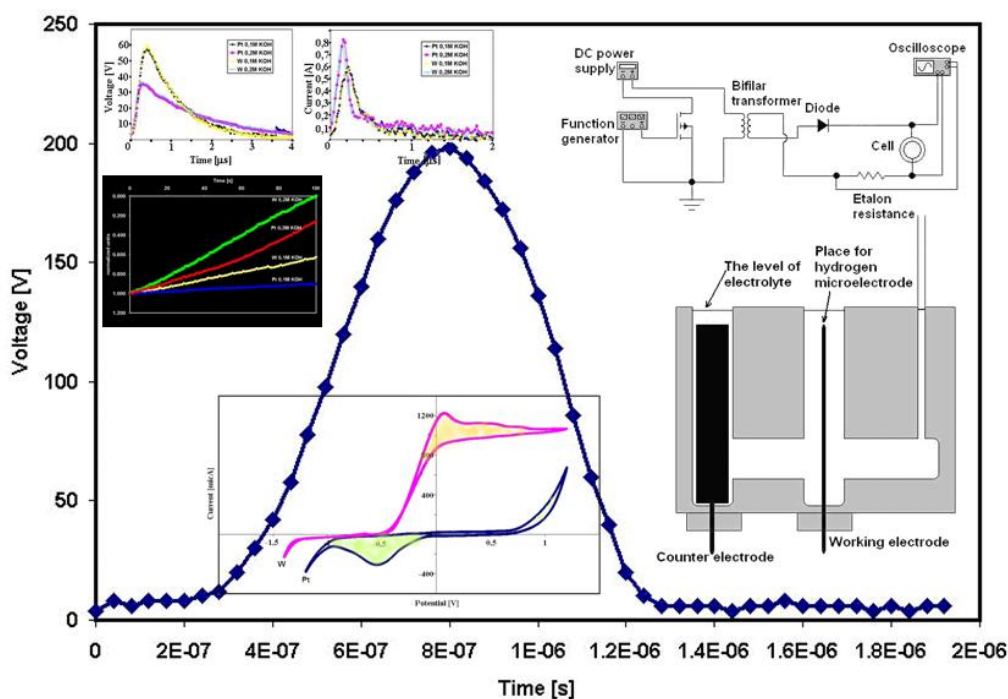


Figure 2. Electrolysis cell, electronic circuit and characteristics of W and Pt electrodes during electrolysis with very short voltage pulses.

Study of structure and electrochemical characteristics of LiFePO_4/C as cathode material for lithium batteries. Recently increased attention has been dedicated to LiFePO_4 as a promising cathode material in lithium-ion batteries for use in consumer electronics and electric vehicles because of the environmental compatibility and low manufacturing cost. In addition, LiFePO_4 has a relatively large theoretical capacity of 170 mAh/g, good thermal stability and little hygroscopic. The main problem restricting the practical application of LiFePO_4 is its low electronic conductivity and poor rate capability. One way to solve the above mentioned problems is to increase the surface area of the cathode by the use of thin film technology. In our present work LiFePO_4 was synthesized from Li_2CO_3 , $\text{FeC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ and $\text{NH}_4\text{H}_2\text{PO}_4$ with different carbon content. LiFePO_4/C thin films prepared under various sputtering conditions were characterized by X-ray diffraction, scanning electron microscope and Raman spectroscopy. The deposited thin films were tested as cathode materials for lithium ion batteries by electrochemical impedance spectroscopy and cyclic voltammetry. The electrochemical characteristics of LiFePO_4/C thin films are related to conditions of preparation, structure, surface morphology and carbon content. An equivalent circuit were found that describes the electrochemical processes on the $\text{LiFePO}_4/\text{Pt}$ and $\text{LiFePO}_4/\text{LiClO}_4/\text{propylene carbonate}$ interfaces.

Parameters of an efficient electrolysis cell for use in internal combustion engine. To produce hydrogen from an alkaline electrolysis cell more efficiently and cheaply, its parameters should be improved. The aim of this work was to create an efficient electrolysis cell by studying and optimizing its parameters: the distance between electrodes, alkaline electrolyte, its temperature, and the operating power. Our electrolysis cell has been made with 63% energy efficiency, using coaxial stainless steel cylinders as electrodes and de-ionized water with KOH as electrolyte.

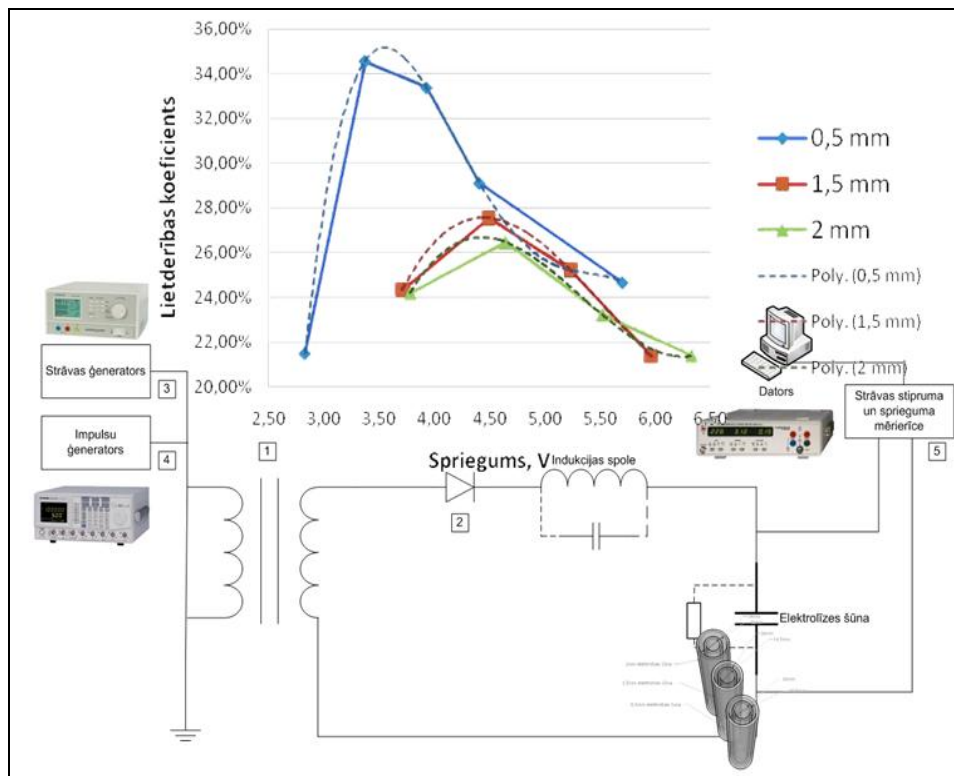


Figure 3. Electrolysis efficiency dependence from voltage between two coaxial stainless steel electrodes, with distance between them 0,5, 1,5 and 2 mm.

Temperature influence on the power efficiency of commercial photo voltage batteries. From May 2009 there are installed 4 Solar panels KS-160 (KoraxSolar, Hungary) with total area 4,5 m² on the roof of Institute of Solid State Physics. Analysis of results collected during 6 months showed that in similar sunny days with different ambient temperatures there are quite different amounts of collected energy. The output (product of electricity and voltage) of a solar cell is temperature dependent. Higher cell temperatures lead to lower output, and hence to lower efficiency. The level of efficiency indicates how much of the radiated quantity of light is converted into useable electrical energy. Regarding information from producer, the output of Solar panel KS-160 reduces by 0,4-0,6% increasing temperature by 1 degree. We experimentally tested panel KS-160 in closed thermal camera equipped with 4 halogen lamps (300W) as light source. An output of Solar panel decrease 2.6 times increasing temperature from 20 to 61 °C. Physical aspects of deterioration of the output power and the conversion efficiency of solar cell and PV module with increasing temperature are discussed in our work. In order to diminish these effects, it is useful to decrease the module temperature by removing the heat produced by non-active absorption of photons, which do not generate pairs, by recombination of electron-hole pairs, by photocurrent (Joule's heat generated during the current flow in the series resistance of the p-n junction) and parasitic currents.

Electron and proton conductive polymer membranes for fuel cells. Global environmental concerns have ignited research to develop energy generation technologies which leave minimal ecological damage concerns of global climate change. These are driving nations to develop electric power generation technologies and transportation technologies which reduce carbon dioxide emissions. Hydrogen is considered the fuel of choice for both the electric power and transportation industries. Nowadays between most expensive materials to be used in hydrogen technologies are membranes and membrane – electrode assemblies. In our work an idea is developed to make multilayered electron/proton conducting membrane from non-expensive and available polymers. Multilayered proton conducting membrane for possible fuel cell applications is made from electron and proton conductive layers on the base of 2 different polymers (sulfonated poly(ether-ether-

ketone) (SPEEK) and polyaniline (PANI)). The sulphonated SPEEK ionomers were synthesized using simple method. The membranes were characterized by FTIR and Raman spectra to confirm sulphonation. Thermogravimetric analysis (TGA) and conductivity measurements of simple SPEEK and complex multilayered membranes PANI/SPEEK/PANI are performed to assess their suitability in fuel cell applications and thermal stability. The proton and electron conductivities of such multilayered membranes were found from impedance measurements.

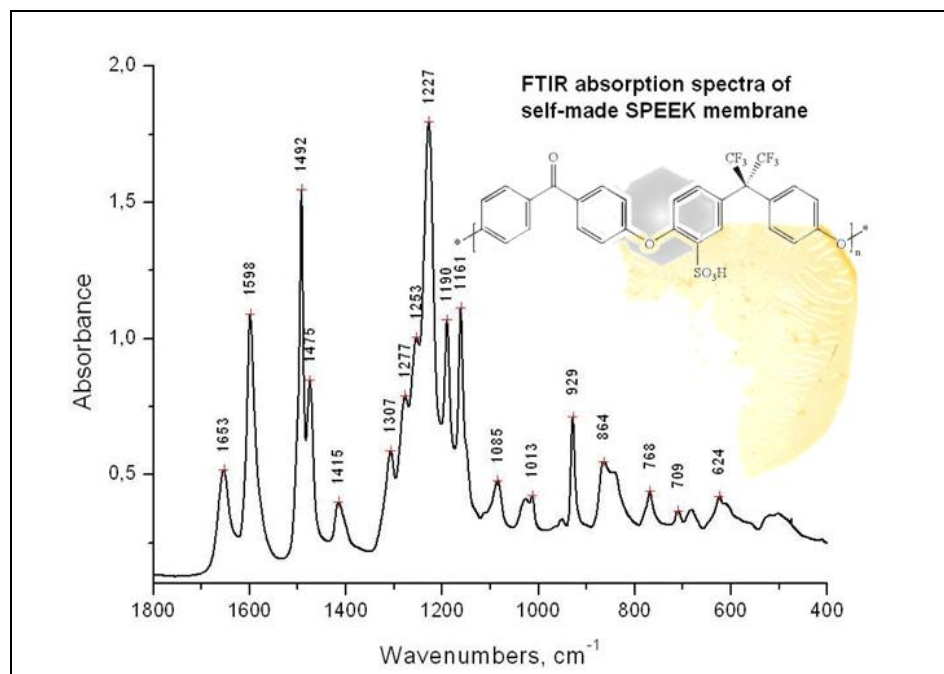


Figure 4. FTIR absorption spectra of self-made sulfonated poly(ether-ether-ketone) membrane

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

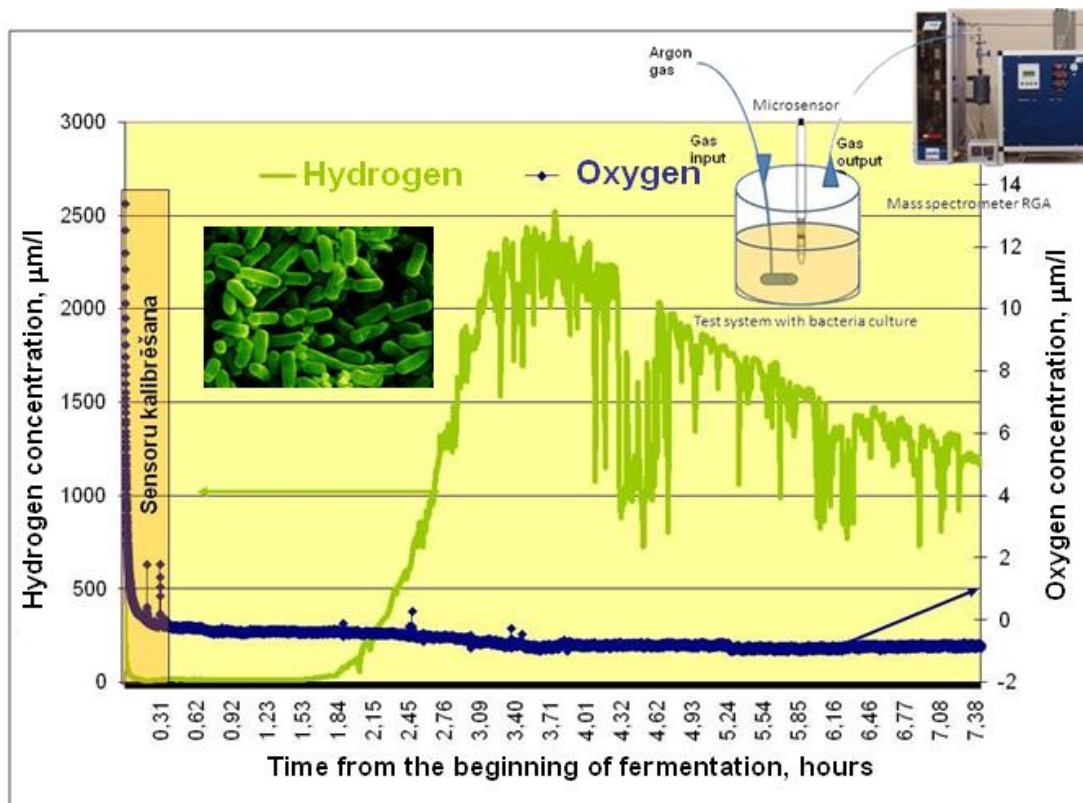


Figure 4. Concentrations of dissolved oxygen and hydrogen gases in bio-reactor with bacteria *E.Coli*, measured with microsensors.

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

J.Kleperis, V.Ogorodņiks

Ecological grain drying on peasant farms using monitoring of the drying process and the obtained results. The computerised system is developed, on the base of sensors DS1923 to perform the monitoring of humidity and temperature into the technological grain drying process. It ensured the operative control of grain drying conditions, allowing to obtain high-quality dry grain with low energy consumption and expenses. Online monitoring of moisture and temperature in the grain storage facility prolonged the drying time by means of active ventilation. Owing to the information obtained from the digital temperature and humidity sensors, the drying period was extended by 15-25% every day. Due to slow desiccation at a low temperature (up to 30 °C) the grain becomes ripe, its quality grows and the grain acquires the properties of food grain and it may be sold at a much higher price. The use of computerised ventilated bins for drying and storing grain is purposeful in the organisational, as well as economical and ecological aspects. It facilitates the farmer to organise the harvesting process, to use favourable weather conditions to a full extent, to obtain a higher-quality product and sell it on more profitable terms. This increases the manoeuvrability of production, makes it less dependent on the weather conditions and the grain reception centres and raises the profitability of grain production.

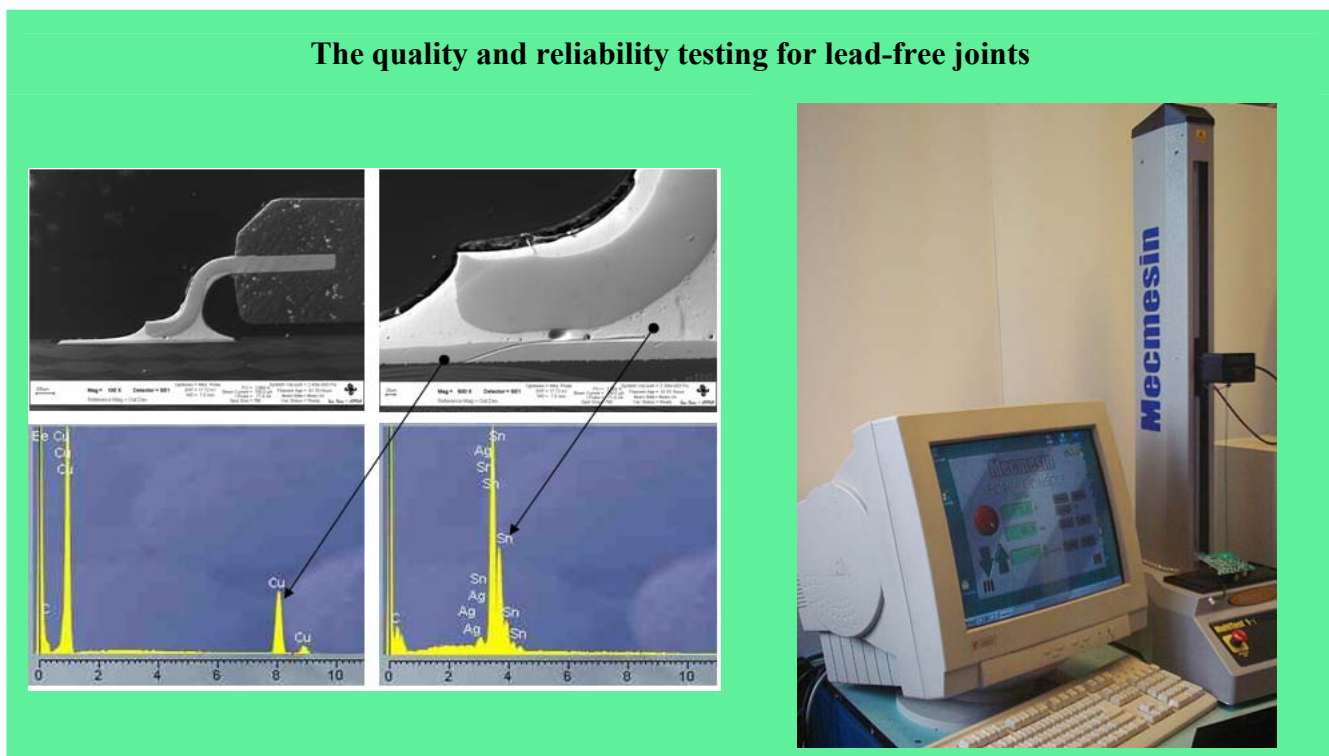
Particle pollution and air quality in Riga. Streets and traffic are the main source of particles in Riga, but not the only source. Database of air pollutants in Riga collected during more than 10 years also includes different point sources with numerous emissions of particles. Particle PM10 monitoring in Riga only started in 2000, but the most reliable data are from 2003, when two street monitoring stations were established with two different PM10 monitors (SM200 and ESM FH62). Results from ESM instrument are with 30 min distinction ability and are analysed together with traffic flow and meteorological data. Higher particle concentrations are registered in the spring

months, but there is a high number of days throughout the year too, when the value used as the European Common Indicator towards a Local Sustainability Profile (50 $\mu\text{g}/\text{m}^3$ for 24h averages of PM10) is exceeded. Road traffic emissions are calculated from detailed information on traffic volumes, vehicle compositions and driving conditions. The database of air pollutants in Riga, hosted by Riga City Council, includes emissions from burning of different fuels in district and residential heating, emissions from industry and traffic (very roughly) that allow approximate estimation of calculated PM10 emissions in Riga. The re-suspension of particulate matter from road dust, which is very important in springtime, wasn't taken into account. Furthermore, black carbon concentrations are analysed from street canyon emissions by optical detection of the blackness of filters; characteristic metal concentrations are determined as well. Black carbon collection directly from exhausts of different transport units demonstrated that not only class of transport and fuel used, but also average agedness is responsible for the concentrations of particles in exhausts.

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

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

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



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

http://www.em.gov.lv/em/images/modules/items/item_file_13148_1.doc

http://www.letera.lv/pic/rohs_direktiva.doc

TRITIUM RELEASE PROPERTIES OF NEUTRON-IRRADIATED BERYLLIUM PEBBLES

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Beryllium pebble beds are considered as a neutron multiplier of the European Helium Cooled Pebble Bed (HCPB) tritium breeding blanket for future fusion power reactors. The tritium accumulated in the beryllium pebbles may cause operational and environmental problems, and therefore tritium release properties of the beryllium pebbles are an important factor for safe operation of the fusion reactor. Under the operating conditions of the HCPB, the beryllium pebbles will be under action of high neutron flux ($10^{18} \text{ n m}^{-2} \text{ s}^{-1}$), high temperature (up to 920 K) and intense magnetic field (up to 7-10 T).

In this study, we present results on tritium release from the beryllium pebbles irradiated for 294 full power days from 17 April 2003 to November 2004 in the pebble-bed assemblies (PBA) experiment in the high flux reactor (HFR) at Petten, the Netherlands. Tritium release of the beryllium pebbles was performed in a continuous flow of 14.5-14.9 L/h of the purge gas He + 0.1% H₂ at a temperature ramp of 2.4-4.8 K/min from room temperature to 1315-1552 K. One PBA Be pebble was investigated in each tritium release experiment.

Histograms of the tritium release rate and curves of the tritium sum release from PBA beryllium pebbles at annealing are given in Figs. 1 and 2. Two distinct stages of tritium release – a stage of gradual increase and a stage of abrupt release peaks are evident in the tritium release of the PBA Be pebbles at a temperature ramp of 2.4-4.8 K/min. These two stages may be related to the tritium release by atomic diffusion and bubble venting respectively. The main maximum of the tritium release rate of the PBA Be pebbles was found to be in the temperature ranges of 1178-1309 K and 1178-1350 K at the temperature ramps of 2.4 and 4.8 K/min respectively.

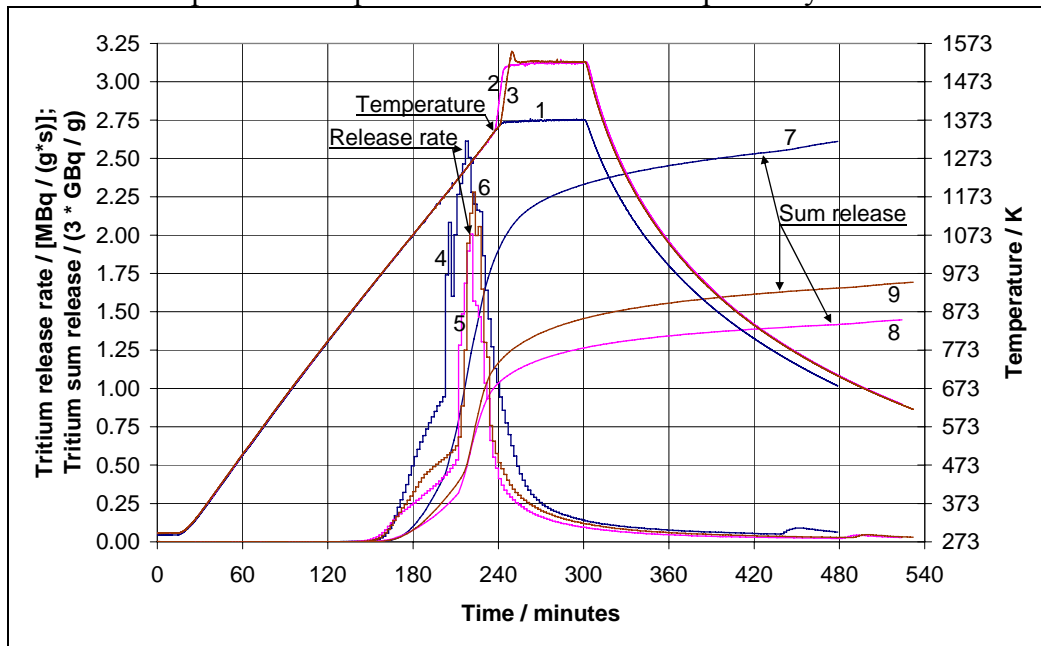


Fig. 1. Tritium release rate (4-6) and tritium sum release (7-9) from the PBA beryllium pebbles heated at the given temperature (1-3) – a linear ramp of 4.8 K/min to an anneal temperature of 1373-1525 K: curves 1, 4, 7 – the PBA Be pebble of 0.86 mg, the tritium sum release 7.83 GBq/g;

curves 2, 5, 8 – the PBA Be pebble of 1.61 mg, the tritium sum release 4.34 GBq/g; curves 3, 6, 9 – the PBA Be pebble of 1.23 mg, the tritium sum release 5.08 GBq/g.

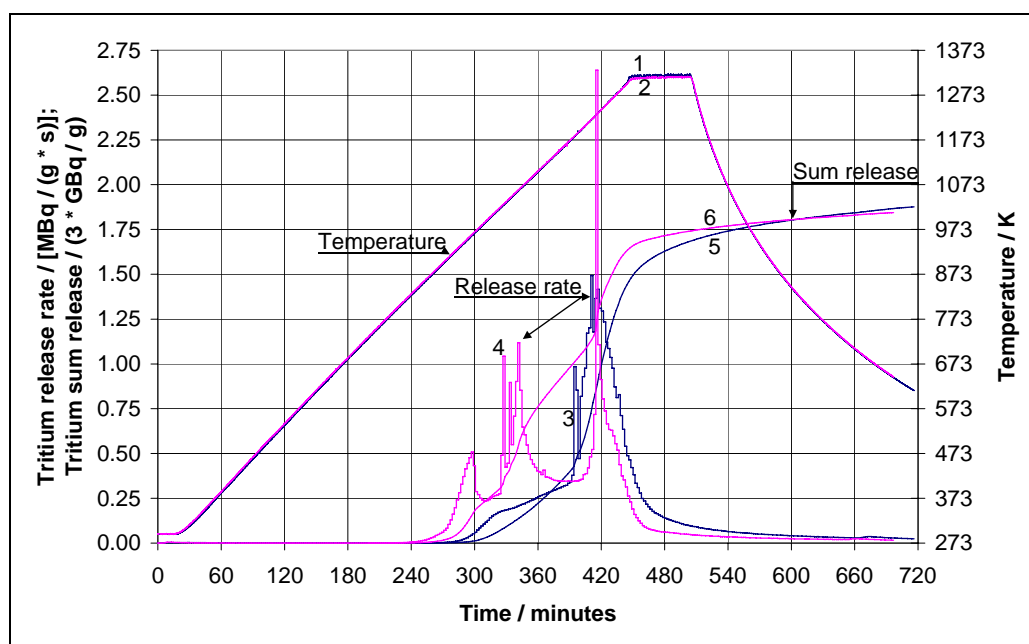


Fig. 2. Tritium release rate (3, 4) and tritium sum release (5, 6) from the PBA beryllium pebbles heated at the given temperature (1, 2) – a linear ramp of 2.4 K/min to an anneal temperature of 1309-1320 K: curves 1, 3, 5 – the PBA Be pebble of 1.22 mg, the tritium sum release 5.63 GBq/g; curves 2, 4, 6 – the PBA Be pebble of 0.87 mg, the tritium sum release 5.53 GBq/g.

Tritium release properties of the beryllium pebbles irradiated in the PBA, EXOTIC 8-3/13 and BERYLLIUM experiments are compared in this study. Total tritium activity in 1 g of sample increases in the sequence of pebbles: EXOTIC 8-3/13 (2.5-20 MBq/g) < BERYLLIUM (0.6-1.5 GBq/g) < PBA (4-10 GBq/g). Abundance ratios of chemical forms of tritium localized in the pebbles were determined with the method of chemical scavengers. A general trend can be concluded that tritium release from the EXOTIC 8-3/13 pebbles takes place at lower temperatures than that of the PBA and BERYLLIUM pebbles. That can be related to a smaller diameter (\varnothing 0.1-0.2 mm) and a higher surface to volume ratio of the EXOTIC pebbles than those of the PBA (\varnothing 0.9-1.1 mm) and BERYLLIUM ($\varnothing \approx 2$ mm) pebbles, and to a higher abundance ratio of atomic tritium in the EXOTIC pebbles.

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18. G. Chikvaidze, J. Kleperis, K. Garkevics, Application of Raman Spectroscopy for Investigation of Lead-Acid Battery Plates. Abstracts of International Baltic Sea Region Conference “Functional materials and nanotechnologies” FM&NT-2009, Riga, March 31 - April 3, 2009, p. 204.
19. V. Kuzmovs, J. Kleperis, M. Vanags, G. Bajars, K. Garkevics, Structural and Morphological Research of Lead/Acid Battery Plates: Pulse Charge Effect. Abstracts of International Baltic Sea Region Conference “Functional materials and nanotechnologies” FM&NT-2009, Riga, March 31 - April 3, 2009, p. 205.
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21. H. Luo, G. Vaivars, M. Mathe, Synthesis and characterization of functional PEEK for Ion-exchange Membranes. Abstracts of International Baltic Sea Region Conference “Functional materials and nanotechnologies” FM&NT-2009, Riga, March 31 - April 3, 2009, p. 207.
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26. Vadim Ogorodnik, Janis Kleperis, Albert Kristinsh, Irina Gvardyna, Aivars Cesnieks, Arvids Vilde. Automated control of the grain drying process. Abstracts of The 6th International Conference on Research and Development in Central and Eastern European Institutes of Agricultural Engineering (CEE AgEng); Raudondvar (Lithuania), June 30 – July 02, 2009, 1 page.
27. Grinberga L., Rancans E., Kleperis J., Particle Dimensions and Metal Hydride Absorption/Desorption Properties, Extended Abstracts of XI International Conference ICHMS'09, Jalta, Ukraina, August 25-31, 2009, p.

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Participation in Conferences

Annual 25th Conference of Institute of Solid State Physics of University of Latvia, February 11-13, 2009, Riga, Latvia:

1. G. Bajars, J. Kleperis, M. Rjabkova. Hydrogen Economy as Environmental Policy Tool.
2. G. Vaivars, Next Generation Proton Conducting Membrane Development Strategy.
3. G. Chikvaidze, G. Vaivars, Study of Diffusion of Methanol in Polymer Membranes using the ATR-FTIR Method.
4. J. Hodakovska, J. Kleperis, Polymer Membrane Protonconductivity Measuring.
5. G. Kisis, M. Zeps, M. Vanags, Research and Development of the Electrolytic Cell using Direct Current and Impulse Mode.
6. E. Rancans, L. Grinberga, J. Kleperis, Research of Hydrogen Sorption Properties using Sievert type Equipment PCTPro 2000.
7. I. Klepere, R. Rutkis, J. Kleperis, Microelectrodes for Gas measurements in an Environment of Algae and Microorganisms.
8. J. Blums, M. Vanags, J. Kleperis, Energy Production and Storage facilities from Solar PV modules in Latvia.
9. G. Narvaiss, A. Purvins, J. Kleperis, Power load and optimization from Fuel Cell in Electric Car.
10. K. Dambis, A. Sokolovs, J. Kleperis, Estimation of driving Distance for Electric Cars using different Power Sources and their Combinations.
11. I. Dirba, M. Vanags, J. Kleperis, Hydrogen Usage in an Internal Combustion Engines – description and optimisation of burning.
12. L. Grinberga, Development of Hydrogen Transport.
13. V. Ogorodniks, J. Kleperis, I. Taivans, N. Jurka, M. Bukovskis, Diagnosing of Diseases by means of Electronic Nose.
14. G. Kizāne, A. Vītiņš, E. Pajuste, S. Kalēja, I. Dušenkova, M. Haļitovs, J. Jansons, Behaviour of tritium in plasma-facing materials of the Joint European Torus (JET). [Oral presentation by G. Kizane].
15. J. Gabrusenoks, Dynamical properties of crystals with ReO₃ lattice.
16. A. Kalinko (poster), A. Kuzmin, Molecular Dynamics Simulation of ReO₃

International Baltic Sea Region Conference “Functional materials and nanotechnologies” FM&NT-2009, Riga, March 31 - April 3, 2009:

17. J. Kleperis, L. Grinberga, J. Klavins, Hydrogen insertion compounds – comparative analysis for storage applications.
18. L. Grinberga, J. Kleperis, G. Chikvaidze, E. Rancans, Hydrogen-metal-substrate interaction studies by PCT and reflection-absorption infrared spectroscopy.
19. G. Chikvaidze, J. Kleperis, K. Garkevics, Application of Raman Spectroscopy for Investigation of Lead/Acid Battery Plates.
20. V. Kuzmovs, J. Kleperis, M. Vanags, G. Bajars, K. Garkevics, Structural and Morfological Research of Lead/Acid Battery Plates: Pulse Charge Effect.
21. J. Hodakovska, J. Kleperis, Research of Power output from Fuel Cell in dependence from Working Conditions.
22. H. Luo, G. Vaivars, M. Mathe, Synthesis and characterization of functional PEEK for Ion-exchange Membranes.

23. M. Vanags, I. Klepere, G. Bajars, G. Chikvaidze, J. Kleperis, Kinetics of Hydrogen Evolution Reaction on Cathode – Electrolysis Model development and testing with Microrespiration Sensors.
24. G. Kizane, A. Zarins, I. Reinholds, A. Supe, A. Vitins, V. Tilika, L. Baumanė, Changes in lithium orthosilicate pebbles under action of radiation. [Poster presentation by G. Kizane]
25. J. Gabrusenoks, Lattice dynamics of $\text{Pb}_2\text{ScTaO}_6$.
26. A. Kalinko, R.A. Evarestov (oral), A. Kuzmin, First principles LCAO calculations of tungstates MeWO_4 (Me = Ca, Mg, Zn)
27. A. Kalinko, R.A. Evarestov, A. Kuzmin, M. Losev, J. Purans, (poster) Structural, electronic and phonon properties of metallic ReO_3

The 6th International Conference of Young Scientists on Energy Issues CYSENI 2009, May 27-28, 2009, Kaunas, Lithuania:

28. E. Rancans, L. Grinberga, J. Kleperis, Research of hydrogen sorption properties using sievert type equipment PCTPro 2000.
29. M. Vanags, J. Kleperis, G. Bajars, G. Vaivars. Water electrolysis – traditional and uncommon aspects.
30. J. Hodakovska, J. Kleperis. Polymer membranes for fuel cells.

The 1st International EJC-PISE Workshop, June 9–10, 2009, Riga:

31. A. Lūsis, E. Pentjuss, J. Balodis, G. Veveris Application of plasma processes for functionalization of technical fibers and textiles, (Published on workshop web site and CD, 6 pp.).

The 6th International Conference on Research and Development in Central and Eastern European Institutes of Agricultural Engineering (CEE AgEng); Raudondvar (Lithuania), June 30 – July 02, 2009:

32. Vadim Ogorodnik, Janis Kleperis, Albert Kristinsh, Irina Gvardyna, Aivars Cesnieks, Arvids Vilde. Automated control of the grain drying process.

The XI International Conference ICHMS'09, Jalta, Ukraina, August 25-31, 2009:

33. M. Vanags, G. Bajars, J. Kleperis. Electrolysis model development for metal/electrolyte interface: testing with micro-respiration sensors.
34. Grinberga L., Rancans E., Kleperis J., Particle Dimensions and Metal Hydride Absorption/Desorption Properties

International Conference “Energy. Scientific and artistic, utopian and critical visions” in frame of International Festival “Energy: Art & Communication” Spikeri Riga (Latvia), October 10, 2009:

35. Janis Kleperis, Liga Grinberga, Imants Dirba, Ilze Klepere. New materials and electro-technology & management software for hydrogen energy systems.

The 3rd International Conference “Environmental Science and Education in Latvia and Europe”, Theme “Education and science for climate change mitigation”. Ministry of Environment, Riga (Latvia), October 23, 2009:

36. Gunars Bajars, Janis Kleperis, Andrejs Lūsis. Ecodesign knowledge and future environmental impact.
37. Janis Kleperis, Gunars Bajars, Ilze Klepere, Biruta Sloka, Justs Dimants. Step by step implementation of Hydrogen Economy as Environmental Policy Tool in Latvia.

The 14th International Conference on X-ray Absorption Fine Structure, Camerino, Italy, 26 – 31 July 2009 (A. Kuzmin, A. Kalinko, J. Purāns)

38. J. Puāns (oral), J. Timoshenko, A. Kuzmin, G. Dalba, P. Fornasini, R. Grisenti, N. D. Afify, F. Rocca, S. De Panfilis, I. Ozhagin, and S. I. Tiutiunnikov, „Femtometer accuracy EXAFS measurements: isotopic effect in the first, second and third coordination shells of germanium.
39. A.Kuzmin (oral) and R.A. Evarestov, Quantum mechanics-classical molecular dynamics approach to EXAFS.
40. A.Kalinko (poster), R.A. Evarestov, A. Kuzmin, and J. Purans, Interpretation of EXAFS From ReO₃ Using Molecular Dynamics Simulations.

The 4th Symposium on Vacuum Based Science and Technology and The 8-th Annual Meeting of the German Vacuum Society – DVG

41. J. Purans (invited), Characterization of thin films and multylayers by advanced synchrotron radiation methods

The 12th International Workshop on Plasma-Facing Materials and Components for Fusion Applications (PFMC-12), Jülich, Germany, 11-14 May 2009:

42. G.Kizane, A. Vitins, E. Pajuste, S. Kaleja, I. Dusenkova, M. Halitovs. Analysis of tritium distribution in carbon based tiles. [Poster presentation by A. Vitins]

The 9th International Symposium on Fusion Nuclear Technology (ISFNT-9), Dalian, China, 11-16 October 2009:

43. A.Vītiņš, G. Ķizāne, E. Pajuste, A. Frolovs, S. Kalēja, Br. Leščinskis, I. Dušenkova. Tritium release properties of neutron-irradiated beryllium pebbles. [Poster presentation by A. Vītiņš]

LABORATORY OF THEORETICAL PHYSICS AND COMPUTER MODELLING

Head of Laboratory Dr. hab. phys. Eugene Kotomin

Research Area and Main Problems

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

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

We combine several different techniques, including analytical formalisms and large-scale computer simulations (quantum chemical methods, stochastic simulations as well as Monte Carlo/cellular automata modeling).

Scientific staff

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

PhD students

12. D. Bocharov
13. A. Gopejenko

Scientific visits abroad

Dr. hab. E. Kotomin, Max Planck Institute for Solid State Research, Stuttgart, Germany (9 months), Universities of Maryland and Michigan, USA (2 weeks), The Eurasian University, Astana, Kazakhstan (2 weeks).

Dr. hab. V. Kuzovkov, Ludwig-Maximilians-Universität (LMU), München, Germany (1 week); University of Hamburg, Germany (1 month).

Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (3 months).

Dr. D. Gryaznov, EC Institute of Transuranium Elements, Karlsruhe, Germany (9 months), Max Planck Institute for Solid State Physics, Stuttgart, Germany (2 months),

Dr. V. Kashcheyevs, Berkeley National Laboratory, USA (2 months), Hebrew University of Jerusalem, Israel (2 weeks), Ben-Gurion University of the Negev, Beer-Sheva, Israel (2 weeks), Physikalisch-Technische Bundesanstalt, Braunschweig, Germany (1 week).

Dr. Yu. Mastrikov, University of Maryland, USA (11 months).

Dr. S. Piskunov, University of Duisburg-Essen (8 months), Northwestern University, Evanston, USA (1 month), LNF Frascati, Italy (1 month).

- Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (1 month), Max Planck Institute for Solid State Research, Stuttgart, Germany (1 month) , Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (6 weeks)
- Dr. Yu. Zhukovskii, Northwestern University, Evanston, USA (1 month), Institute for Materials Research-I, Karlsruhe, Germany (1 month), St. Petersburg State University, Russia (3 weeks), Max Planck Institute for Solid State Research, Stuttgart, Germany (2 weeks), Technical University of Braunschweig, Germany (2 weeks), EC Institute of Transuranum Elements, Karlsruhe, Germany (1 week).
- Dr. G. Zvejnicks, University of Michigan, USA (1 week).
- D. Bocharov, Max Planck Institute for Solid State Research, Stuttgart, Germany (2 weeks), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (1 week), EC Institute of Transuranum Elements, Karlsruhe, Germany (1 week).
- A. Gopejenko, Forschungszentrum Karlsruhe, Institut für Materialforschung I, Karlsruhe, Germany (4 months).

International Cooperation

Finland	1. Helsinki University of Technology (Dr. T. Kurki-Suonio)
France	2. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober)
	3. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)
	4. Physikalisch-Technische Bundesanstalt, Braunschweig (Dr. Bernd Kästner).
	5. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm)
	6. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov)
Germany	7. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. Van Uffelen).
	8. Max Planck Institut für Plasmaphysik, Garching (Dr. V. Igochine, Prof. Dr. K. Lackner, Dr. R. Mayer-Spasche, Prof. Dr. H. Zohm)
	9. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk)
	10. Institut für Materialforschung I (KIT), Karlsruhe (Dr. A. Möslang)
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)
Japan	14. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	15. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Poland	16. Warwaw University, Dept of Chemistry (Dr A. Huczko)
Romania	17. University of Craiova (Dr. D. Constantinescu)
Russia	18. St. Petersburg University (Prof. R.A. Evarestov)
UK	19. Cavendish Laboratory, University of Cambridge (Dr. M.R. Buitelaar)
	20. University College London (Prof. A.L. Shluger)
Ukraine	21. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)
	22. Idaho National Laboratory (Dr. S.N. Rashkeev)
USA	23. Northwestern University, Evanston, Illinois (Prof. D.E. Ellis)
	24. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

THE MAIN RESULTS

KINETIC MONTE-CARLO SIMULATION OF OXIDIZED SILICON STRIPE FORMATION ON PD(111)

G. Zvejnicks

Recently several papers were published on room temperature decomposition of silane (SiH_4) on oxidized Pd and Pt(111) surfaces. Room temperature fits into a narrow temperature where silane already decomposes, but the temperature is insufficient for formation of various silicides. The most striking result of these experiments was the discovery of Si-O stripe structure. This result was confirmed by vibrational spectra measurements and supported by density functional theory (DFT) calculations.

We propose the model with two interaction constants (nearest neighbor pair repulsion of SiO complexes, v , and their trio attraction in a line, v_t) which demonstrates stripe formation during silane decomposition on oxidized Pd(111) surface. The simplest (2×1) stripe phase is obtained by kinetic Monte Carlo simulation in absence of longer-range attractive interactions which are usually necessary for stripe structure formation. Despite higher energy, this phase is shown to be very stable. Phase diagram for this model is obtained, Figure 1, and (2×1) phase stability is analyzed varying coverage and reaction rate parameters.

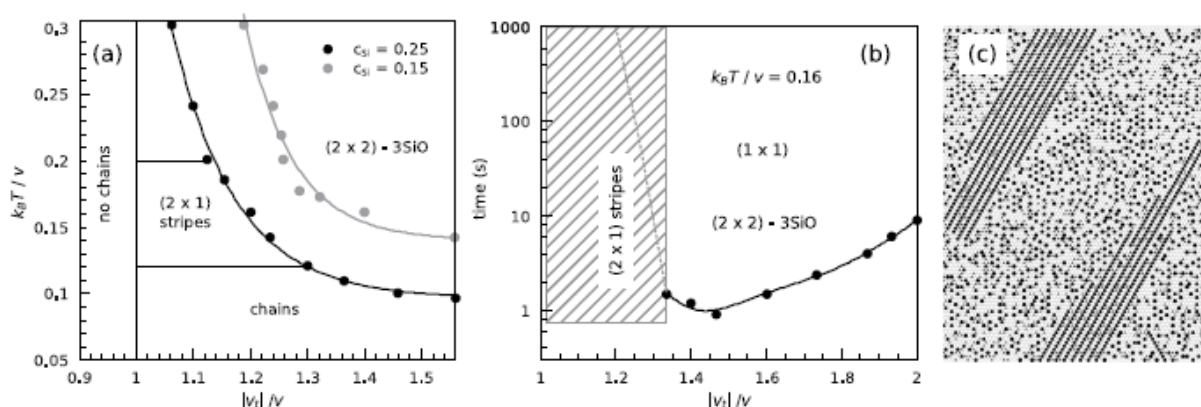


Figure 1 (a) Phase diagram obtained after 10s. (b) Time of (2×1) stripe structure stability (dashed region) and time of (2×2) structure formation from chains at $k_B T / v = 0.16$. (c) Snapshot of (2×1) structure at $|v_t| / v = 1.13$ and $k_B T / v = 0.16$ after 1000 s. Black dots correspond to SiO complexes.

THE ANDERSON LOCALIZATION PROBLEM, THE FERMI-PASTA-ULAM PARADOX AND THE GENERALIZED DIFFUSION APPROACH

V. Kuzovkov

Based on the interpretation of a quantum tight-binding model in terms of a classical Hamiltonian map, we have considered the Anderson localization (AL) problem as the Fermi-Pasta-Ulam (FPU) effect in a modified dynamical system containing both stable and unstable (inverted) modes. Delocalized states in the AL are analogous to the stable quasi-periodic motion in FPU; whereas localized states are analogous to thermalization, respectively. Our second aim was to use the classical Hamilton map for a simplified derivation of *exact* equations for the localization operator $H(z)$. The letter was presented earlier [J.Phys.: Condens. Matter **14** (2002) 13777] treating the AL as a generalized diffusion in a dynamical system. We have demonstrated that the counter-intuitive results of our studies of the AL are similar to the FPU counter-intuitionism.

ELECTRON DYNAMICS IN THE PROCESS OF MODE SWITCHING IN GYROTRONS

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The present study was devoted to the analysis of electron interaction process in the course of gyrotron switching from one mode to another. This analysis is based on the use of the Hamiltonian formalism that allows one to construct Poincare plots for different instants of switching time. The study is carried out for a 170 GHz, MW-class gyrotron for the International Thermonuclear Experimental Reactor (ITER).

Simulations were done for the following set of gyrotron operating parameters: $B = 6.76T$, $I_b = 42A$, $R_{el} = 9.50mm$, and $\alpha = 1.3$ at $U_b = 79kV$. In solving (1)-(2) we used 25 electrons with different entrance phases ϑ and 7 groups of electrons with different azimuthal coordinates of guiding centers ϕ uniformly distributed between 0 and 2π . In Figs. 2-4 we show Poincare plots at four cross sections of the resonator and three time moments; it is shown electron distribution for electrons having two azimuthal angles of guiding centers: $\phi = 2\pi/7$ (black dots) and $\phi = 2\pi \cdot 4/7$ (empty diamonds). Crosses mark the electron number one, whose entrance phase is $\vartheta = 2\pi/25$. Here the lower cat's eye shows the separatrix of the operating mode and the upper cat's eye shows the separatrix of the parasitic mode.

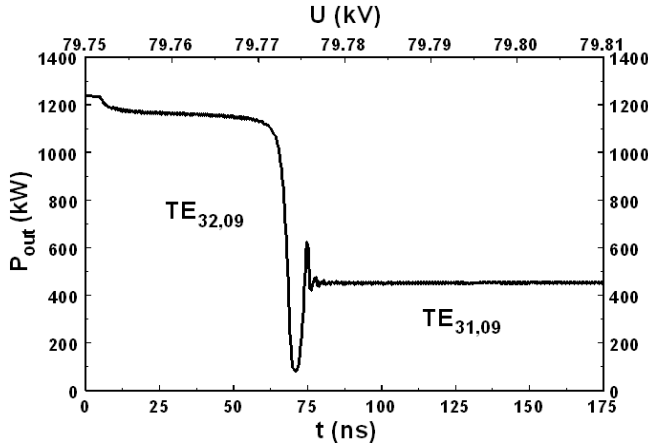


Figure 1. Switching from the operating $TE_{32,09}$ mode at $170.027GHz$ to the parasitic $TE_{31,09}$ mode at $166.985GHz$.

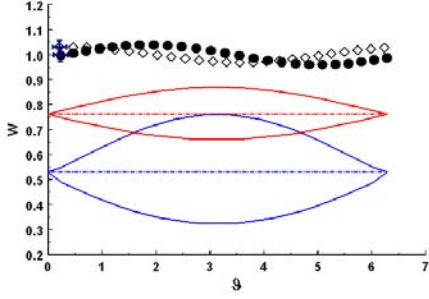


Fig. 2a

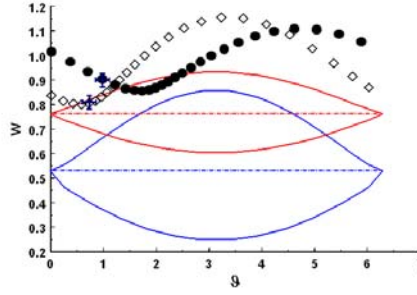


Fig. 2b

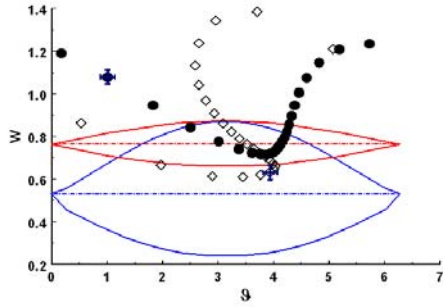


Fig. 2c

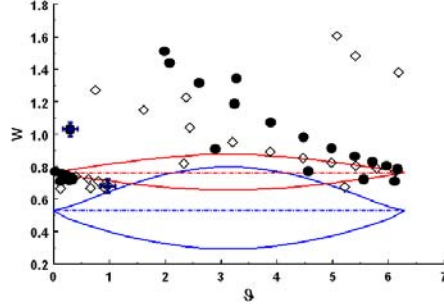


Fig. 2d

FIGS. 2a-d.. Poincaré plots at four cross sections of the resonator: $\zeta = \zeta_{out}/4, \zeta_{out}/2, 3\zeta_{out}/4, \zeta_{out}$ for the time moment $t = 70 ns$.

It should be noted that electrons with different azimuthal coordinates of guiding centers exhibit different dynamics in the process of mode switching. This can be considered as a specific feature of the electron interaction with the fields of more than one mode. In the case of single-mode operation, electrons with different azimuthal coordinates of guiding centers exhibit the same behavior in the phase space. However, in the process of mode switching, where two modes are present, electron dynamics depends on the azimuthal coordinate of the guiding center. This can be explained by the fact that the phase difference of these modes is azimuthally dependent. This conclusion can be illustrated by the right figure in the second row in Fig. 2 showing electron distribution at the exit for $t=72 ns$: here the lowest value of w for black dots is larger than 0.8, while a corresponding minimal value of w for empty diamonds is about 0.5.

When the guiding magnetic field is chosen properly, the voltage rise results, first, in fulfillment of self-excitation conditions for the operating $TE_{32,09}$ mode; then, at higher voltages, it operates with a high efficiency (possibly, in the region of hard self-excitation). In this regime, the difference between the frequency of this mode and the electron cyclotron frequency is rather large. For the parasitic $TE_{31,09}$ mode with a lower frequency this difference is smaller. Therefore, electrons, which enter the interaction region with the initial value of w equal to unity, in the process of their deceleration by the $TE_{32,09}$ mode first enter the region occupied by the separatrix of the $TE_{31,09}$ mode (red) and, hence, interact with it in spite of the presence of the $TE_{32,09}$ mode. This gives the preference to the $TE_{31,09}$ mode and so it starts to grow.

Growth of the $TE_{31,09}$ mode is accompanied by significant disturbances in the electron distribution in the phase space. Therefore, when electrons enter the region occupied by the separatrix of the $TE_{32,09}$ mode (blue), they have much less free energy to be transformed to this mode radiation. Thus, the $TE_{32,09}$ mode begins to decay.

It is shown that the electron dynamic in the process of simultaneous interaction with two modes depends on the azimuthal coordinate of electron guiding centers. Correspondingly, the kinetic energy in a spent electron beam at the exit from the interaction space is azimuthally dependent. When the switching process is rather slow, this azimuthal non-uniformity in the energy of spent electrons can be important for collector operation.

FIRST-PRINCIPLES CALCULATIONS OF PURE AND DEFECTIVE PEROVSKITE SURFACES

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J. Maier, R. Merkle, V. Alexandrov, E. Heifets (*Max Planck Institute, Stuttgart, Germany*)
R.A. Evarestov (*St. Petersburg University, Russia*),
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ABO₃-type perovskites continue to attract a considerable attention as materials for catalytic and electrochemical applications, *e.g.*, in solid oxide fuel cells (SOFC), ceramic membranes for gas separation, actuators, sensors, *etc.* Mixed oxides with the ABO₃ perovskite structure are flexible systems as their properties can be adjusted or enhanced for specific applications by chemical doping at the A or B cation sites. Alternatively, these oxides can also contain *point defects* in the form of vacancies and trapped electrons/ holes depending on the A, B cation- and dopant nature. In all these applications surfaces play a key role. We performed a series of perovskite studies with a focus on defects and surface properties which are important for high tech applications.

Using Hartree-Fock and DFT hybrid exchange-correlation functionals as incorporated into LCAO computer code *CRYSTAL*, we performed *ab initio* calculations of a surface relaxation and rumpling for (001) and (011) surfaces of BaZrO₃ and ATiO₃ (A=Sr, Ba, Pb, Ca). The (001) surface energies of AO, TiO₂ and ZrO₂ terminations are close to each other for all five materials. The energies for BaZrO₃, SrTiO₃, BaTiO₃, PbTiO₃ and CaTiO₃ polar (011) surfaces for all terminations are much larger than the (001) surface energies. The considerable increase in the Ti-O (Zr-O) chemical bond covalency is predicted near the (011) surface as compared to the bulk and the (001) surface.

In a close cooperation with Prof. D.E. Ellis (Northwestern University, USA), using the same *CRYSTAL* code, we performed large-scale computer calculations of bulk and surface O vacancies with trapped electrons (known as the *F* centers) in three key perovskite crystals: SrTiO₃, PbTiO₃ and PbZrO₃. The local lattice relaxation, charge redistribution and positions of defect levels within the band gap have been compared. We have demonstrated that difference in a chemical composition of host materials leads to quite different defect properties: the *F* center is a shallow defect in titanates but a deep defect in zirconite. All three perovskites show a considerable trend in O vacancy segregation to the surfaces which important for the interpretation of the experimental data on mass-charge transport in nanocrystalline materials. The same trend of defect segregation towards surfaces (or internal grain boundaries) was observed in our joint study with V. Alexandrov and Prof. J. Maier (Max Planck Institute, Germany) for the charged *F*⁺ centers in SrTiO₃ (O vacancy with a single trapped electron).

Magnetic perovskites play an important role in spintronics, catalysis and other applications. One of widely used materials, *e.g.*, as a cathode for Solid Oxide Fuel Cells (SOFC), is LaMnO₃, both pure and Sr-doped. In a close collaboration with Dr E. Heifets and Prof. J. Maier (Max Planck Institute, Germany), we have used plane-wave *VASP* computer code in

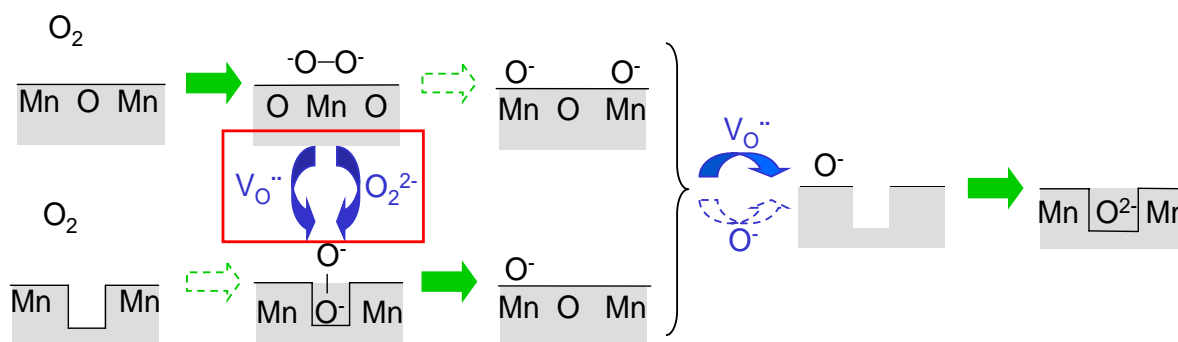


Figure 1: The most probable mechanism of oxygen incorporation on $\text{MnO}_2[001]$ -terminated $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ follows the solid arrows. Straight arrows indicate reaction steps (chemisorption, dissociation, O incorporation), bent arrows describe transport (diffusion parallel to the surface). The rate-determining step in the red box is the encounter of an adsorbed molecular oxygen species O_2^- or O_2^{2-} and a surface oxygen vacancy.

a pioneering study of the atomic, electronic and thermodynamic properties of three types of LaMnO_3 surfaces in both cubic and (low-temperature) orthorhombic phases. In particular, thermodynamic analysis demonstrated that the O-terminated (011) surface in both cubic and orthorhombic phases is stable only under very poor O- and Mn-conditions (Fig. 1), whereas under normal SOFC operational conditions O_2 -terminated (011) and MnO_2 -terminated (001) surfaces are the most thermodynamically stable. This study was accompanied with the modeling of oxygen incorporation into LaMnO_3 -based SOFC cathode. Based on the *ab initio* calculations of adsorbates, surface defects, and their migration, several mechanisms of the O_2 molecule dissociation on the surface and penetration into the cathode were suggested, with a focus on the rate-determining step.

POINT DEFECT MODELLING IN NUCLEAR FUELS

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Uranium oxide (UO_2) and nitride (UN) are two actinide materials used as the nuclear fuels in fission reactors. Improvement of reactor performance and development of advanced fuels for future (generation IV) reactors needs better understanding the fuel physico-chemical properties, *e.g.*, UN oxidation and UO_2 thermo-mechanical properties under self-irradiation. To this end, we performed *ab initio* VASP modeling of both materials.

In collaboration with Prof. R.A. Evarestov and Dr A.V. Bandura (St. Petersburg University, Russia) we have studied oxygen adsorption on the UN (001) surface using the slab periodic model (Fig. 2). We have studied the binding energies, atomic displacements, and charge redistribution and demonstrated a strong O atom chemisorption typical for metallic surfaces

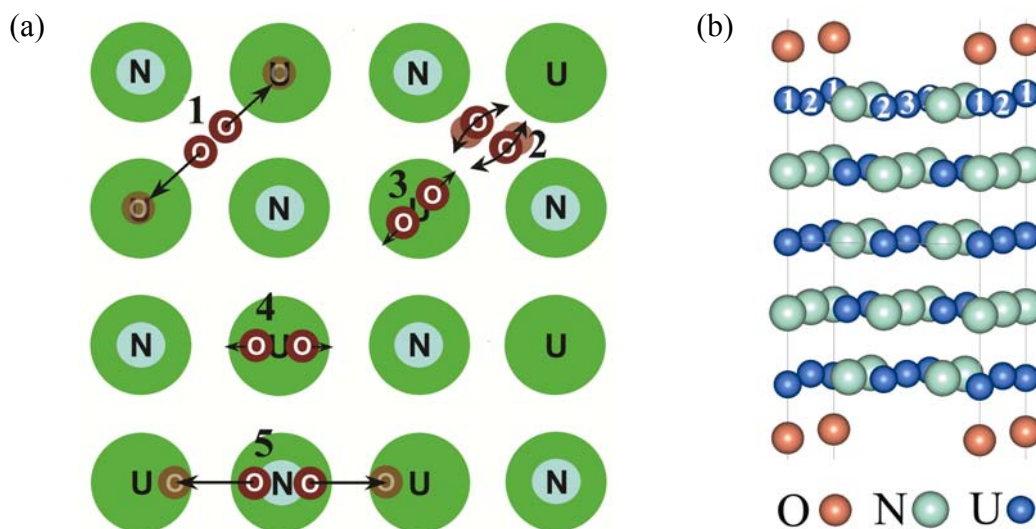


Fig.2. Two periodic slab models: (a) five different horizontal configurations for the O_2 molecule adsorption on the UN(001) surface including those with spontaneous molecular dissociation (1 and 5) and (b) two-side periodic adsorption of O atoms (0.25 ML) atop the surface U cations.

which is an important step in the surface oxidation process (O atoms replace for surface N atoms). To check reliability of the plane wave calculations, we employed also the *CRYSTAL* LCAO code and obtained very good agreement with the *VASP* calculations. To shed more light on the initial stage of the adsorbed O_2 molecule dissociation, we have studied this process for different possible molecule configurations on UN surface (Fig. 2a) and demonstrated that the dissociation occurs spontaneously when the molecular centre lies above the surface hollow site or atop N ions, certain activation barrier arises when a molecule sits atop the surface U ion. Besides the UN interaction with oxygen, we studied also basic defect migration (U, N vacancies and interstitials, as well as O impurities). These *ab initio* energies were used in the fuel performance code *TRANSURANUS* for the analysis of the role of O impurities in the thermal creep in UN. Therefore, a concrete example is provided of how *ab initio* calculations can contribute directly to improve design tools of advanced nuclear fuels.

Lastly, in collaboration with Dr. S.N. Rashkeev (Idaho National Laboratory, USA) and Dr. P. Van Uffelen (EC Institute for Transuranium Elements, Karlsruhe, Germany) a detailed study of the He incorporation into UO_2 fuel has been performed using the DFT+U formalism. We have demonstrated that careful modelling of the fuel structure is necessary for a reliable calculation of the He incorporation energy.

CARBON NANOTUBE TECHNOLOGY FOR HIGH-SPEED NEXT-GENERATION NANO-INTERCONNECTS (CATHERINE, EC FP7 PROJECT)

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Carbon nanotubes (CNTs) become an important constituent of future nanoelectronics which is still hindered by inability to reproduce a growth of CNT with predetermined chirality indices since existing methods of nanotube synthesis yield a mixture of metallic and semiconducting nanotubes. The chemical vapor deposition (CVD) growth of CNTs above the particles of metallic catalyst is believed to be the promising approach for gaining a control over the properties of nanotubes. In collaboration with Dr S. Bellucci (Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di

Frascati, Italy), we have performed the large-scale DFT-LCAO calculations on 2D-periodic models of the nanostructured C/Ni(111) interface (Fig. 3, values of E_{bind} describe carbon species bonding per C atom).

Initial appearance of carbon atoms upon the catalyst surface (when using the CVD method) follows from the dissociation of hydrocarbon molecules, e.g., CH₄. As a next step, we have simulated the C/Ni(111) interface, where carbon adatoms initially form periodic 2D islands then transforming to nanotube embryos, looking as semi-fullerenes, and finally to capped CNTs ($d_{C-C} \approx 1.42 \text{ \AA}$) of either armchair (*ac*) or zigzag (*zz*) chirality. Periodicity of this system results (Figs. 3,4) in models of infinite bundles of single-walled (SW) CNT (Fig. 4) with diameter 1.0-1.1 \AA and inter-tube distance 3.4-3.8 \AA (depending on chirality).

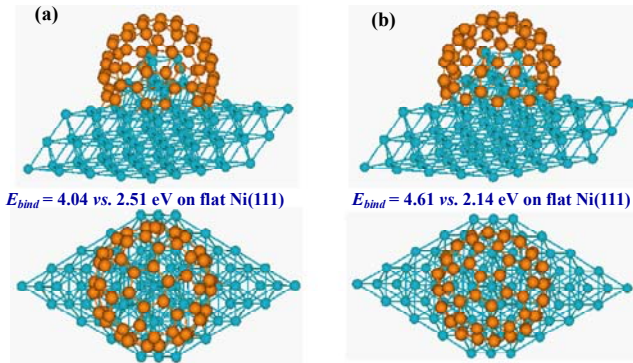
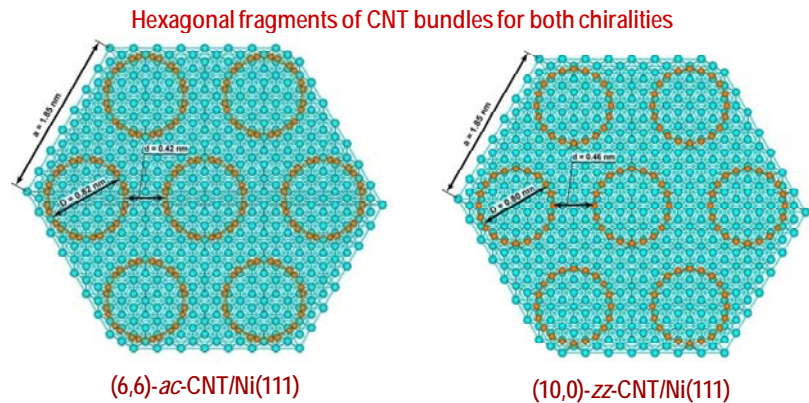


Fig. 3. Aside (upper) and atop (lower) views of 2D supercells containing CNT of either *ac* (a) or *zz* (b) type chirality upon the nanostructured Ni(111) surface.

Fig. 4. Hexagonal fragments of the CNT/Ni(111) interconnect sectioned across the bundle junctions and containing seven supercells shown in Fig. 3 for both *ac*- and *zz*-type chiralities.



Excellent conductivity properties of metallic CNT are the main reason for choosing them as the next-generation material for interconnects. However, the state-of-the-art estimates for the number of conducting channels in existing literature, which so far have been used in electrodynamical simulations, are based upon the limited microscopic modeling (room temperature, low voltage only, limited ensemble of chiralities, no doping). In collaboration with Prof. M.S. Sarto and Dr A. Tamburrano (La Sapienza Università, Roma, Italy), we have performed in-depth simulations (based on the orthogonal tight-binding, OTB, simulations, validated for simple examples by *ab initio* DFT calculations) producing the new quantitative analytic and numerical results which allow us to lift the above limitations. The key quantity, connecting CNT transport properties with the band structure is the number of conducting channels, $N(E)$, at particular energy E . It is defined by the positions of the bottoms for the conduction sub-bands and those on the tops of valence sub-bands. The values of $N(E)$ are not only the functions of energy, but also the nanotube diameter, temperature, bias voltage and chemical potential.

Based on the formalism of scattering theory, we have developed the coherent-potential approach considered as an effective-medium-approximation (CPA EMA). The first step of CPA-EMA modeling is the construction of potentials, both atomic and crystalline which uses the special well-tested analytical procedures. For proper description of CNT-Ni interconnect, including its

resistivity, the CPA-EMA model has been developed in the current study, in collaboration with Dr S. Bellucci (Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, Italy). Within the formalism of electronic transport it consists of two regions supporting two different electron transport mechanisms: ballistic (elastic, valid for carbon nanotubes *per se*) and collisional (non-elastic, valid for metal-CNT junctions). Taking into account that not all the electrons participate in a conduction process with the Fermi velocity, we have defined the so-called “thermally activated electrons” responsible for conductivity in the interconnect area. In the framework of this formalism, the interconnect resistance between the various transition metal substrates and either single-walled (SW) or multi-walled (MW) CNTs have been quantitatively estimated.

CsPbCl₃ NANOCRYSTALS DISPERSED IN Rb_{0.8}Cs_{0.2}Cl MATRIX STUDIED BY FAR-IR SPECTROSCOPY

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The comparative far-infrared spectroscopy studies of Rb_{0.8}Cs_{0.2}Cl and Rb_{0.8}Cs_{0.2}Cl containing CsPbCl₃ nanocrystals between 170 and 320 K are performed. Far infrared reflectivity of Rb_{0.8}Cs_{0.2}Cl crystals was measured at the Daphne Light IR station, Laboratori Nazionali di Frascati in Italy. Obtained reflectivity spectra have been analyzed using FOCUS software. Detailed analysis of FIR spectra allows to determine and analyze, in particular, the temperature dependences of phonon frequencies (in cm⁻¹), damping constants and optical dielectric constants of Rb_{0.8}Cs_{0.2}Cl and Rb_{0.8}Cs_{0.2}Cl:Pb. The effect of cesium lead chloride nanocrystals on the phonon modes of the host matrix, particularly manifested in different temperature behavior of LO–TO splitting and the temperature dependence of high frequency dielectric constant, was demonstrated as well.

SILICON CARBIDE NANOWIRES: SYNTHESIS AND CATHODOLUMINESCENCE

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Silicon carbide which exist in several polytypes (3C, 4H, 6H etc.) is recognized as a technologically relevant material. In optoelectronics, SiC can be used for creating LEDs covering the entire visible range. This possibility is now of particular interest whereas the progress in the producing of various silicon carbide based nanostructures opened a new way of obtaining tunable emission from the material at the same time providing improved luminescence yield.

The β-SiC (or 3C-SiC) nanowires were efficiently produced using the thermal-explosion mode of self-propagating high temperature combustion synthesis (SSH) from elemental Si and poly(tetrafluoroethylene) powder mixtures combusted under different operational parameters [A. Huczko et al., *J. Phys.: Condens. Matter* 19, 2007, 395022].

We present the study of one-dimensional β-SiC structures by means of cathodoluminescence (CL) technique. CL spectra of several nano 1D-SiC samples and of a reference commercially available 3C-SiC, measured at 77 K, are compared. It was demonstrated that the emission band at 1.97 eV related to irradiative transitions between the deep defect level (silicon vacancy) and the conduction band (weakly detected in the spectrum of the commercial SiC) becomes, under 10 keV electron beam irradiation, the prevailing band in CL of the purified silicon carbide nanowires. After the final stage of purification process the intensity of 1.97 eV band is almost 10 times stronger with respect

to the 2.38 eV peak which, in turn, corresponds to band-to-band transition in 3C-polytype of silicon carbide. Observed behavior confirms that produced nanowires are defects-enriched. Summarizing, a morphological characterization of the fabricated 3C-SiC 1D nanostructures has been performed by combining electron microscopy with CL measurements. Using those techniques as complementary tools can be helpful in the analysis of various nanomaterials having pronounced defect structure.

FAR-IR SPECTRA OF Ag_2CdI_4 IN TEMPERATURE RANGE 10–420 K: COMPLEMENTARY EXPERIMENTAL AND FIRST-PRINCIPLES STUDY

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Ag_2MX_4 compounds, where $M = \text{Cd}, \text{Hg}, \text{Zn}, \text{etc.}$, belong to a class of *superionic solids* which are promising materials for use in *solid state batteries and fuel cells* due to extraordinarily high ionic conductivity at supercritical temperatures.. We have performed a complete IR characterization of the ternary superionic compound Ag_2CdI_4 . Far IR spectroscopy was performed at the Daphne Light synchrotron IR facility. The influence of temperature on the far-infrared (FIR) spectrum of polycrystalline Ag_2CdI_4 has been investigated in details. We complement FTIR spectroscopy with Kramers-Kronig analysis and complex dielectric response modeling with a number of quantum-chemical DFT calculations of the central-zone vibrational spectrum of Ag_2CdI_4 . This combination of different techniques allowed us to validate the IR-active optical modes, describe mode splitting in polycrystalline Ag_2CdI_4 , obtain dielectric parameters in the IR-range and thus bridge the gap in studying of Ag_2MX_4 superionic compounds. The present approach can be further applied to study the lattice dynamics in other complex polycrystalline solids.

FUNDAMENTAL AND APPLIED NANOELECTRONIC ELEMENTS

V. Kashcheyevs

M.R. Buitelaar (*Cavendish Laboratory, University of Cambridge, UK*)

B. Kästner (*Physikalisch-Technische Bundesanstalt, Braunschweig, Germany*)

We have studied the coherent electron transport in time-dependent nanoelectronic elements – nanotubes and quantum dots. In collaboration with Dr. Mark Buitelaar (Cavendish Laboratory, University of Cambridge, UK), we have investigated charge pumping in carbon nanotube quantum dots driven by the electric field of a surface acoustic wave. It was found that, at small driving amplitudes, the pumped current reverses polarity as the conductance is tuned through a Coulomb blockade peak using a gate electrode. This behavior was systematically investigated as a function of wave amplitude, frequency, and direction and a model was developed in which our results can be understood as resulting from adiabatic charge redistribution between the leads and quantum dots on the nanotube. In collaboration with Dr. Bernd Kästner (Physikalisch-Technische Bundesanstalt, Braunschweig, Germany) we have described a new mechanism for charge quantization in dynamic quantum dots. These elements can be formed by time-dependent electrostatic potentials in nanoelectronic devices, such as gate- or surface-acoustic-wave-driven electron pumps. Ability to control the number of captured electrons with high precision is required for applications in fundamental metrology and quantum information processing, but the available models are limited. We have described stochastic decrease in the electron number of a shrinking dynamic quantum dot by a nuclear decay cascade model with "isotopes" being different charge states of the dot. Unlike the natural nuclei, the artificial confinement is time-dependent and tunable, so the probability distribution for the final "stable isotopes" depends on the external gate voltage. An explicit fitting formula was derived to extract the sequence of decay rate ratios from the measurements of averaged

current in a periodically driven device. This provides a microscopic fingerprint of the initialization process, allows to compare different devices and architectures, and predict the upper limits of initialization accuracy.

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I. 25th ISSP Conference (Riga, Latvia, February, 2009).

1. R.I. Eglitis, "First-principles calculations of BaZrO₃, SrTiO₃, BaTiO₃, PbTiO₃, CaTiO₃ (001) and (011) surface microstructures". Abstracts: p. 53.

2. D. Bocharov, Yu.F. Zhukovskii, and E.A. Kotomin, "Chemisorption of a molecular oxygen on the UN (001) surface". Abstracts: p. 54.

3. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Simulation of yttrium and oxygen solute atoms in *fcc* Fe lattice in support of ODS steel development. Abstracts: p. 55.

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5. S. Piskunov, T. Jacob, and E. Spohr, "First-principle simulations of oxygen adsorption on LaMnO₃ and LSM (x=1/8) (001) surfaces under SOFC operating p/T conditions". Abstract: p.57.

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11. G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, K.D. Li, and L.M.Wang, "Initial stage of void superlattice formation as self-organization phenomenon". Abstracts: p. 74.
12. Yu.F.Zhukovskii, V. Kashcheyevs, S. Piskunov, Yu.N. Shunin, and E.A. Kotomin, "Participation of ISSP group in the EC FP7 project: carbon nanotube technology for high-speed next-generation nano-interconnects (*CATHERINE*) ". Abstracts: p. 89.
13. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, "Perfect and defective (001) surface of uranium nitride: *ab initio* calculations". Abstracts: p. 100.
14. A. Gopejenko, Yu.F. Zhukovskii, P. Vladimirov, E.A. Kotomin, and A. Moslang, "Simulations on solution of yttrium and oxygen atoms in fcc iron lattice". Abstracts: p. 101.
15. V. Pankratov, A.I. Popov, A. Kotlov, S.A. Chernov, A. Zharkouskaya, and C. Feldmann, "Luminescence and energy transfer processes in LaPO₄: Ce,Tb nanocrystals". Abstracts: p. 111.
16. A.I. Popov, V. Pankratov, A. Kotlov, I. Karbovnyk, and I. Bolesta, "Time-resolved luminescence of CdI₂ single crystal under the excitation of synchrotron radiation". Abstracts: p. 112.
17. I. Karbovnyk, S. Piskunov, I. Bolesta, S. Bellucci, M. Cestelli Guidi, M. Piccinini, E. Spohr, and A.I. Popov, "Far IR spectra of Ag₂CdI₄ at temperature range 10-420 K: complementary experimental and first principles theoretical study". Abstracts: p. 113.

VI. The 7th International Conference "Information Technologies and Management", IT&M'2009 (Riga, Latvia, April, 2009).

18. Yu. F. Zhukovski, S. Piskunov, E.A. Kotomin, and S. Bellucci, "Carbon nanotubes in project *CATHERINE*: 2D periodic model of CNT bundle growth on the nanostructured Ni(111) surface: *ab initio* simulations". Abstracts: p. 15-16.
19. Yu.N. Shunin, Yu.F. Zhukovskii, and S. Bellucci, "Theoretical simulations of carbon nanotubes devices". Abstracts: p. 17-18.
20. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Simulation of yttrium oxide particle formation in iron in support of ODS steel development". Abstracts: p. 30-31.
21. D. Bocharov, D. Gryaznov, Yu.F. Zhukovskii, and E.A. Kotomin, "*Ab initio* calculations on the atomic and electronic structure of defective UN(001) surface". Abstracts: p. 32-33.

VII. The European Future Technologies Conference, FET'2009 (Prague, Czech Republic, April, 2009).

22. Yu.N. Shunin, Yu.F. Zhukovskii, and S. Bellucci, "Theoretical simulations on conductivity and resistivity of carbon nanotubes and CNT-Ni interconnects using effective media approach". Abstract. p. 115.

VIII. International Workshop "Modeling of Carbon and Inorganic Nanotubes and Nanostructures" (Lausanne, Switzerland, May, 2009).

23. S. Piskunov, Yu.F. Zhukovskii, E.A. Kotomin, and S. Bellucci, "First principles modeling of initial stage of CNT growth on nanostructured Ni(111) catalyst". Abstracts: p. 47

IX. Technische Sitzungen JK 2009 (Leipzig, Germany, May, 2009).

24. S. Kern, M.H. Beringer, E. Borie, G. Dammertz, O. Dumbrajs, G. Gantenbein, S. Illy, J. Jin, W. Leonhardt, B. Piosczyk, H. O. Prinz, T. Rzesnicki, M. Schmid, S. Alberti, J.-P. Hogge, M. Q. Tran, H. Braune, V. Erckmann, H. P. Laqua, G. Michel, E. Giguët, F. Legrand, C. Lievin, J. Flamm, M. Thumm, "Gyrotrons for Fusion Plasma Heating - Status of Development at the Forschungszentrum Karlsruhe (FZK)".

X. 108th Annual Meeting of German Physical Chemistry Society (Köln, Germany, May, 2009).

25. E.A. Kotomin, R. Merkle, Yu. Mastrikov, E. Heifets, and J. Maier, "First principles modelling of oxygen incorporation into SOFC cathode". Abstracts: p. 75.

XI. 5th International conference on Quantum Theory of Solids (Aarhus, Denmark, May, 2009).

26. E.A. Kotomin, Yu.F. Zhukovskii, and S. Piskunov, "Hybrid functional calculations of point defects in ABO₃ perovskites".

XII. 15th International Semiconducting and Insulating Materials Conference (Vilnius, Lithuania, June 2009).

27. E.E. Tornau, V. Petrauskas, G. Zvejnieks, "Simulation of oxidized silicon stripe formation on Pd(111)".

XIII. 13th ICQC International Congress of Quantum Chemistry (Helsinki, Finland, June, 2009).

28. S. Piskunov, E. Heifets, T. Jacob, E.A. Kotomin, and E. Spohr, "Hybrid density functional calculations of thermodynamic stability and oxygen adsorption on LaMnO₃ and La_{1-x}Sr_xMnO₃ (001) surfaces". Abstracts: p. 115.

XIV. 36th EPS Conference on Plasma Physics (Sofia, Bulgaria, June 2009).

29. V. Igochine, O. Dumbrajs, K. Lackner, G. Pereverzev, H. Zohm, and ASDEX Upgrade team, "Structure of incomplete sawtooth crashes in ASDEX Upgrade".

XV. 3rd National Conference on Nanotechnology NANO 2009 (Warsaw, Poland, June 2009)

30. V. Savchyn, I. Karbovnyk, A.I. Popov and A. Huczko. Combustion Formation of Novel Nanomaterials: Synthesis and Cathodoluminescence of Silicon Carbide Nanowires. Abstract.

XVI. 7th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation LUMDETR 2009 (Krakow, Poland, July 2009)

31. V. Savchyn, I. Karbovnyk, A. Huczko, A.I. Popov, Cathodoluminescence from nano-SiC powders: temperature study. Abstract. P2-42

XVII. 17th conference on Solid State Ionics (Toronto, Canada, July 2009).

32. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, E. Heifets, and J. Maier, "First principles modeling of pathways for oxygen incorporation into SOFC cathode". Abstracts: p. 255.

XVIII. International Conference on Magnetism (Karlsruhe, Germany, July 2009).

33. D. Gryaznov, D. Sedmidubsky, E. Heifets, and E.A. Kotomin, "Density functional theory calculations on magnetic properties of actinide compounds". Abstracts: p. 220.

XIX. International Conference "Radiation Defects in Insulators" REI-15 (Padova, Italy, August-September, 2009).

34. A.I. Popov, E.A. Kotomin, and J. Maier, "Basic properties of radiation-induced point defects in halides and oxides". Abstracts: O9

35. E.A. Kotomin, Yu.F. Zhukovskii, S. Piskunov, and J. Maier, "First principles calculations of point defects in ABO_3 perovskites". Abstracts: O11.

36. Kun-Dar Li, Weixing Li, Lumin Wang, R. Ewing, and E.A. Kotomin, "Dynamics of microstructural evolution in electron-irradiated fluor-apatite". Abstracts: P-A25.

37. E.A. Kotomin, V.N. Kuzovkov, G. Zvejnieks, Kun-Dar Li, and Lumin Wang, "Void superlattice formation in electron irradiated CaF_2 : theoretical analysis". Abstracts: P-A34.

38. S. Rashkeev, E.A. Kotomin, and Yu.A. Mastrikov, "First principles calculations of defect migration in UN nuclear fuels". Abstracts: P-C3.

39. D. Gryaznov, E.A. Kotomin, S. Rashkeev, E. Mauger, and T. Wiss "Radiation defects behavior in oxide nuclear fuels: first principles modelling and helium release measurements". Abstracts: P-C8.

XX. International Workshop "DFT modelling of actinide solid solutions with the emphasis to bulk properties and helium behaviour" (Karlsruhe, Germany, September, 2009).

40. Yu.F. Zhukovskii, E.A. Kotomin, D. Bocharov, and V.N. Kuzovkov, "The DFT+U calculations on defects in PuO_2 and MOX".

41. D. Gryaznov, "Density functional theory calculations on UO_2 , UN and $UZrN$ ".

XXI. 13th European Fusion Theory Conference (Riga, Latvia, October, 2009).

42. O. Dumbrajs, V. Igochine, A. Gude, K. Lackner, M. Maraschek, G. Pereverzev, H. Zohm, and ASDEX Upgrade team, "The role of stochastization in fast MHD phenomena on ASDEX Upgrade". Abstracts: I-4, p.6.

43. D. Constantinescu, O. Dumbrajs, V. Igochine, K. Lackner, R. Meyer-Spasche, H. Zohm, "A low-dimensional model system for quasi-periodic plasma perturbations". Abstracts: P1.06, p.31

XXII. 9th International Conference 'Reliability and Statistics in Transportation and Communication' (Riga, Latvia, October, 2009).

44. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Shunina, "Theoretical simulations of nanoelectronic devices: quantum dots, nanowires and carbon nanotubes". Abstracts: p. 98-99.

XXIII. 216th Electrochemical Society Meeting (Vienna, Austria, October, 2009).

45. R. Merkle, Yu.A. Mastrikov, E. Heifets, E.A. Kotomin, M. Kuklja, and J. Maier, "Oxygen incorporation reaction into mixed conducting perovskites: a mechanistic analysis for $(La,Sr)MnO_3$ based on DFT calculations".

XXIV. International conference "Fermions 2009: From Correlated Electrons to Cold Atoms" (Oberurgl, Austria, October, 2009).

46. V. Kashcheyevs, "Dynamic quantum dot spectroscopy via strongly non-adiabatic electron counting".

XXV. Workshop on Nanoscience and Nanotechnology INFN-LNF (Frascati, Italy, October, 2009).

47. R.A. Evarestov and Yu.F. Zhukovskii, "Symmetry of inorganic nanotubes: from bulk crystal space group to monolayer diperiodic group and nanotube line group" Abstracts p. 38.

48. V. Kashcheyevs and B. Kaestner, "Decay cascade theory for dynamical quantum dot initialization and quantized charge transport". Abstracts: p. 45.

49. S. Piskunov, Yu.F. Zhukovskii, E.A. Kotomin, and S. Bellucci: "Theoretical predictions for initial stage of CNT growth on nano-structured Ni catalyst and inside the nanopore of alumina membrane". Abstracts: p. 46.

50. R.A. Evarestov, A.V. Bandura, M.V. Losev, S. Piskunov, and Yu.F. Zhukovskii. "Atomic and electronic structure of anatase- and fluorite-type TiO₂ nanotubes: Comparative analysis based on *ab initio* LCAO calculations". Abstracts: p. 75.

XXVI. 14th International conference on physics and chemistry of inorganic materials (Astana, Kazakhstan, October, 2009).

51. E.A. Kotomin, Yu. Zhukovskii, S. Piskunov, Yu.A. Mastrikov, and J. Maier, "First-principles calculations of radiation defects in perovskites

XXXVII. International conference of Materials Science and technology (Pittsburg, USA, October, 2009).

52. E.A. Kotomin, Yu.F. Zhukovskii, D. Fuks, D. Ellis, and J. Maier, "First principles modeling of metal ceramic interfaces: growth mode and surface defects. Abstracts: p. 58.

53. E.A. Kotomin, R. Merkle, E. Heifets, Yu.A. Mastrikov, and J. Maier, "Modeling of oxygen incorporation reaction into SOFC cathode: A first principles study". Abstracts: p. 64.

54. S. Rashkeev, E.A. Kotomin, and Yu.A. Mastrikov "First principles calculations of defect migration in UN nuclear fuels". Abstracts: p. 112.

55. E.A. Kotomin, Yu.A. Mastrikov, E. Heifets, R. Merkle, M. Kuklja, and J. Maier, "First principles modeling of SOFC cathode". Abstracts: p. 135.

56. E.A. Kotomin, V. Alexandrov, Yu.F. Zhukovskii, S. Piskunov, and J. Maier, "First principles calculations of the static and dynamic properties of oxygen vacancies in ABO₃ perovskites". Abstracts: p. 123.

XXXVIII. 3rd International conference "Innovative information technologies IIT-2009" (Vilnius, Lietuva, December, 2009).

57. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burluckaya, and R. Muhamediyev, "Simulations of nanoelectronic devices: quantum dots, nanowires and carbon nanotubes for computer technologies". Abstracts: p. 8-9.

XXXIX. International workshop "Towards Reality in Nanoscale Materials'09" (Levi, Finland, December, 2009).

58. S. Piskunov, Yu.F. Zhukovskii, E.A. Kotomin, and S. Bellucci, "Carbon adsorption on nano-structured Ni(111) catalyst and inside the nanopore of alumina membrane: Predictions from first principles calculations". Abstracts: p. 60.

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

Scientific Staff

1. Dr. M.Reinfelde
2. Dr. J.Teteris
3. Dr. O.Balcers

PhD Students

- A.Gerbreders
- E.Sledevskis

Technical Staff

1. J.Gurovs
2. D.Popele

Students

1. U.Gertners
2. J.Aleksejeva
3. A.Danilovs
4. V.Duboviks
5. M.Vdovičenko

Scientific visits abroad

1. Dr. K.Jefimovs, post-doc researcher, Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, Switzerland (12 months).

Cooperation

Latvia

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

Finland

3. University of Joensuu (prof. T.Jaaskelainen and prof. J.Turunen).

USA

4. University of Arizona, Optical Science Center, Tucson (Dr. O.Nordman and Dr. N.Nordman)
5. National Renewable Energy Laboratory, Colorado (Dr. P. Stradins).

Lithuania

6. Institute of Physics, Vilnius (Dr. R.Petruskevicius).

THE MAIN RESULTS

SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

Mara Reinfelde and Janis Teteris

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

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

The recording of the subwavelength gratings with a period of $0.15 \mu m - 1 \mu m$ was performed by holographic method. The fringe period for two intersecting light beams in a media with high refractive index n can be expressed as $\Lambda = \lambda_0 / 2n \sin \theta$, where 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.

AMORPHOUS CHALCOGENIDE THIN FILMS IN OPTICAL RECORDING TECHNOLOGIES

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 discussed. The laser interference lithography is used as a low-cost method for the exposure of large surfaces with regular patterns like subwavelength-gratings and microsieves. The regular features with the sizes of about 50 nm and less can be fabricated by this method. The Bragg reflection gratings were recorded and studied in amorphous 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.

IMMERSION HOLOGRAPHIC LITHOGRAPHY IN AMORPHOUS CHALCOGENIDE THIN FILMS

J.Teteris, J.Aleksejeva, M.Reinfelde

The recording of the surface-relief and refractive index modulated gratings with a period of 0.15 – 1.0 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 $\Lambda = \lambda_0 / 2n \sin\theta$, 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° , 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, 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°C . Results have shown that the surface relief formation efficiency is many times larger in case of extra softening by additional incoherent light during recording. The mechanism of the direct recording of surface relief on amorphous chalcogenide films based on the photoinduced plasticity has been discussed.

NANOSTUCTURED SURFACES FOR OPTICAL ANTIREFLECTION

J.Aleksejeva, J.Teteris

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

etc.) At present work we show the results obtained for surface patterning consisting of nano-structural elements smaller than incident light wavelength. The decreasing of light reflection for such structures results from light diffraction on above mentioned structures. Nanostructured antireflective elements are formed by holographic recording in chalcogenide photoresist. The next step is electrochemical growing of Ni shim used as a stamp for printing of nanostructures into organic polymer – laminate which can be pasted on glass surface. Nano-relief surface are transferred into transparent polymer films by hot embossing at 100-120⁰C 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 SPIROPYRAN AND POLYMER COMPOSITE FILMS

A. Gerbreders, J. Teteris

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

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

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

Scientific Publications

1. J.Teteris, Immersion holography based on amorphous chalcogenide films. Journ. of material Science: Materials in Electronics, vol. 20 (issue 1), 2009, 149-152.
2. Vj.Gerbreders, E.Sledevskis, V.Kolbjonoks, J.Teteris, A.Gulbis, Second harmonic generation in selenium-metal structures. Journ. Non-Cryst. Sol., 355 (2009) 1959-1961.
3. A.N.Trukhin, J.Teteris, A.Fedotov, D.L.Griscom, G.Buscariono, Photosensitivity of SiO₂-Al and SiO₂-Na glasses under ArF (193 nm) laser. Journ. Non-Cryst. Sol., 355 (2009) 1066-1074.
4. U.Gertners, J.Teteris, Surface relief formation during holographic recording. JOAM, 12 (2009) 1953-1956.
5. A.Gerbreders, J.Teteris, E.Aleksejeva, A.Danilovs, Optical recording in spiropyran and polymer composite films. JOAM, 12 (2009) 2145-2148.
6. A.Gerbreders, J.Teteris, E.Aleksejeva, A.Danilovs, Latvian Journal of Physics and Technical Sciences. 3 (2009) 23-29.
7. V.Gerbreders, E.Sledevskis, V.Kolbjonoks, J.Teteris, A.Gulbis, Second harmonic generation in selenium-metal structures. Journal of Non-Crystalline Solids, 355 (2009) 1959-1961.

8. U.Gertners, J.Teteris, Mass transport in amorphous chalcogenide thin films during holographic recording, *Latv.Journ.Phys. Techn. Sciences*, 46 (2009) 30-36

Lectures on Conferences

International Baltic Sea Region Conference “Functional materials and nanotechnologies” FM&NT-2009, Riga, Latvia, March 31 -April 3, 2009.

J.Teteris, Photoinduced mass transport in soft materials.

A.Gerbreders, J.Aleksejeva, A.Daņilovs, J.Teteris, Holographic recording in organic polymer, chalcogenide and photochrome composites.

M.Reinfelde, J.Teteris, M.Vdovičenko, E.Sledevskis, Holographic recording in amorphous As-S-Se and As-S films by 632.6 nm laser.

Internat. Student conference „Developments in optics and communications 2009”, Apr. 24-26, 2009, Riga

A.Danilovs, Optical recording in organic materials by ultraviolet laser light.

A.Gerbreders, J.Aleksejeva, A.Danilovs, J.Teteris, Feature of holographic recording in photochromr-chalcogenide composites.

J.Aleksejeva, Holographic recording in organic polymers by UV laser light.

V.Duboviks, J.Teteris, Photoinduced mass transport in liquids.

U.Gertners, J.Teteris, Mass transport in amorphous chalcogenide thin films during holographic recording.

4th International Conference on Amorphous and Nanostructured Chalcogenides, Constanta, Romania, June 29- July 3, 2009

U.Gertners, J.Teteris, Surface relief formation during holographic recording.

J.Aleksejeva, J.Teteris, Nanostructured surfaces for optical antireflection.

I.Mihailova, V.Gerbreders, E.Sledevskis, V.Kolbjonoks, E.Tamanis, Second harmonic generation in selenium-copper structures.

23rd Intern.Conf. Amorphous and Nanocrystalline Semiconductors, Ultrecht, Netherlands, 23.-28.08.2009

J. Teteris, Photoinduced mass transport in amorphous materials.

Int.Conf.”Northern Optics 2009”, Vilnius, 26-28 August, 2009.

A.Gerbreders, J.Aleksejeva, A.Daņilovs, J.Teteris, Holographic recording in photochrome-chalcogenide composites.

U.Gertners, J.Teteris, Photoinduced surface relief modulation in amorphous chalcogenide thin films during holographic recording.

LABORATORY OF VISUAL PERCEPTION

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

Research Area and Main Problems

Laboratory is trying to find synergies between material science (physics), vision research (perception) and everyday optometry (profession). Human vision is a complex phenomenon. Its optical part is essential, however optical image stays only at the very beginning of the visual pathway and information processing in the cortex. We see with our brains, and as a result in some provocative cases it is very hard for us to accept the final outcome.

Research in laboratory is focused on following problems:

- investigation of advanced optical materials and designs of vision appliances – tinted, high refractive glasses, antireflective coatings, multifocal and progressive, and contact lenses;
- effect of aberrations in eye structures and appliances on retinal image formation and on the psychophysically detected human visual response;
- effect of stimuli blurring and decrease of contrast and colour contrast on the stereo threshold;
- designs of software to display visual stimuli on computer screen for studies of monocular vision perception, suppression and rivalry mechanisms of binocular vision;
- digital visual stimuli image processing determinant for analyse of the human visual response;
- evaluation of suppression strength and depth on quality of vision binocular functions and on dominant eye;
- evaluation of accommodation/convergence mechanisms reading print materials and for regular computer users;
- eye kinematics studies for children and adults without and with several disorders of visual perceptions, eye kinematics studies in sports vision.

Scientific Staff:

1. Prof. I.Lācis
2. Prof. M.Ozolins
3. Dr. G. Krūmiņa
4. M.Sc. R.Paeglis

PhD Students:

1. M.Sc. A.Švede
2. M.Sc. G.Ikaunieks
3. M.Sc. S.Fomins
4. M.Sc. V.Karitāns

Educational.

Every year up to 25 bachelor and 10 master students of Department of Optometry and Vision science are graduated from University of Latvia. Lot of them performs their diploma experimental works tied with research topics of Laboratory of Visual perception.

Partners abroad

Italy	Florence University, Italy, (Prof. S. Villani) Universita` di Roma "Tor Vergata" (Prof. I. Davoli)
Sweden	Chalmers TH, Sweden (Prof. L.Komitov)
Norway	Buskerud Høgskolan, Institutt for Optometri (Prof. J.R.Bruehich).
Spain	Laboratorio de Optica, Universidad de Murcia, Spain (Prof. P. Artal) Universidad Complutense Madrid, Spain (Prof. Miguel Ángel Muñoz)
Scotland	Psychology Department, University of Glasgow, Scotland (Dr.D.Simmons)
Finland	Colour Research Laboratory, University of Joensuu (Prof. J.Parkkinen)

Germany	Institut für Arbeitsphysiologie an der Universität Dortmund
The Netherlands	Utrecht University (Prof. R. van Ee)
France	Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand (Dr.M.Colomb).

International projects.

Staff of laboratory participated in following international projects:

- Student and teacher exchange program ERASMUS between University of Latvia and Universidad Complutense Madrid, Escuela Universitaria de Optica and Institut für Arbeitsphysiologie an der Universität Dortmund;
- EU Program "ACCORD". Cooperation with Moscow State University Adaptive Optics laboratory;
- Latvian-France governmental program "OSMOSE".
"Visual performances in simulated and real adverse visibility to analyze traffic accidents and improve traffic safety". Cooperation with Clermont-Ferrand LRPC Fog Chamber.

THE MAIN RESULTS

FERROELECTRIC LIQUID CRYSTAL GLASSES FOR AMBLYOPIA RESEARCH

Sergejs Fomins, Maris Ozolinsh, Gunta Krumina, Varis Karitans
University of Latvia, 8 Kengaraga Str., LV-1063 Riga, Latvia

Ferroelectric Liquid Crystal (FLC) filters offer the speed of electronic light shutters and the vibration free operation. These characteristics make them ideal for applications requiring short exposure times and minimal blur, offering switching times of 0.002 of a second. FLC filters can be used as the optical shutter for machine vision purposes, also in vision research. On the basis of FLC filters we have developed ferroelectric glasses, allowing temporal differentiation of optical information for both eyes. In the case of amblyopia („lazy eye”) the only way to oblige the „lazy” eye to work is to close the other better-seeing eye. We advice the appliance for dynamic visual system training to promote the functionality of the worse-seeing eye. For fast switching the filters are powered by bipolar voltage power supply separate for two left and right channel switch optical isolation for higher safety reasons. The duration of the shutters open-close state are controlled through the PC parallel port. The main application of the system is use for amblyopia research and training.

LATVIAN AND RUSSIAN TEXTBOOKS: EYE MOVEMENTS IN READING TEXT FORMATTED IN TWO COLUMNS

Roberts Paeglis, Irina Gorshanova, Kristine Bagucka, Ivars Lacis
*Department of Optometry and vision science, University of Latvia
Inst.of Solid State Physics, University of Latvia*

Research of eye movements in reading textbooks suggests that reading the Cyrillic-based Russian language differs from reading the extended Latin-based Latvian texts. Ten bilingual students were asked to start reading a book passage in

Latvian and to continue reading the text in Russian. Key parameters in information processing have been analyzed. Even though the difference in duration of fixations does not reach statistical significance, saccade size and regression rate are smaller in Russian.

EYE MOVEMENTS DURING SILENT AND ORAL READING WITH STABILIZED VERSUS FREE HEAD MOVEMENT AND DIFFERENT EYE-TRACKERS

Roberts Paeglis, Inita Jokste, Kristine Bagucka, Ivars Lacis
Department of Optometry and vision science, University of Latvia
Inst. of Solid State Physics, University of Latvia

Eye movement research of reading has been done on a battery of eye-tracking setups during last decades. We compared reading data of the same group of six students, their eyes were tracked by a video-based helmet-mounted system with the data sampling frequency of 50 Hz and a setup with a chin-rest at 240 Hz. We found that not only the number of fixations may decrease after reading practice, but so does also the mean duration of fixations. In spite of the short duration of saccades, their distributions and changes in them are similarly reported in the two experimental conditions. Lack of significant correlation in the HED data testifies to the result variability due to measurement technique. We conclude that the head-free setup is applicable in reading research but has insufficient precision to track changes in reading patterns.

INTRAOCULAR LIGHT SCATTERING FROM DIFFERENT COLOUR STRAYLIGHT SOURCES

Gatis Ikaunieks, Maris Ozolinsh
Department of Optometry and vision science, University of Latvia
Inst. of Solid State Physics, University of Latvia

Important optical parameter of the eye is intraocular light scattering. To assess the effect of light scattering and stimulus colour on visual functions, visual acuity and retinal straylight were measured with and without light scattering occluder (polymer dispersed liquid crystal plate). For visual acuity measurements black Landolt optotypes on red, green and blue background were used. Retinal straylight was measured with a direct compensation method using the same colours. Light scattering for blue colour is the greatest in all light scattering conditions. Light scattering occluder changes spectral dependency of intraocular straylight – intraocular light scattering increases for green light and reduces for red light. These changes have no direct effect on visual acuity for coloured stimuli. One of the factors which causes the changes in spectral dependency is spectral transparency of occluder. Occluder has the greatest transparency for long wavelengths and smallest for short wavelengths. Another factor could be the changes in amount of light which penetrate through sclera and iris and which is important source of straylight for red light. To evaluate more this effect, additional studies of retinal straylight measurements with light projected directly on pupil and on iris are in progress.

ELECTRONIC EYE OCCLUDER WITH TIME-COUNTING AND REFLECTION CONTROL

V. Karitans¹, M. Ozolinsh¹, G. Kuprisha²
¹*Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., 1063 Riga*
²*Department of Optometry and Vision Science, University of Latvia*

In pediatric ophthalmology 2 – 3 % of all the children are impacted by a visual pathology – amblyopia. It develops if a clear image isn't presented to the retina during an early stage of the development of the visual system. A common way of treating this pathology is to cover the better-seeing eye to force the „lazy” eye to learn seeing. However, children are often reluctant to

wear such an occluder because they are ashamed or simply because they find it inconvenient. This fact requires to find a way how to track the regime of occlusion because results of occlusion is a hint that the actual regime of occlusion isn't that what the optometrist has recommended. We design an electronic eye occluder that allows to track the regime of eye occlusion. We employ real-time clock DS1302 providing time information from seconds to years. Data is stored in the internal memory of the CPU (EEPROM). The MCU (PIC16F676) switches on only if a mechanical switch is closed and temperature has reached a satisfactory level. The occlusion is registered between time moments when the infrared signal appeared and disappeared.

DYNAMICS AND ACCURACY OF EYE ABERRATION MEASUREMENTS

M.Ozolinsh, S.Fomins, and V.Karitans
University of Latvia

Deviations of the eye aberration terms that are determined using the Hartman-Shack wavefront sensors can be explained either due to methodological reasons: non-stability of the eye positioning, the validity criteria of the hartmanogram spots for the waveform reconstruction; or that can have physiological origins - eye tearfilm breakup process, feedback to keep eye in focus, breathing and heartbeats. We have studied eye aberrations using a fast (up to 30 frames per second) aberrometer "Multispot-2500" simultaneously together with records of the heart beat rhythmus. The Fourier and correlation analyses were applied to characterize the aberration dynamics during the tearfilm formation (first 2-3 sec after eye blinks) and to detect possible correlation of the aberration terms to various physiological factors. Spectral power analyze reveals inverse proportionality to frequency beyond 10 Hz. In some cases (for defocus and astigmatism terms) a maximum in the power spectrum is observed at frequencies close to arterial pulse frequency. However the correlation analyze does not reveal a clear correspondence of the heart beat and aberration time sequences. It is confirmed that the accurate determination of the aberration terms is possible after statistical processing of high speed measurements done between two sequent eye blinks.

SUMMATION OF RETINAL AFTER-EFFECTS AND CORTICAL MECHANISMS IN CONTRAST ADAPTATION

Didzis Lauva¹, Maris Ozolinsh²

¹*Department of Optometry and Vision Science, University of Latvia*

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We investigated perception of Gabor gratings after adaptation to high contrast gratings. Four symmetrically positioned achromatic and R, G and B adaptation Gabor stimuli were presented for 8 sec on a monitor. After that a lower contrast test stimulus – one Gabor grating of the same spatial frequency and direction - was presented spatially coinciding with one of the previously demonstrated gratings of the adaptation stimuli. Subjects had to detect the position of the test stimulus. We measured two time parameters: the time of recovery of retinal after effects (RRA) and the instant of appearance of the test stimuli (ATS time). When test and adaptation gratings were spatially in-phase, we observed a weak diminishing of RRA (0.6-0.8s) and a pronounced decrease in ATS times (7 to 2s) when the contrast of the test stimuli increased up to 70%. When test and adaptation gratings were spatially in counterphase (*i.e.*, the retinal aftereffect image in phase with the modulation of the test stimuli attenuated by adaptation) RRA time revealed a slight increase with the test stimulus contrast. To separate cortical mechanisms and retinal effects in contrast adaptation, red and green colour filters were used for the right and left eye, and adaptation and test stimuli were presented - red and green, correspondingly. Thus the right eye was contrast adapted, but the ATS time was measured for the non-adapted left eye only. Results were qualitatively similar

to the tests mentioned previously, confirming the high contribution of cortical mechanisms in contrast adaptation. Measurements for monochromatic (R,G,B) stimuli did not reveal significant differences in ATS and RRA time values.

LIGHT SCATTERING EFFECT ON COLOR PATTERN VEP RESPONSE

G.Ikaunieks, M.Ozolinsh, and S.Fomins

University of Latvia

To assess the effect of light scattering on colour pattern VEP (CP-VEP), the quality of stimuli was reduced with a light scattering occluder. The results were compared with results of visual acuity and retinal stray light measurements. In CP-VEP studies white-black, red-black, green-black and blue-black gratings were used. For visual acuity measurements black Landolt optotypes on the coloured backgrounds were used. Retinal stray light was measured with a compensation comparison method (Van den Berg, T.J.T.P. et al, 2005, IOVS, 46:ARVO, E-Abstract, 4315).

We found good correlation between CP-VEP and psychophysical visual acuity test results. Our results show, that reduction of different colours stimuli perception due to light scattering is not related only with the presence of retinal stray light effect in the eye and physiological behaviour of spatially organized neural receptive fields should be taken into account.

THE PERCEPTION OF ISOLUMINANT COLOURED STIMULI OF AMBLYOPIC EYE AND DEFOCUSED EYE

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University of Latvia, Kengaraga St. 8, 1063 Riga, Latvia

In routine eye examination the visual acuity usually is determined using standard charts with black letters on a white background, however contrast and colour are important characteristics of visual perception. The purpose of research was to study the perception of isoluminant coloured stimuli in the cases of true and simulated amblyopia. We estimated difference in visual acuity with isoluminant coloured stimuli comparing to that for high contrast black-white stimuli for true amblyopia and simulated amblyopia. Tests were generated on computer screen. Visual acuity was detected using different charts in two ways: standard achromatic stimuli (black symbols on a white background) and isoluminant coloured stimuli (white symbols on a yellow background, grey symbols on blue, green or red background). Thus isoluminant tests had colour contrast only but had no luminance contrast. Visual acuity evaluated with the standard method and colour tests were studied for subjects with good visual acuity, if necessary using the best vision correction. The same was performed for subjects with defocused eye and with true amblyopia. Defocus was realized with optical lenses placed in front of the normal eye. The obtained results applying the isoluminant colour charts revealed worsening of the visual acuity comparing with the visual acuity estimated with a standard high contrast method (black symbols on a white background).

SPECTRAL AND TEMPORAL CHARACTERISTICS OF LIQUID CRYSTAL GOGGLES FOR VISION RESEARCH

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²*Chalmers TH, Göteborg, Sweden*

Spectral and switching characteristics of two manufacturer liquid crystal goggles are tested. Experimentally the human stereovision acuity and threshold were studied for the case, when one

eye random dot stereo stimulus simulated on the display is continuously blurred or the stimulus contrast is decreased. In order to determine the artefacts of two eye channel crosstalk on the stereostimuli separation the contrast ratio limits for the computer display phosphors wavelengths are determined.

Scientific Publications

1. S. Fomins, M.Ozolinsh, G.Krumina, and V.Karitans. Ferroelectric liquid crystal glasses for amblyopia training. *Integrated Ferroelectrics*, V.103, pp.10-17 (2009).
2. J. M. Bueno, M. Ozolinsh, and G. Ikaunieks, „Scattering and Depolarization in a Polymer Dispersed Liquid Crystal Cell,” *Ferroelectrics*, V.370, pp.18-28 (2008).
3. G. Ikaunieks and M. Ozolinsh. Effect of Light Scattering Simulation in the Eye on Different Color Stimuli Perception. *Proc. IFMBE*, V.20, pp.367-370 (2008).
4. R. Paeglis, A. Spunde, A. Klavinsh, L. Vilkausha, and I. Lacis. Eye Kinematics of Athletes in Non-Familiar Sports Situations. *Proc. IFMBE*, V.20,, pp.146-149 (2008).
5. R. Paeglis, A. Kotelnikovs, A. Podniece, and I. Lacis .What Conclusions does Rapid Image Classification by Eye Movements Provide for Machine Vision? *Proc. IFMBE*, V.20, pp.299-302 (2008).
6. V. Karitans, M. Ozolinsh, and G. Kuprisha. Electronic Eye Occluder with Time-Counting and Reflection Control. *Proc. SPIE* , V.7142 (2008).
7. R. Paeglis, I. Gorshanova, K. Bagucka, and I. Lacis. Latvian and Russian Textbooks: Eye Movements in Reading Text Formatted in Two Columns. *Proc. SPIE* , V.7142 (2008).
8. R. Paeglis, I. Jokste, K. Bagucka, and I. Lacis. Eye Movements During Silent and Oral Reading with Stabilized Versus Free Head Movement and Different Eye-Trackers. *Proc. SPIE*, V.7142 (2008).
9. G. Krumina, M. Ozolinsh, G. Ikaunieks. The Perception of Isoluminant Coloured Stimuli of Amblyopic Eye and Defocused Eye. *Proc. SPIE* , V.7142 (2008).
10. S.Fomins, M.Reinfelde, A.Larichev, N.Iroshnikov, A.Gerbreders, M.Ozolinsh Photoinduced AsSeS Thin Film Phase Plates as Adaptive Optics Mirrors for Eye Aberration Correction. *Proc. SPIE* , V.7142 (2008).
11. G.Ikaunieks, M.Ozolinsh, and S.Fomins. Factors Affecting Intraocular Light Scattering from Different Color Straylight Sources. *Proc. SPIE* , V.7142 (2008).
12. S Fomins. Masking Study of Instant Stimuli Texture Segmentation. *Perception*, V.37, S80(2008).
13. M. Ozolinsh, G. Andersson, G. Krumina, and S. Fomins. Spectral and Temporal Characteristics of Liquid Crystal Goggles for Vision Research. *Integrated Ferroelectrics*, V.103, pp.1 – 9 (2009).

Lectures on conferences

Results are presented in conferences.

1. **International Baltic Sea Region conference "Functional materials and nanotechnologies"**. April 1-4, 2008, Riga, Latvia.
2. **14th Nordic-Baltic Conference on Biomedical Engineering and Medical Physics: NBC 2008**. 16-20 June 2008. Riga, Latvia.
3. „**Developments in Optics and Communications**”, Riga, April 24 - 26, 2009.
4. **4th European Meeting in Visual & Physiological Optics**. Heraklion, Crete, 31 Aug.-2 Sept., 2008.
5. **The 6th International Conference "Advanced Optical Materials and Devices"**, 24-27 August 2008, Riga, Latvia.
6. **ECVP-2008**. Utrecht. The Netherlands, Aug. 2008.
6. Annual **OSA-Vision**, Rochester, Oct. 2008.
7. **13th Applied Vision Association Meeting**, Bristol, Dec. 2008.

LABORATORY OF WIDE BAND GAP MATERIALS

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

Research Area and Main Problems

The research interests of the Laboratory of Wide Band Gap Materials are focused on spectral characterization of compounds formed from the III-V group elements (AlN, h-BN) and some related materials such as Al₂O₃. Recently it was shown that some optical properties of nitride compounds are prospective for its application as new UV light and visible light emitters (Watanabe, Taniguchi), besides, features of AlN could rate it among materials available for UV light dosimetry (our results). Presently different forms of these materials are synthesized including a bulk material and its nanostructured forms and it is also known that their optical properties could be different. The interests of our research are largely focussed on revealing of the difference between the optical properties of the bulk material and its nanostructured forms. The spectral investigations performed in this laboratory are based on luminescence studies (photoluminescence (PL) and its excitation (PLE), optically stimulated luminescence (OSL) and thermo-luminescence (TL)) including also optical absorption. This complex can give essential information about the defects and optical properties of the material, containing revealing of light-induced processes, luminescence mechanisms, energy accumulation and its release mechanisms. These problems could be prevalently related to the fundamental physics. In the field of innovations the interests are focussed on application of AlN and related-materials for the UV light dosimetry and h-BN – as light emitter; AlN and Al₂O₃ seems to be prospective for elaboration of new luminescent materials for energy saving compact luminescent lamps. Part of investigations was performed together with the collaboration partners from abroad.

Scientific Staff:

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

Students - Technicians:

1. D.Jakimovica (assistant)

Collaborations

Latvia

Institute of Inorganic Chemistry, Riga TU (Dr. E.Palcevskis, Prof. J.Grabis)

Institute of Solid State Physics, University of Latvia, Lab. of Nonlinear Processes Theory, (Prof. Y.Zhukovskii, Dr. S.Piskunov)

France

University of Nice-Sophia Antipolis, Nice (Prof. M.Benabdesselam, Prof. P.Iacconi)

USA

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

Wake Forest University, Center of Nanotechnologies, Winston-Salem (Prof. D. Carroll).

Belarus

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

Italy

INFN-Laboratori Nazionali di Frascati, Italy (Prof. S.Bellucci)

THE MAIN RESULTS

LUMINESCENCE PROPERTIES OF Al_2O_3 BULK AND NANOSIZE POWDERS

L.Trinkler, B.Berzina, D.Jakimovica

Photoluminescence (PL) and thermoluminescence (TL) have been studied in the alumina (Al_2O_3) bulk and nanosize powders irradiated with UV light. The PL and TL properties of the studied alumina powders are determined mainly by presence of impurity defects (iron, chromium and titanium ions). Intrinsic and surface defects also contribute to the luminescence processes. PL spectra of both bulk and nanosize powders consist of two broad complex emission bands (300-600 nm and 650-900nm), containing overlapping bands of different origin. The study of thermal evolution of PL in the range of 300-7 K has shown that with the decrease of temperature 1) PL intensity increases by factor of 2 to 4, 2) relative yield of emission bands changes, 3) the long wavelength band becomes resolved into fine structure. Analysis of these features help to ascribe emission subbands to definite defects taking part in the luminescence process. At low temperatures the decisive role of the surface defects in nanosize alumina powder becomes ever more pronounced. The studies of the luminescence processes in alumina powders are in progress. Materials used for investigation are synthesized in Institute of Inorganic Chemistry RTU (Dr J. Grabis).

SPECTRAL CHARACTERIZATION OF MULTI-WALLED h-BN NANOTUBES AND ITS RAW MATERIAL - BULK h-BN POWDER

B. Berzina, L.Trinkler, V.Korsak, R.T.Williams¹, B.Ucer¹, D.Carroll², S.Bellucci³

¹ *Department of Physics, Wake Forest University, USA*

² *Center of Nanotechnologies, Wake Forest University, USA*

³ *INFN-Laboratori Nazionali di Frascati, Italy*

Photoluminescence (PL) spectra of h-BN powder and multi-walled BN nanotubes made from this powder were investigated. A similarity of complex luminescence spectra was found for both the BN nanotubes and its raw material – h-BN powder. Three main spectral groups can be distributed from the complex luminescence spectra. It was established that the first group around 300 nm presents a phonon-induced fine structure and could be related to the intrinsic luminescence of carbon impurity characterizing the bulk material. The second group of spectra around 400 nm also presents the phonon-induced sub-structure. According to our previous results and literature data the 400 nm luminescence could be related to the excitonic processes influenced by some sorts of defects such as nitrogen vacancies and appropriate luminescence centers could be related to the bulk material. The third part from the luminescence spectra forms a wide structureless band around 500 nm and its intensity and maximum location highly depend on previous treatment of material: ageing, previous irradiation with UV light, heating etc. It allows conclusion that this luminescence is caused by surface defects. All these spectral groups are common for both the macrosized h-BN powder and nanomaterial, nevertheless, a ratio of luminescence intensities characterizing these spectral groups is different for both the bulk and nanomaterial. In the nanomaterial the 400 nm luminescence is predominant.

Currently the low temperature luminescence (beginning from 7 K) is investigated. The same spectral groups mentioned above are observable also at low temperatures and the fine structure of 300 nm and 400 nm bands is better pronounced than at room temperature. These investigations are in progress.

All of the photoluminescence investigations were performed in ISSP University of Latvia; the infrared (IR) light absorption measurements were performed in INFN National Laboratory Frascati, Italy; the bulk and nanomaterial samples were made in Center of Nanotechnologies, Wake Forest University, USA.

Scientific Publications

1. B Berzina, L Trinkler, D Jakimovica, V Korsaks, J Grabis, I Steins, E Palcevskis, S Bellucci, Li-Chyong Chen, Surojit Chattopadhyay, and Kuei-Hsien Chen. „*Spectral characterization of bulk and nanostructured AlN*”. Journal of Nanophotonics 3 (2009) 0031950.
2. Yu.F.Zhukovskii, S.Piskunov, N.Pugno, B.Berzina, L.Trinkler, S.Bellucci. "Ab initio simulations on the atomic and electronic structure of single-walled BN nanotubes and nanoarches" Journal of Physics and Chemistry of Solids 70 (2009) 796-803.
3. Yu. F. Zhukovskii, S. Bellucci S. Piskunov, L. Trinkler and B. Berzina "Atomic and electronic structure of single-walled BN nanotubes containing N vacancies as well as C and O substitutes of N atoms" European Physical Journal B67 (2009) 519-525.
4. L. Trinkler, B. Berzina, D. Jakimovica, J. Grabis, I. Steins „UV light induced luminescence processes in Al₂O₃ bulk and nanosize powders”. Optical Materials (accepted).

Lectures on Conferences

25th LU Scientific Conference of Institute of Solid State Physics, University of Latvia, February 11-13, 2009, Riga, Latvia

1. V.Korsaks, B.Berzina, L.Trinklere, D.Jakimovica. “*Phonon structure of luminescence spectra of h-BN powder and nanomaterial*”. Book of Abstracts, 2009 p. 82.
2. D.Jakimovica, L.Trinklere, B.Berzina. “*Termoluminescence of Al₂O₃ macrosize and nanosize powders*”. Book of Abstracts, 2009 p. 83.

International Baltic Sea Region Conference Functional Materials and Nanotechnologies (FM&NT), March 31 - April 3, 2009, Riga, Latvia

3. V.Korsaks, B. Berzina, L. Trinkler, R.Williams, B.Ucer, and D.Carroll, S. Bellucci, and M.Piccinini. „*Phonon structure of luminescence spectra of hexagonal BN and multiwalled BN nanotubes*”. Book of Abstracts 2009, p. 114.
4. L. Trinkler, B. Berzina, D. Jakimovica, J. Grabis, I. Steins. „UV light induced luminescence processes in Al₂O₃ bulk and nanosize powders”. Book of Abstracts 2009, p. 46.

7th international Conference on Luminescent Detectors and Transformers of Ionizing Radiation (LUMDETR 2009), 12-17 July, 2009, Krakow, Poland.

5. V.Korsaks, B.Berzina, L.Trinkler, R.T. Williams, K,B, Ucer. „*Luminescence and its possible mechanisms in bulk h-BN powder and BN nanotubes.*” Book of Abstracts 2009, p.149.

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 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 with EDX option, XRD and optical microscopy.

Main research topics in 2009

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

Scientific Staff

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

Technical Staff

A.Petersons

PhD Students

Mg.Phys.G.Bakradze

Students

1. B.sc.R.Zabels
2. B.sc.R.Lisovskis

Scientific visits abroad

1. Dr.F.Muktepavela, Chernogolovka, ISSP, Moscow (12 days)

Visitors from Abroad

1. Dr.V.Sursajeva, ISSP, Chernogolovka, Russia (2 weeks).

Cooperation

Latvia

Daugavpils University (Dr. E.Tamanis).

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

Riga Technical University (Prof.V.Mironovs).

Germany

GSI, Darmstadt (Prof. K.Schwartz).

France

CIRIL, Caen (Prof. M.Toulemonde).

Israel

Technion, Haifa (Dr.S.Stolyarova).

Russia

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

Bulgaria

University of Chemical technology and Metallurgy, Sofija (Dr.P.Petkov).

THE MAIN RESULTS**PROPERTIES OF ZnO COATINGS OBTAINED BY
MECHANOACTIVATED OXIDATION**

F. Muktepavela¹, G. Bakradze¹, L.Grigrorjeva¹, R.Zabels¹, E. Tamanis²

¹*Institute of Solid State Physics, University of Latvia*

²*Daugavpils University*

A simple and cost-effective mechanoactivated oxidation method (MAOM) has been developed for obtaining ZnO coatings on glass. To achieve the transparency of initially opaque mechanoactivated ZnO coatings they were annealed at the temperatures modifying the surface morphology of nanostructured coatings. Investigation of nanomechanical properties revealed that MAOM coatings in as-obtained state have higher hardness (up to 3 GPa) as compared with bulk metallic zinc (160 MPa). In the annealed state the coatings showed stable high adhesion with glass, with the ability to form a grained structure (hardness 8-10 GPa) or a whiskers nanostructure (hardness 18-20 GPa). The Young modulus of coatings ranged from 80 to 120 GPa. The optical properties of ZnO films with a whiskers structure are typical for a transparent high-quality ZnO single crystal. The high intensity luminescence band at 3.26 eV (blue luminescence) is LO-phonon associated free exciton luminescence (1LO-Ex). In spectra measured at 12K the main band is due to the exciton bound at neutral donor (ExD⁰) and its phonon replica (1LO_ExD⁰). PL intensity related to oxygen vacancies was very low.

The obtained coatings have high electrical resistance, which decreases in response to the UV exposure. The photocurrent increases by two orders of magnitude, which is easily detectable and makes it possible to use these coatings for creating relatively easily manufacturable UV – emission detectors.

**NANOSTRUCTURING AND HARDENING OF LiF CRYSTALS
IRRADIATED WITH 3-15 MeV Au IONS**

I.Manika¹, J.Maniks¹, R.Grants¹, R.Zabels¹, K.Schwartz², M.Sorokin³

¹*Institute of Solid State Physics, University of Latvia*, ²*GSI, Darmstadt, Germany*,

³*Russian Research Centre “Kurchatov Institute”, Moscow, Russia*

The change of structure and micromechanical properties of LiF single crystals irradiated with 3-15 MeV Au ions at 10^{12} - 10^{14} ions/cm² has been studied using AFM and nanoindentation techniques. The nanoindentation shows remarkable (up to 160%) ion-induced increase of hardness typical for the aggregation stage of radiation defects. The thickness of hardened layer coincides with the range of Au ions in LiF calculated using SRIM 2008. In contrast to GeV ions, which deposit their energy

mainly by inelastic interactions with target electrons, thereby causing excitation and ionization processes, the MeV ions deposit a significant fraction of their energy by elastic collisions with the target atoms. The depth profile of hardness correlates with that for total energy loss (Fig.1) thus indicating that both the elastic and electronic mechanism contribute the hardening. AFM studies revealed generation of dislocations and nanostructuring in irradiated layer where columnar grains with a cross-section of 100-150 nm were observed. The annealing experiments showed an increase of the thermal stability of ion-induced modifications with increasing the fluence and beam current density. Accordingly, formation of colloids and other thermally stable aggregates is promoted under conditions of high ion fluence and flux as it was established earlier by optical absorption spectroscopy

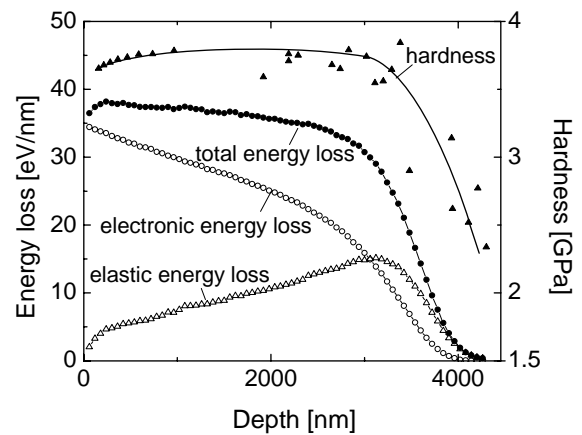


Fig.1 Depth profiles of hardness and energy loss of ions in LiF crystal irradiated with 15 MeV Au ions at a fluence of $5 \times 10^{13} \text{ cm}^{-2}$

Scientific publications

SCI publications

1. I.Manika, J.Maniks, M.Toulemonde, K.Schwartz. Dislocation mobility study of heavy ion induced track damage in LiF crystals.- *Nuclear Instruments and Methods in Physics Research B* 267 (2009) 949–952
2. M. Shorohov, F. Muktepavela, L. Grigorjeva, J. Maniks, D. Millers. Surface processing of TlBr single crystals used for radiation detectors.. *Nuclear Instruments and Methods in Physics Research A* 607 (2009) 120–122.
3. F. Muktepavela, G. Bakradze, L. Grigorjeva, R. Zabels, E. Tamanis. Properties of ZnO coatings obtained by mechanoactivated oxidation. *Thin Solid Films* 518 (2009) 1263-1266.

Other publications

4. R.Zabels, F.Muktepavela, M. Chubarov Nanomechanical properties and possible applications of mechanoactivated ZnO coatings. *Latvian Journal of Physics and Technical Sciences*, 3 (2009) p.55-63.
5. F Muktepavela., G.Bakradze, R. Zabels. The role of interphase boundaries in the deformation behaviour of fine-grained Sn–38wt.%Pb eutectics. *Latvian Journal of Physics and Technical Sciences*, 1 (2009)33-43.
6. R. Krishbergs, E. Ligere, F. Muktepavela, E. Platacis, A. Shishko, A. Zik. Experimental studies of the strong magnetic field action on the corrosion of RAFM steels in Pb17Li melt flows. *Magnetohydrodynamics* 45, No. 2, (2009) 289-296.
7. K.Kravalis, F.Muktepavela, E.Platacis, A.Shishko Experimental results on the magnetic field influence on the corrosion of EUROFER steel in Pb17Li flow. Proc.6th Int.Conf. Electromagnetic Processing in Materials Dresden, Oct. 19-23. 2009, pp. 473-475.
8. V.Mironovs, F.Muktepavela, E.Mihailova, V.Filipovs. Ligatūra un tās izgatavošanas paņēmieni. Latvijas patents Nr.13980, publ.20.11.2009 (Pieteicējs RTU).

Lectures on Conferences

5th International Conference “Diffusion in Solids and Liquids; Nanodiffusion and Nanostructured Materials DSL-2009”, Italy, Rome, June 24-26, 2009.

1. F.Muktepavela, R. Zabels. The role of diffusion accommodation and phase transformation in the deformation behaviour of the interphase boundaries in ultrafine grained Sn-Pb eutectic. Abstracts p. 50 (oral)

International conference “Functional Materials& Nanotechnologies (FM&NT-2009), Riga, Latvia, March 31- April 3., 2009.

2. R.Zabels, F. Muktepavela, L. Grigorjeva, E. Tamanis, M. Mishels-Piesins. Nanoindentation and photoluminescence characterisation of ZnO thin films and single crystals.. Abstracts p. 60 (oral)
3. I.Manika, J.Maniks, R.Zabels, J.Gabrusenoks, M.Tomut, K.Schwartz.. Nanoindentation study of graphite irradiated with swift ^{238}U ions. Abstracts p. 92 (oral).

5th Intern Student Conf “ Developments in Optics and Communications” DOC-, Riga, April 24-26, 2009

4. R. Zabels, F.Muktepavela, M. Cubarovs. Nanomechanical properties and possible applications of mechanoactivated ZnO coatings. Abstracts p. 21 (oral).

Международ. Симпозиум „ Перспективные материалы” Витебск, Беларусь 25-29 мая, 2009

5. Страумал Б., Внуков В.И., Калниньш Я., Шотанов Ф,Е., Аслунд А.,Костюченко В.Г., Первезенцев В.Н., Муктепавела Ф.О., Сурсаева В.Г. Сплавы Cu-Zn-Pb , Sn-Pb для реставрации старинных органов., Сб-к тезисов с. 183 .

Международ. Симпозиум * Перспективные материалы* Витебск, Беларусь 25-29 мая 2009

6. Муктепавела Ф., Сурсаева В.Г. Исследование деформационного поведения границ в мелкодисперсной Sn-Pb эвтектике и поликристаллическом Zn методом наноиндентирования., Сб-к тезисов с. 184. (oral)

6th International conference “Electromagnetic Processing in Materials ,Dresden, Oct. 19-23. 2009”.

7. K.Kravalis, F.Muktepavela, E.Platacis, A.Shishko Experimental results on the magnetic field influence on the corrosion of EUROFER steel in Pb17Li flow (oral).

25th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 11-13, 2009.

8. R.Zabels, F.Muktepavela, L.Grigorjeva, E.Tamanis. Evolution of structure during annealing and nanomechanical characterization of ZnO films. Abstracts p.63 (oral).

DEPARTMENT OF RADIATION PHYSICS

Head of laboratory Dr. habil. J.Berzins

Research Area and Main Problems

The Department includes two research groups – the Laboratory of nuclear reactions and Laboratory of Transition Metals Compounds Physics. The following main investigations are developed in the department:

- experimental and theoretical investigation of nuclear structure at medium and high excitation energies;
- development of the nuclear spectral 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;
- iron group ions in inorganic and organic compounds are studying by the optical absorption, luminescence;
- EPR and Raman spectroscopies the magnetic ions exchange interaction in the antiferromagnetic oxides MeO-MgO solid solutions were studied using of optical absorption, luminescence;
- EPR and Raman spectroscopies exchange interaction between radiation defects and transition metals ions in the dielectric crystals doped with the transition metals ions;
- retrospective biodosimetry.

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

- | | |
|--------------------------------|---|
| 1. Dr.hab. J.Berzins | 8. Dr. D.Riekstina |
| 2. Dr.hab. M.Balodis | 9. Dr. V.Skvortsova |
| 3. Dr.hab.V.Bondarenko | 10. Dr. O.Veveris |
| 4. Dr.hab. A.Afanasjevs | 11. Dr.Ing. A.Pavlenko |
| 5. Dr.hab. N.Mironova - Ulmane | 12. Mag. M.Polakovs |
| 6. Dr. L.Simonova | 13. LU PhD student, Mag.phys. J. Proskurins |
| 7. Dr. T. Krasta | 14. LU PhD student, Mag.phys. A. Andrejevs |

Technical Staff

1. S.Afanasjeva

Students

1. D. Magone
2. K. Bavrins

Scientific visits abroad

Dr. hab. J. Berzins, European Commission Euratom, Brussels,Belgium (10 days).

Dr. hab. J. Berzins, Cyclotron Workshop, Ispra, Italy (3 days).

Dr. hab. J. Berzins, 41. Tagung des FS “Leben mit Srahlung – von den Grundlagen zur Praxis” Alpbach, 21 – 25 September, 2009.

Dr. D. Riekstina, 41. Tagung des FS “Leben mit Srahlung – von den Grundlagen zur Praxis” Alpbach, 21 – 25 September, 2009.

Dr. hab. J. Berzins, International Symposium on Gamma spectroscopy Oslo, 15 -16 September 2009.

Dr. D. Riekstina, International Symposium on Gamma spectroscopy Oslo, 15 -16 September 2009.

J. Berzins, Cyclotron Networking Meeting, Ispra, Italy, 3-5 December, 2009.

Cooperation

Latvia

1. Medical Academy of Latvia (Dr.hab., Prof. M.Eglite, Dr. hab. Prof. I. Cema, Dr.T.Zvagule).
2. Hazardous Waste Management State Agency “BAPA”.
3. Radiation Safety Center (I. Kisite)
4. Riga Technical University, Institute of Inorganic Chemistry (Dr. I.Vitina,).
5. University of Latvia, Chemical faculty (Dr. A.Viksna,)
6. Institute of Wood Chemistry (Dr. hab. G. Dobele, Dr.hab. G. Telesheva, Dr.hab.T.Dizbit)
7. Riga Technical University, Faculty of Material Science and Applied Chemistry (Dr.Berzina-Cimdina r).
8. National Diagnostic center.
9. Institute of Technical Physics, Rīga Technical University (Dr.J.Ruža).

USA

1. Lawrence Livermore National Laboratory, California (Prof. R. W. Hoff).
2. Brookhaven National Laboratory, Upton (Prof. R.F. Casten).

Germany

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

Brasil

1. Instituto de Fisica Teorica, Universidade de Sao-Paulo (Dr.Castilho-Alcaras).

Lithuania

1. Institute of Theoretical Physics and Astronomy, Vilnius (Dr.O.Katkevičius)

France

1. Institute Laue-Langevin, Grenoble, France (Prof. H. Börner, Dr. M. Jentchel).

Canada

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

Czech Republik

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

Estonia

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

Italy

1. Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Frascati (M. Cestelli Guidi, A. Marcelli)

2. Dipartimento di Scienze Geologiche, Università Roma Tre, Rome (M. Piccinini)
3. INFN and Dipartimento di Fisica, Università di Trento, Povo (Trento)(G.Mariotto)
4. INFN and Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (Cosenza) (E.Cazzanelli)

Ukraine

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

Russia

1. Ural State University, Ekaterinburg (Prof. A. Nikiforov).
2. Ural Technical University, Ekaterinburg (Prof. B.Shulgin)
3. St.Petersburgh Nuclear Physics Institute, Gatchina (Dr.V.Bunakov, Dr.A.Sushkov)
4. Institute of Metal physics . Yekaterinburg (prof. Goscitkii).

Denmark

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

THE MAIN RESULTS

DEVELOPMENT OF THE ^{188}Re NUCLEUS LEVEL SCHEME USING THE $(n,\gamma\gamma)$ -REACTION DATA

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

Low-high and low-low energy $\gamma\gamma$ -coincidences, following the $^{187}\text{Re} (n,\gamma) ^{188}\text{Re}$ reaction with thermal neutrons, have been measured at the research reactor in Rež near Prague. The target was made of 500 mg rhenium with enrichment to 97.5% of ^{187}Re . The γ -ray spectra in the energy range from 50 to 2600 keV and from 4500 to 6500 keV have been recorded using 28% HpGe detector and 25% Ge(Li) detector. The analysis of measurement results allowed to obtain energies and possible quantum characteristics (spins and parities) for 134 ^{188}Re excited levels in the energy range up to 1590 keV. The previously known (E.B.Shera et al, 1972) level scheme of the odd-odd nucleus ^{188}Re has been essentially corrected and extended. The proposed level scheme of ^{188}Re contains 61 levels up to ~ 800 keV excitation energy, including 20 levels, which are completely new, and 11 levels with changed interpretation. The complete level scheme for up to ~ 400 keV energy and spins ≤ 5 is obtained and supported by the results of two-quasiparticle rotational-vibrational interaction model calculations. The theoretically predicted level scheme up ~ 1 MeV excitation energy has been obtained. Some ^{188}Re states display features indicating the nuclear shape phase transition from the strong axial-deformation to the γ -soft form.

STUDY OF NUCLEAR STRUCTURE EFFECTS DUE TO THE NUCLEON ISOSPIN SYMMETRY

T.Krasta

The properties of light $Z \sim N$ nuclei in the $4 \leq A \leq 40$ region have been studied in the frameworks of microscopic Strictly Restricted Dynamics Model (SRDM), which employs for the classification of nuclear states the supermultiplet scheme. For the determination of parameters of effective NN-potential including central, vectorial and tensor terms, the calculated values of nuclear binding energies and energies of levels, belonging to the pseudo-bands of the ground SU(3)-configuration, have been fitted to the experimental binding energies and low-lying level energies of even-even ($Z=N$ and $Z=N\pm 2$), odd ($Z=N\pm 1$) and odd-odd ($Z=N$) nuclei, which form isospin singlets ($T=0$), doublets ($T=1/2$) and triplets ($T=1$). The SRDM values for nuclear binding energies, Coulomb

energy displacements, nuclear symmetry energy shifts, low-lying level spectra, electric quadrupole and magnetic dipole moments, as well as the B(E2) and B(M1) reduced transition probabilities have been compared with the predictions of other model approaches (shell model, collective model, boson model). It was found that many effects, which are traditionally related with collective excitations of the core (rotations and vibrations) and single particle motion in the nuclear mean field, can be successfully reproduced in the frameworks of microscopic approach based on SU(3) classification scheme.

THE USE OF SYMMETRY AND CHAOS CONCEPTIONS FOR THE STUDY OF NUCLEAR PHASE TRANSITIONS

J.Proskurins, T.Krasta, K.Bavrins, A.Andrejevs

The behavior of statistical and dynamical quantum chaos criteria (level spacing distributions, wave function entropy and fragmentation of basis states) in the vicinity of nuclear shape phase transitions has been studied in the frameworks of interacting boson model (IBM-1) and collective rigid triaxial rotator models. Quantum chaos calculations have been performed employing the Bravin-Fedorov triaxial rotator model, which considers both quadrupole shape parameters β and γ . The results have been compared with previously obtained results of calculations using Davidov model, where only the triaxiality angle γ is taken into account. Also, the study of quantum chaos criteria in the frameworks of complete IBM-1 version, when the boson interaction terms are taken into account, have been performed, employing the catastrophe theory approach for the analysis of phase transitions between different nuclear shapes, corresponding to IBM-1 limiting cases (U(5), O(6) and SU(3)). The dependence of dynamical nuclear chaos criteria from the nuclear shape quadrupole deformation parameters β and γ have been analyzed using the Peres lattice method.

RADIATION CONTROL OF SOME CONTAMINATED TERRITORY OF LATVIA

J.Berzins, D.Riekstina, O.Veveris, J.Malnacs¹
¹*Radiation Safety Centre, Latvia*

Control of radioactive contaminated territory and monitoring of artificial radionuclide Cs-137 and Ra-226 in the soil and tritium in the groundwaters around the potentially most polluted regions of Latvia was carried out: in the areas of the shut-down (1998) Salaspils research nuclear reactor, the radioactive waste repository "Radons" and one of the former medical facilities.

The pollution by radium-226 and its decay products in the rooms, sewage and special ventilation systems of the former medical facility as well as the migration of pollution in the soils around this object was investigated. The total area of the facility occupies 3525 m². The laboratory building and five more auxiliary buildings are located there in this territory. The special purpose laboratory in Dubulti was originally established as radon production facility at the beginning of the seventies of the 20th century, which supplied medical and rehabilitation institutions of the Baltic region with Rn-222 solution. Several accidents occurred during the operational period of the laboratory. Those accidents and minor incidents resulted in radium contamination. In 1994 experts shut down the laboratory.

RAMAN MICROSPECTROSCOPY OF HAEMOGLOBIN

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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 bands [1]. In this work, we report the application of the Raman technique to study Hb using three different laser excitation lines (441.6, 514.5, 830 nm). The Raman spectra of the hemoglobin in single erythrocytes were recorded on "Nanofinder-S" using the 441.6 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. The 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 [2]. We observed the unusual enhancement of several bands in Raman scattering spectra of hemoglobin at excitation line 830 nm compared with the 441.6 and 514.5 nm wavelengths investigated. The origin of unusual enhancement of Raman scattering bands of hemoglobin will be discussed.

1. Streckas, T. C. & Spiro, T. G. *Biochim. Biophys Acta* 263, 830-833 (1972)
2. Abe M, Kitagawa T, Kyogoku K. *J. Chem. Phys.* 1978; 69: 4526.

PHONON AND MAGNON EXCITATIONS IN BULK AND NANOSIZED NICKEL OXIDE

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J. Grabis³ V. I. Voronin⁴

¹*Latvian State Institute of Wood Chemistry,*

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

Raman spectra were measured at room temperature through 50 \times microscope objective using Renishaw inVia micro-Raman spectrometer equipped with argon laser (514.5 nm, max cw power $P_{\text{ex}}=10$ mW). The spectral signal was dispersed by the 2400 grooves/mm grating onto Peltier-cooled (-60°C) CCD detector. The rhombohedral distortion of the crystal structure and the presence of magnetic ordering at room temperature have been confirmed in all samples by x-ray and neutron diffraction.

The room temperature Raman spectrum for bulk NiO consists of several bands: a one-magnon (1M) band at ~ 34 cm^{-1} (not shown in the figure); five vibrational bands – one-phonon (1P) TO at 440 cm^{-1} and LO at 560 cm^{-1} modes, two-phonon (2P) 2TO at 740 cm^{-1} , TO+LO at 925 cm^{-1} and

2LO at 1100 cm^{-1} modes; a two-magnon (2M) band at $\sim 1500\text{ cm}^{-1}$. The frequency and shape of the phonon bands do not vary with temperature, whereas the magnon scattering intensities are strongly temperature dependent - they shift to lower frequencies and decrease in intensity with increasing temperature, disappearing completely close to the Néel point. More accurate Raman studies suggest unambiguously the presence of an additional band at about 200 cm^{-1} . To our knowledge, this band was not observed previously, and the interpretation of its origin requires reassessment of the lattice dynamics calculation for bulk NiO, performed previously only for cubic *Fm-3m* phase. Note that in the cubic phase the first-order Raman scattering is forbidden by symmetry selection rules and no phonon density of states (DOS) is present at Γ -point around 200 cm^{-1} . We have performed the lattice dynamics simulation for NiO using the shell model [20], in which an Ni and O ions were described by a core and a shell having the electronic charges and coupled by the harmonic spring. In the *R-3m* phase two modes (E_g and A_{1g}) at 361 and 527 cm^{-1} are Raman active, corresponding to the experimental bands at 440 and 560 cm^{-1} , respectively. The doubling of the unit cell due to magnetic ordering is responsible for the appearance of the DOS at Γ -point around 191 cm^{-1} (E_u mode), observed experimentally due to defect induced Raman scattering.

The room temperature Raman spectra of NiO nanopowders, produced at different annealing temperatures are rather similar except a narrow band around 500 cm^{-1} . The phonon related part of the Raman spectra (1P and 2P bands in figure 2) in nanosized NiO powders is also close to that in the single-crystal. However, the 1P bands become slightly more pronounced in nanopowders due to the presence of defects or surface effect, but the three 2P bands appear to be more broadened. At the same time, the two-magnon (2M) band in nanopowders has about two times smaller intensity than in the crystal and disappears on heating caused by the laser excitation power increase.

Scientific Publications

1. J.Barea, R.Bijker, A.Frank, G.Graw, R.Hertenberger, H.F.Wirth, S.Christen, J.Jolie, D.Tonev, M.Balodis, J.Berzins, N.Kramere, T.Von Egidy. New supersymmetric quartet of nuclei in the $A=190$ mass region. *Phys.Rev.C*, Vol.79, No.3 (2009) 031304 (R).
2. J.Proskurins, A.Andrejevs, T.Krasta, J.Tambergs. Phase transitions in the framework of complete version of IBM-1. *Bulletin of the Russian Academy of Sciences: Physics*, Vol.73, No.2 (2009), pp. 241-244.
3. N. Mironova-Ulmane, A. Kuzmin, M. Grube, Raman and infrared spectromicroscopy of manganese oxides, *J. Alloys Compd.* 480 (2008) 97-99.
4. V. Skvortsova, N. Mironova-Ulmane, L. Trinkler, L. Grigorjeva, Optical properties of hydrogen-containing MgO crystal, *Proc. SPIE 7142* (2008) 71420E:1-7.
5. M. Polakovs, N. Mironova-Ulmane, N. Kurjane, E. Reinholds, M. Grube, Micro-Raman scattering and infrared spectra of hemoglobin, *Proc. SPIE 7142* (2008) 714214:1-8.
6. G. Telysheva, T. Dizhbite, D. Evtuguin, N. Mironova-Ulmane, G. Lebedeva, A. Andersone, O. Bikovens, J. Chirkova, L. Belkova, Design of siliceous lignins – Novel organic/inorganic hybrid sorbent materials, *Scripta Materialia* 60 (2009) 687-690.
7. Telysheva G., Dizhbite T., Jashina L., Andersone A., Volperts A., Ponomarenko J., Mironova-Ulmane N. Synthesis of lignin-based inorganic/organic hybrid materials favorable for detoxification of ecosystem components. *BioResources* Nov. 2009., Vol. 4, Issue 4, pp. 1276-1284. [<http://ncsu.edu/bioresources>].
8. V. Skvortsova, L. Trinkler, D. Jakimovica. Luminescence of impurity in irradiation magnesium oxide. *Proc. Int. Conf. "Actual problems of solid state physics-2009"*, 20-23 October, Minsk, Belarus, pp.97-99.
9. N. Mironova-Ulmane, A. Kuzmin, T. Dizhbite, I. Sildos, M. Pärs, J. Grabis. Phonon and magnons in bulk and nanosized nickel oxide. *Proc. Int. Conf. "Actual problems of solid state physics-2009"*, 20-23 October, Minsk, Belarus, pp.93-95.

10.A.Pavlova, N. Mironova-Ulmane, L.Berzina-Cimdina, J. Locs. Micro-Raman spectroscopy of TiO₂. Proc. Int. Conf. "Actual problems of solid state physics-2009", 20-23 October, Minsk, Belarus, pp.90-92.

Submitted manuscripts:

1.T.Krasta, J.Tambergs, J.Ruža, O.Katkevičius, J.A.Castilho Alcaras. Study of Z~N isospin multiplets in the frameworks of strictly restricted dynamics model. Int.J.Mod.Phys.E (35 lpp. – submitted 1.12.2009).

Conference Publications

1.M.Balodis, T.Krasta, Ļ.Simonova, V.Bondarenko, J.Bērziņš. Improved model interpretation of ¹⁸⁸Re nucleus. 25-th Scient. Meeting of ISSP, Univ. of Latvia, Riga, 11.–13.02.2009. p.14.

2.A.Jakimovičs, T.Krasta, J.Tambergs. Residual interaction of unpaired nucleons in 184≤A≤192 region nuclei. 25-th Scient. Meeting of ISSP, Univ. of Latvia, Riga, 11.–13.02.2009. p.13.

J.Proskurins, A.Andrejevs, K.Bavrins, T.Krasta, J.Tambergs. Study of nuclear phase transitions employing Peres lattices method. 25-th Scient. Meeting of ISSP, Univ.of Latvia, Riga, 11.–13.02.2009. p.38.

3.J.Berzins, D.Riekstina, O.Veveris, J.Malnacs. Radiation control of some contaminated territory of Latvia. Int. Conf. Leben mit Strahlung – von den Grundlagen zur Praxis, Alpbach, Austria, 21-25. September, 2009, pp.182-186.

Conference Presentations

25-th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, 11-13 February, 2009.

1. A.Jakimovičs, T.Krasta, J.Tambergs. Residual interaction of unpaired nucleons in 184≤A≤192 region nuclei.

2. M.Balodis, T.Krasta, Ļ.Simonova, V.Bondarenko, J.Bērziņš. Improved model interpretation of ¹⁸⁸Re nucleus.

3.J.Proskurins, A.Andrejevs, K.Bavrins, T.Krasta, J.Tambergs. Study of nuclear phase transitions employing Peres lattices method.

4. M.Balodis, J.Bērziņš, Ļ.Simonova, V.Bondarenko, T.Krasta, J.Tambergs, A.Jakimovičs, I.Tomandl, M.Jentschel, P.Mutti, H.Boerner. Structure of the odd-odd nucleus ¹⁸⁸Re. Proc.13th Int. Conf. on "Capture Gamma-Ray Spectroscopy and Related Topics", Eds. A.Blazhev, J.Jolie, N.Warr and A.Zilges, AIP Conference Proceedings Vol.1090 (2009), pp.609-610.

5. J.Proskurins, K.Bavrins, A.Andrejevs, T.Krasta, J.Tambergs. Study of quantum chaos in the framework of triaxial rotator models. Proc.13th Int. Conf. on "Capture Gamma-Ray Spectroscopy and Related Topics", Eds. A.Blazhev, J.Jolie, N.Warr and A.Zilges, AIP Conference Proceedings Vol.1090 (2009), pp.635-636.

6. J. Berzins, „Multipurpose cyclotron center in Latvia” Cyclotron Networking Meeting, Ispra, Italy, 3-5 December, 2009.

7.V. Skvortsova, L. Trinkler, D. Jakimovica. Impact of fast neutrons and annealing on optical properties of MgO crystals with transition ions. 15th International conference "Radiation Effects in Insulators REI-2009", Padova (Italy), 30 august- 4 september 2009, P-A5, p.7.

8.V. Skvortsova. Impurity and radiation defects influence on luminescence of irradiated MgO crystals. . LU CFI 25. zin. konf. 2009 g. febr. Tēzes, lp.84

9.N. Mironova-Ulmane, A. Kuzmin, T. Dizhbite, I. Sildos, M. Pārs phonon and magnon excitations in nanosized NiO First International conference Nanostructured Materials & Nanocomposites ICNM 2009 (April 6-8 2009), Kottayam, Kerala, India, p. 182-183.

- 10.N. Mironova-Ulmane, A. Kuzmin, T. Dizhbite, I. Sildos, M. Pārs, J. Grabis Magnons and phonons in nanosized NIO International Scientific Workshop "Oxide Materials for Electronic Engineering - fabrication, properties and application" (OMEE-2009) Lviv, Ukraine, in June 22-26, 2009.
- 11.V. Skvortsova, L. Trinkler, D. Jakimovica. Luminescence of impurity in irradiation magnesium oxide. Proc. Int. Conf. "Actual problems of solid state physics-2009", 20-23 October, Minsk, Belarus, pp. 97-99.
- 12.N. Mironova-Ulmane, A.Kuzmin, T. Dizhbite, I. Sildos, M. Pārs, J. Grabis. Phonon and magnons in bulk and nanosized nickel oxide. Proc. Int. Conf. "Actual problems of solid state physics-2009", 20-23 October, Minsk, Belarus, pp.93-95.
- 13.A.Pavlova, N. Mironova-Ulmane, L.Berzina-Cimdina, J. Locs. Micro-Raman spectroscopy of TiO₂. Proc. Int. Conf. "Actual problems of solid state physics-2009", 20-23 October, Minsk, Belarus, pp.90-92
- 14.M. Polakovs, N. Mironova-Ulmane, I. Sildos, M. Pārs. Raman microscopy of hemoglobin. International Baltic Sea Region conference „Functional materials and nanotechnologies 2009” 31.March-3.April , Riga, Latvia, p.143
- 15.N. Mironova-Ulmane, A. Kuzmin, J. Grabis, I. Sildos, M. Pārs, V. I. Voronin. Phonon-magnon coupling in nanosized NiO International Baltic Sea Region conference „Functional materials and nanotechnologies 2009” 31.March-3.April , Riga, Latvia, p.61.
- 16.M. Polakovs, N. Mironova-Ulmane, I. Sildos, M. Pārs. Raman microscopy of hemoglobin. Three excitation wavelengths. XIII European Conference on the Spectroscopy of Biological Molecules 28. August – 2. September 2009, Palermo Italy, p. 81

Physics Doctor students:

1. Jevgenijs Proskurins – Study of quantum chaos and phase transitions in nuclear models. Supervised by Dr.T.Krasta. Submission of thesis planned in 2010.
2. Andrejs Andrejevs – first year studies, supervised by Dr.hab.phys J.Bērziņš. Studies interrupted in Autumn 2009.

Lectures at Universities, Institutes ...

- During 2009, 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 chaos and phase transitions in nuclear models” (continued in 2010);
- 2) supervision of A. Andrejevs started his Ph.D. studies – proposed theme „Study of the quantization conditions for phase integrals”;
- 3) supervision of physics masters work of LU Physics and Mathematics Faculty student
- K. Bavrins.

LABORATORY OF ORGANIC MATERIALS

Head of Laboratory Dr.habil.phys.I.Muzikante

Scientific Staff

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

PhD students

Elīna Laizāne
Jānis Latvels
Andrejs Tokmakovs
Aivars Vembris

Technical Staff

Edgars Nitišs
Jurgis Sīpols

Students

Baiba Niparte
Martins Porozovs
Kaspars Pudžs

Scientific projects of the Latvian Council of Sciences

05.0026.5	Nanomaterials and nanotechnologies - Nanostructured thin layers of organic molecules and polymer for molecular electronics (2005-2009)
09.1210	Photo and electrophysical processes of multilayer structures and their components (2009-2012)

National Research Program in Materials Science (2005-2009), Project No.3

Materials for photonics and nanoelectronics based on novel functional low molecular organic compounds and polymers

International projects

Projects of Mutual scientific co-operation fund of Republic of Lithuania and the Republic of Latvia with R.O.C. (Taiwan):	
1. ISSP LU & RTU Institute of Physics, Vilnius, Lithuania Institute of Atomic and Molecular Science Taipei, Taiwan	Structural organization and optical nonlinearities of low-dimensional molecular structures (2007-2009)
2. ISSP LU Kaunas Technology University Institute of Chemistry, Academia Sinica, R.O.C., Taiwan	Design, Synthesis and Studies of New Effective Materials for Organic (Opto)electronics (2008-2011)

Main equipments:

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 system.
4. Computer-controlled Kelvin probe setup with the temperature control up to +130°C and measuring the surface potential in a range between -9.6 and +9.6V with the accuracy ±1mV. The diameter of vibrating gold electrode was 2mm
5. Scanning Kelvin Probe SKP5050
6. Surface Profile Measuring System Dektak 150
7. Computer-controlled SHG setup ($\lambda=1064$ nm) allows us to measure SHG ($\lambda=532$ nm) intensity as function of the fundamental power, incidence angle, fundamental and SH light polarization as well as sample surface mapping by SHG intensity. The detection threshold of equipment is 1×10^{-6} pm/V

Cooperations

Latvia:

1. Institute of Applied Chemistry, Riga Technical University (Prof. V.Kampars).
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).
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, B.Stiller).

Taiwan

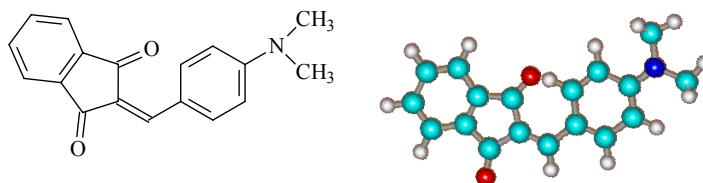
1. Institute of Atomic and Molecular Science Taipei (Prof. S.H.Lin)
2. Institute of Chemistry, Academia Sinica, (Prof.. Chao-Ping Hsu)

Japan

1. Institute for Chemical Research, Kyoto University, Uji, Kyoto (prof. N.Sato)

THE MAIN RESULTS

OPTICAL PROPERTIES OF THIN FILMS CONTAINING IPB AND DMABI DERIVATIVES



DMABI

VOLTAGE INDUCED FLUORESCENCE CHANGES OF N,N-DIMETHYLAMINO BENZYLIDENE 1,3-INDANDIONE FILMS

V. Gulbinas, R. Karpicz, **I. Muzikante**, L. Valkunas

In co-operation with

Institute of Physics, Vilnius, Lithuania

Institute of Materials Science and Applied Research, Vilnius University, Vilnius, Lithuania

Effects caused by the applied voltage on the steady state and time resolved fluorescence of vacuum evaporated N,N-dimethylaminobenzylidene 1,3-indandione films sandwiched between gold and aluminium electrodes are investigated and discussed. Fluorescence enhancement and quenching as well as the fluorescence band narrowing have been observed depending on the applied voltage. Fluorescence decay and recovery take place on a time scale of tens of seconds after voltage is switched on and off. Similar decay kinetics is also appreciable after switching on the excitation light. These fluorescence changes are attributed to the exciton quenching by trapped charge carriers. Voltage-induced fluorescence quenching and enhancement have been observed in DMABI films sandwiched between Al and Au electrodes. The fluorescence changes have been attributed to the exciton quenching by trapped charge carriers. The trapped carrier concentration and the quenching rate are determined by several parameters, which depend on the material morphology and on the electric field strength. Common action of several field dependent processes causes nonmonotonical voltage dependence of the quenching efficiency, which appears as the fluorescence enhancement at low applied voltages and its weakening at high voltage values. The fluorescence band narrowing is also observed at the applied voltage. The band narrowing is attributed to the quenching by trapped carriers of the fluorescence originating from particularly disordered material sites forming edges of the fluorescence band.

Our investigation demonstrates that the trapped carrier concentration may be much higher than that of mobile carriers and may cause significant fluorescence quenching. Therefore, the fluorescence quenching by charge carriers cannot be simply ignored even at very low current densities, moreover that quenching dependences on applied voltage and excitation wavelength may closely resemble those caused by the exciton dissociation.

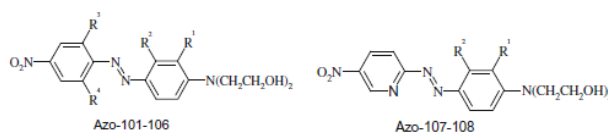
The work is supported by the Taiwan—Lithuanian—Latvian collaboration project.

NOVEL AZOBENZENE PRECURSORS FOR NLO ACTIVE POLYURETANES: SYNTHESIS, QUANTUM CHEMICAL AND EXPERIMENTAL CHARACTERIZATION

E.Jecs, J.Kreicberga, V.Kampars, A.Jurgis, M.Rutkis

*In co-operation with
Institute of Applied Chemistry, Riga Technical University*

For the development of electro optical active polyurethanes six new derivatives of 2-{(2-hydroxyethyl)-[4-(4-nitrophenylazo)phenyl]amino}ethanol and two of 2-{(2-hydroxyethyl)-[4-(5-nitropyridin-2-ylazo)phenyl]amino}ethanol were synthesized by azocoupling reaction. Molecular geometry, hyperpolarizability, β_{FF} and ground state dipole moment μ_g were acquired by **RHF *ab initio*** (6–31G**) calculations using HyperChem software package. To characterize **NLO** performance of synthesized azo compounds second order non linear coefficients d_{31} and d_{33} were measured as function of chromophore load in guest–host films (**PMMA**). Eight synthesized compounds can be grouped in four similar gross formula pairs (different position of octyloxy group) with almost equal $\mu_g \beta_{FF}$ product and different μ_g values. At low chromophore concentrations higher dipole moment compounds perform better. Lower dipole moment compounds have better **NLO** efficiency at high chromophore loads. Accurate ranking of all chromophores, based on two-level model corrected zero frequency $d_{33}(0)$ values, was not viable due to overestimation of the dispersion factor.



Azocompound	R ¹	R ²	R ³	R ⁴
Azo-101	OC ₈ H ₁₇	H	H	H
Azo-102	H	OC ₈ H ₁₇	H	H
Azo-103	OC ₈ H ₁₇	H	CN	H
Azo-104	H	OC ₈ H ₁₇	CN	H
Azo-105	OC ₈ H ₁₇	H	CN	CN
Azo-106	H	OC ₈ H ₁₇	CN	CN
Azo-107	OC ₈ H ₁₇	H	-	-
Azo-108	H	OC ₈ H ₁₇	-	-

Scheme 1.

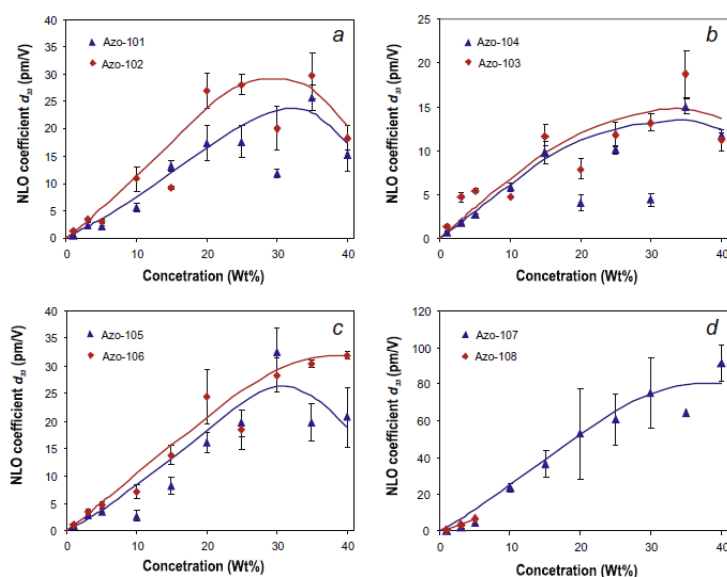


Fig. 4. Nonlinear coefficient d_{33} of guest–host films of investigated azo dyes in PMMA matrix. Solid lines are just for eye guiding.

This work is supported by national research program in Materials Sciences

DETERMINATION OF ELECTRO – OPTIC COEFFICIENT OF THIN ORGANIC FILMS BY MACH – ZEHNDER’S INTERFEROMETRIC METHOD

E.Nitišs, M.Rutkis, O.Viltis

The theoretical analysis of numerous methods existing for determination of the electro-optic coefficients of thin organic films is shortly reported and reasoned argumentation in favor of the Mach-Zehnder interferometric (**MZI**) method is given. The **MZI** method has successfully been implemented after we had found solutions to the key setup problems (to reduce extremely high sensitivity to acoustical and mechanical vibrations, attenuate rf and mechano-optical signals, etc.). Further increase in the reliability of effective determination of **EO** coefficients was achieved by setting-up measurements in the **MZI** phase scanning mode. First investigations of the test organic **NLO** active host-guest polymers have shown that the necessary conditions for good sandwich sample preparation by “baking” two slides are the high surface quality and compatibility of films. Finally, we can report the value $r_{13} = 6.4$ pm/V immediately after poling of 5 wt% tBu-DMABI in PMMA. This value decays with characteristic time $\tau \approx 17$ h to a constant value $r_{13} = 2.4$ pm/V after 48 h.

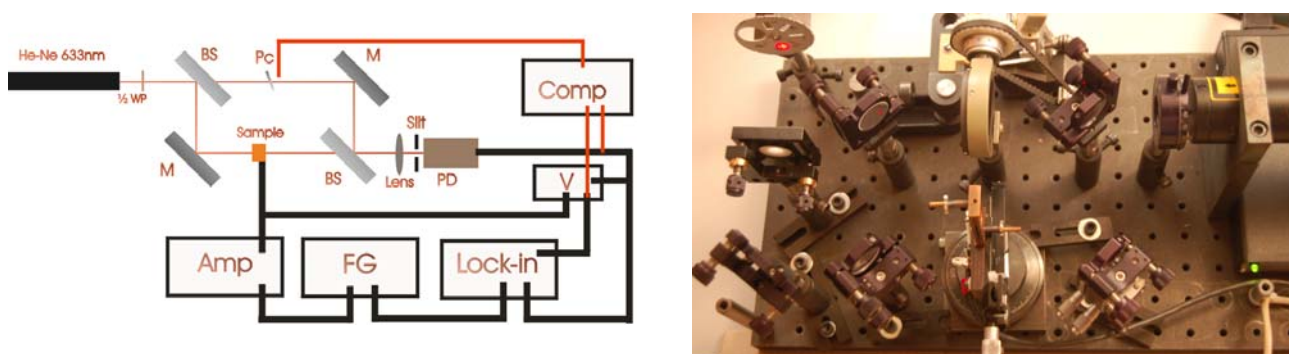


Fig.1. Scheme and photo of setup. He-Ne, helium-neon laser $\lambda=633$ nm; $\frac{1}{2}$ WP, half-wave plate; BS: 50/50 beam splitter; Pc: phase compensator (wedge); M: mirror; Sample; Lens; PD: photodiode; Slit; V: voltmeter; Comp: computer; FG: function generator; Amp: signal amplifier; Lock-in: lock-in amplifier.

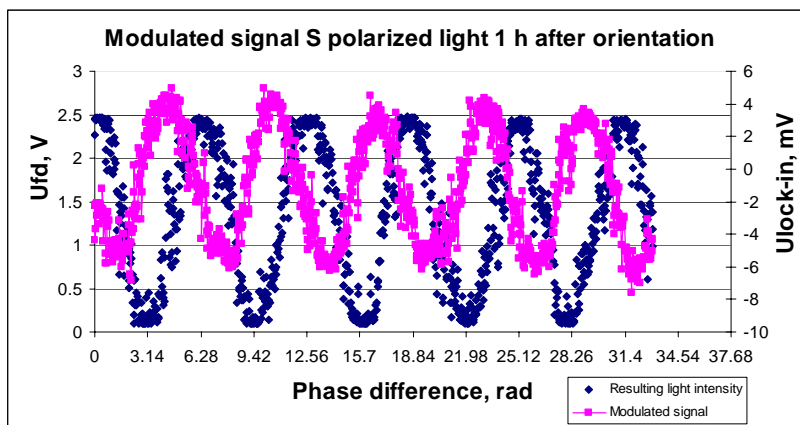


Fig. 6. EO modulated signal in the MZI; incidence angle: 0° ; 1 h after poling; modulation voltage: 49.22 V rms.

The work is supported by Project 05.0026.5 of the Latvian Council of Sciences.

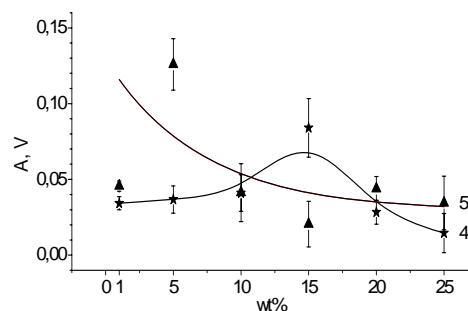
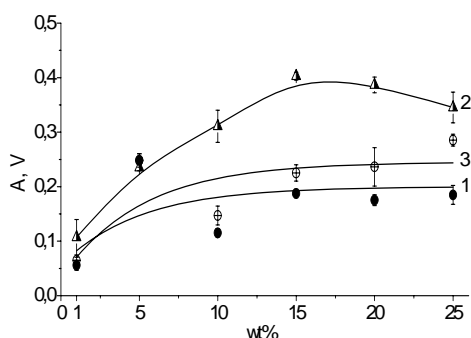
PHOTOELECTRICAL PROPERTIES OF THIN FILMS CONTAINING IPB AND DMABI DERIVATIVES

PHOTOELECTRICAL PROPERTIES OF INDANDIONE CHROMOPHORE IN SOLID STATE

J.Sipols, I.Muzikante, E.Fonavs

*In co-operation with
Institute of Applied Chemistry, Riga Technical University*

The optically induced switching of electrical properties of indandione type molecules, which consist of acceptor and donor groups, are investigated. Both calculation and experimental results show a reversible highly dipolar photoinduced intramolecular electron transfer in 2-(4'-N,N-dimethylaminobenzylidene)indan 1,3 dione molecule (DMABI). Kelvin probe technique is applied to investigate surface potential of host-guest polymer film with 4 different DMABI derivatives. Derivatives are chosen to compare influence of geometry, concentration and values of dipole moment of molecule in ground and excited state on response time and amplitude of photoinduced surface potential. The values of the fast response time to irradiation are independent on concentration of molecules in polymer film and last to several seconds. The dependence of the values of amplitude of photoinduced changes of surface potential on concentration of molecules is observed for DMABI and its 3 derivatives. The optimal concentration of guest molecules in polymer matrix is in range 10 – 25wt% in dependence of molecule.



Dependence of amplitude A characterizing fast response of surface potential on irradiation of DMABI (1), DMABI-dPh (2), tBu-DMABI-dPh (3), N-DMABI (4) and N-DMABI-dPh (5) molecules in PMMA matrix.

This work is supported by Project No.09.1210 of the Latvian Council of Sciences and national research program in Materials Sciences

STUDIES OF PHYSICSL PROPERTIES OF CARBAZOLE DERIVATIVE MATRIX FOR ELECTROLUMINESCENCE SYSTEMS

K.Pudzis, A.Vembris, M.Porozovs, I.Muzikante, J.V.Grazulevicius

In co-operation with

Department of Organic Technology of Kaunas University of Technology, Kaunas, Lithuania

Bi-polar organic material (electron and hole mobility is of same order) is very important for organic light emitting diodes (OLED). Carbazole derivatives are one of them. We study electrical properties and energy structure of novel carbazole derivative SJ97 (synthesized in Kaunas University of Technology) thin films. The organic films were prepared by spin-coating method with the thickness of the order of 0.5 μm . It allows applying space charge limited current method to characterise charge carrier injection and energy distribution of traps in the thin films. For injection of holes ITO, Ag electrodes and for injection of electrons Al electrodes were applied. For application of carbazole derivative thin film in OLED structure, the matrix of bipolar compound SJ97 with incorporated electrofluorescent Alq3 molecules or electrophosphorescent Ir(ppy)₃ molecules are studied as well.

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

Scientific publications

1. E.Jecs, J.Kreichberga, V.Kampars, A.Jurgis, M.Rutkis, Novel azobenzene precursors for NLO active polyuretanes: Synthesis, quantum chemical and experimental characterization, *Optical Materials*, 31 (2009) 1600–1607, doi:10.1016/j.optmat.2009.03.010
2. V.Gulbinas, R.Karpicz, I.Muzikante, L.Valkunas, Voltage induced fluorescence changes of N,N-dimethylaminobenzylidene 1,3-indandione films *Thin Solid Films*, 2009, doi:10.1016/j.tsf.2009.09.081

3. Jyn'ya Tsutsumi, Takahiro Sasamori, Hiroyuki Yoshida, Motihiro Tokitoh, Naoki Sato, Shigeki Kato, Inta Muzikante, Ojars Neilands, A noncentrosymmetric crystal structure of a zwitterionic compound, pyridinium 5,7-dihydro-5,7-dioxo-6H-cyclppenta[b]pyridin-6-ylide, realized by weak hydrogen bonds, *J. Molecular Structure*, Vol. 920, Iss.1-3, 52-60, 2009, doi:10.1016/j.molstruc.2008.10.021
4. J.Sipols, I.Muzikante, E.Fonavs, Photoelectrical properties of indandione chromophore in solid state, *Latvian Journal of Physics and Technical Sciences*, 2009, Vol. 46, no.3, pp. 16-22.
5. E.Nitišs, M.Rutkis, O.Vilītis, Determination of electro – optic coefficient of thin organic films by Mach – Zehnder's interferometric method, *Latvian Journal of Physics and Technical Sciences*, 2009, Vol. 46, no.3, pp. 5-14

Abstracts:

25th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, Latvia, February 11-13, 2009

1. J.Latvels, V.Kampars, I.Muzikante, K.Pudžs, New indandione heterojunction in molecular diode), Book of Abstracts, p.85
2. E.Nitišs, M.Rutkis, O.Vilītis, Determination of the electro-optic coefficients of polymer films bu Mach-Zehnder inteferometric method, Book of Abstracts, p.86
3. J.Sīpols, V.Kampars, I.Muzikante, Analysis of photoelectrical properties of polymer films consisting of indandione derivatives by Kelvin probe, Book of Abstracts, p.87
4. E.Laizāne, K.Kundziņš, I.Muzikante, J.Teteris, Holography recording in azobenzene containing polymer films, Book of Abstracts, p.88
5. A.Vembris, I.Muzikante, New trends of improvement of organic light emitting diodes and its realization in Laboratory of Organic Materials, Book of Abstracts, p.89
6. G.Zelča, A.Vembris, J.Latvels, I.Muzikante, J.V.Grazulevicius, V.Kokars, Study of electroluminescence in new synthesized organic materials, Book of Abstracts, p.90
7. A.Tokmakov, M.Rutkis, V.Kampars, V.Kokars, Characterization of the novel indandione derivatives based binary chromophore organic glass material, Book of Abstracts, p.91

Young Optical Scientists Conference YOSC-2009, Baumann Moscow State Technical University, Moscow, Russi, February 2-7, 2009

1. A.Vembris, J.Latvels, G.Zelca, I.Muzikante, J.V.Grazulevicius, V.Kokars, Optoelectrical properties of new synthesized mono-polar and bi-polar organic materials, Proramme, p. 30

**International Conference on Functional materials and Nanotechnologies
FM&NT 2009, Riga, Latvia, March 31 – April 3, 2009**

1. M.Rutkis, A.Jurgis, Computer modeling of external electrical field chropophore poling, Book of Abstracts, p 71.
2. I.Muzikante, I.Bidermane, E.Fonavs, D.Gustina, V.Kampars, J.Sipols, Host-guest polymer films of low molecular polar organic molecules. Structure and photoelectrical properties, Book of Abstracts, p 68.
3. B.Polakov, J.Sipols, A.Kuzmin, I.Muzikante, I.Tale, Kelvin probe AFM investigations of nanostructures, Book of Abstracts, p 91.
4. I.Muzikante, V.Gulbinas, R.Karpicz, L.Valkunas, Voltage induced fluorescence changes of DMABI thin films, Book of Abstracts, p 118.
5. E.Laizane, D.Gustina, K.Kundzins, I.Muzikante, J.Teteris, Optically induced patterning of polymer films doped with azobenzene molecules, Book of Abstracts, p 125.
6. I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, M.Plotniece, M.Roze, J.Kalnachs, A.Murashov, P.Shipkovs, G.Rozite, Electrode influence of bi-layer GaOHPc:C₆₁(CO₂Et)₂ and P3HT:PCBM organic photosensitive system, Book of Abstracts, p 129.
7. A.Tokmakov, M.Rutkis, E.Jecs, J.Kreicberga, V.Kampars, V.Kokars, Binary chromophore supramolecular systems as promising route for obtaining electro-optically active polymer composites, Book of Abstracts, p 185.

International Student Conference “Developments in Optics and Communications DOC-5”, Riga, Latvia, April 24-26, 2009

1. A.Vembris, G.Zelca, J.Latvels, I.Muzikante, Preparation and study of organic electroluminescent systems, Abstract book, p. 54
2. A.Tokmakov, M.Rutkis, E.Jecs, J.Kreicberga, V.Kampars, V.Kokars, Binary chromophore organic systems as a promising route for obtaining electro- optically active polymer composites, Abstract book, p. 26-27
3. E.Nitiss, M.Rutkis, O.Vilitis, Implementation of Mach – Zehnder’s interferometric technique for electro – optic measurement on thin organic films, Abstract book, p. 25
4. J.Sipols, I.Muzikante, E.Fonavs, V.Kampars, Photoelectrical properties of indandione chromophore in solid state, Abstract book, p. 15-16.

The 11th International Conference-School „Advanced Materials and Technologies”, Palanga, Lithuania, August 27-31, 2009,

1. G.Garda (Zelca), A.Vembris, J.Latvels, I.Muzikante, Studies of materials for hole and electron injection in Alq3 OLED systems, Abstracts, p.75.

2. K.Pudzs, I.Muzikante, J.Latvels, J.V.Grazulevicius, J.Simokaitiene, A.Vembris, G.Garda (Zelca), Electrical properties of thin films based on derivatives of carbasole oligomers, Abstracts, p.87.
3. J.Sipols, I.Muzikante, J.Latvels, Photo-electrical properties of DMABI thin films, Abstracts, p.89.

The international conference “Baltic Polymer Symposium 2009”, Ventspils, Latvia, September 22-25, 2009

1. I.Muzikante, M.Rutkis, Polymer composites of polar organic chromophores, Abstracts, p. 12
2. A.Sternberg, I.Muzikante, Research of Functional Materials and Composites in Latvian Research Programme in Materials Sciences, Abstracts, p.18

Patent:

1. I.Kaulachs, I.Muzikante, L.Gerca, G.Slihta, J.Kalnacs, P.Shipkovs, G.Rozite, Solution-proceeded bulk heterojunction layer consisting of hydroxy gallium phtalocianine and solulable fullerene derivatives for light sensing and solar cells, method for producing the same and bi-layer bulk heterojunction organic solar cell containing hydroxy gallium phtalocianine, (submitted by the Institute of Physical Energetics, Latvia), Latvian Patent No. 13995, 20.11.2009.

ELECTRONIC ENGINEERING

Head of Department Dr. phys. A. Kristins

Main Problems

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

Scientific Staff

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

Technical Staff

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

Cooperation

Latvia

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

Denmark

DanBalt Electronics

Russia

St. Petersburg I. Joffe's
Institute of Physics and Techniques

Estonia

1. Tallinn University of Technology
2. Competence Centre ELIKO

The prospects of the instruments look at appendix.

Our Clients

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

Lectures on Conferences

25th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2009

1. I.Gvardina, A.Kristiņš, J.Melderis *Room Access Control System with Ethernet communication*. Abstracts, p.27.
2. P.Annus, M.Min, A.Kristiņš. *RF Communication in Embedded Systems*. Abstracts, p.28.
3. E.Garkājs, I.Gvardina, A.Kristiņš. *Unit for Proxy Card Data Inpu*. Abstracts, p.49.
4. D.Gusevs, J.Veinbergs, J.Melderis, I.Gvardina *Electric Motor Starting by a Three-Phase Soft Starter in Current Restriction Mode*. Abstracts, p.29
5. A.Zeļenkovs, S.Zeļenkovs..*Choice of Noise Generator in Digital Modelling of Radiosystem Signal Processing*. Abstracts, p.50

9th International Scientific Conference „Engineering for Rural Development” 27.-28.05.2010. Jelgava, LATVIA

Vadim Ogorodnik, Janis Kleperis, Albert Kristinsh, Irina Gvardyna, Aivars Cesnieks, Arvids Vilde *Automated control of the grain drying process*. P. 324 – 327

Other publications:

1. A.Kluga, A.Zelenkovs, E.Grab, V. Belinska. *Accuracy Estimation of GPS Receiver Parametrs with Simulator in Dynamic Mode*. // Electronics and Electrical Engineering. – Kaunas: Technologija, 2009, No. 6(94), pp. 9-14.
2. A.Zeļenkovs, S.Zeļenkovs. *The noise generator for model – based signal processing in linear radio channels with viterbi detection as output* –Rīga Technical University 50th International Scientific Conference. Section «Electronics, Telecommunications and e-Society» Riga, 14 – 16 October 2009, pp. 41-50



**Electronic Engineering Department
Institute of Solid State Physics
University of Latvia**

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*TM identification code keys.

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

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

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

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

Technical Specification

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

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

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

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

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

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

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

Technical Specification

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

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Car parking and access control systems

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

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

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

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

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

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Electronic Documentation

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

TM replaces paper documents that are difficult to attach to objects and are prone to damage or illegibility. If copying is undesirable, lock bits, add-only memory, passwords and encryption can be employed.

TM based electronic documents are very convenient and safe for persons who have contacts with confidential or strict registration papers.

Each TM chip has a unique registration number up to $2,81 \cdot 10^{14}$ variants.

A personal computer with special interface and special software can read and write data from/to Touch Memory.

TM is housed in a durable hermetic stainless steel case (\varnothing 17,4 x 5,89 mm) and is tolerant to mechanical shock, static electricity, and electromagnetic fields and to other harmful environmental factors.

TM has an ambient temperature range -40°C to $+85^{\circ}\text{C}$.

Touch Memories can accommodate over one million data changes.

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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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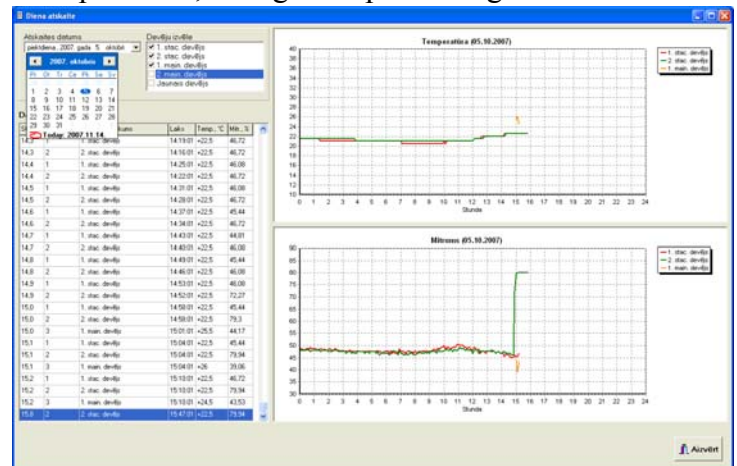


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Monitoring of the environment temperature and relative humidity

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 $+85^{\circ}\text{C}$ 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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**Device for Authorized One-Door Access System
with TM Identification Code Keys**

The device is constructed for creation of authorized access system for apartments.

The device controls electromagnetic keys of any construction.

Accessing in the apartment is implemented with the aid of the *Dallas Semiconductor* Touch Memory™ identification code keys. In the emergency case it is possible to enter the apartment with the aid of ordinary mechanical key.

Exiting of the apartment is provided either with the button or with the TM (if the second reader is available).

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

The device has a sound and light indication and it provides an electrical signal for security service.

This device is cheaper than most of similar ones.

Technical Specification

Power supply:	+ (10 - 15) V
Consumption:	
System armed in waiting state:	≤ 8 mA
System activated in access mode (defined by el. mech. lock):	< 0,5A (typically)
Access time:	5 seconds
Sound signal on non-authorized opening of the door:	Immediately
Sound signal delay after authorized opening of the door:	5 seconds
Possible combinations of keys:	$2,8 \cdot 10^{14}$
User keys:	≤ 56 pcs.
Dimensions:	83x55x35 mm

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**Device for Authorized One-Door Access System
with TM Identification Code Keys and Event Registering**

The device is constructed for creation of authorized access system for apartments.
The device controls electromagnetic keys of any construction.

Accessing in the apartment is implemented with the aid of the *Dallas Semiconductor Touch Memory™* identification code keys. In the emergency case it is possible to enter the apartment with the aid of ordinary mechanical key.

Exiting of the apartment is provided either with the button or with the TM (if the second reader is available).

Reprogramming of the TM list, setting of the time and time access zones (optionally) and also transferring of the data on the events registered from the device to PC is realized with the assistance of the special identification Master-key with 64K bits of read/write nonvolatile memory.

This device is cheaper than most of similar ones.

Technical Specification

Power supply:	+(10 - 15) V
Consumption of system activated in access mode (defined by el. mech. lock):	< 0,5A (typically)
Access time (standard):	5 seconds
Sound signal on non-authorized opening of the door:	Immediately
Sound signal delay after authorized opening of the door:	5 seconds
Possible combinations of keys:	$2,8 \cdot 10^{14}$
Number of user keys (standard):	56 pcs.
Number of events registered:	500
Time of data retention in Master-key:	over 10 years

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High-voltage Breaker Analyzer Device "OSKARS"

The device was designed for the verification of high-voltage (110 and 330 kV) breakers. 14 timing channels and the current in the driving solenoid are simultaneously controlled and necessary time parameters calculated.

Only one minute - and you have the operating sequence and the time control results printed out on the A4 format (210 x 297 mm) paper sheet by ordinary printer without using of the computer.

The device has four modes of operation: *OPEN (O)*, *CLOSE (C)*, *OPEN-CLOSE-OPEN (O-C-O)*, *CLOSE-OPEN (C-O)*. The delay time between pulses (O-C) and (C-O) can be set on the thumbwheels ($0 \div 0,15$ s).

The device can be used for testing of 10 types of breakers: BBIII-110; BBБ-110; BBY-110; BBH-110/6; BB-330Б; BBH-330/15; HGF-115/2B; HPL-362/B2; LTB-145D1.

The time resolution is 0,001 s.

Dimensions are 490 x 480 x 165 mm.

Weight is 20 kg.

The device specifications may be changed according to customer's requirements.

The device may be used to study reaction velocity, delay and vibrations of different kinds of the relays and for registration of different processes in other branches of science and technique.

These devices are put into operation by power engineering departments of "LATVENERGO" and "LIETUVOS ENERGIJA".

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**Operating with remote objects
based on TCP/IP communication protocol**

Usage of this communication protocol makes possible to work without wiring of additional communication lines and allows to transmit information in far distances practically without difficulties.

In the developed remote control systems “Rabbit” controllers are used.

Different modifications of microcontrollers permit to collect information due from contact sensors (hercons, magnetic loop controllers, move detectors etc.), from data carriers based on DS19XX protocol (i-Buttons, thermometers and others) or based on Viegand protocol (Proximity cards).

It is possible to connect the system with other peripheral devices via standard RS232/485 ports.

Controllers can provide communication with main server via TCP/IP ports by using local, corporate or world wide nets.

Practical applications:

1. The system of access, control and management is worked out for LatRosTrans company. The system consists of 24 controllers (number of technological blocks on Russia-Ventspils oil pipeline), dispatcher program (in Daugavpils) and some client applications.
2. Entrance in/out system for “Latvijas Gāze” company is worked out, which consists of three in/out gates with automatic barriers, server administrator and guard programs and some other client applications.
3. The system including checkpoint, the authorized access in cabinets and the security signal system for two buildings of the Latvian Shipping Company with a unified database.

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Security Drawers and Safes for the Cash Points

There are some versions of safes produced by Solid State Physics Institute & Co for storage of banknotes, coins and forms. A safe has an electromechanical lock, activated by electronic system with time delay.

The safe-drawer SF-1 has the keys based on Dallas Semiconductor firm Touch Memory™ identification chips with unique registration number (up to $2,81 \cdot 10^{14}$ numbers), but safes KT-2F may be completed both TM and mechanical key. The electronic time delay system can be activated by TM or control button, then a red LED flashes intermittently until the delay time has run out. At that moment a buzzer beeps and a green LED flashes for access time. During of that time the safe may be pulled open.

	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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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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Register system on supervision of route checkpoints

This system is designed to monitor the schedule of visiting route checkpoints by guard patrol. The system also allows monitoring arrivals (and optionally leavings) the object (optionally remote) if there is a checkpoint at this object.

The system consists of one or more portable data readers (DR), identification keys (IK) as checkpoints and software.

The system doesn't require permanent use of computer. Data readers are completely autonomous and the information about attendance of checkpoints (codes of checkpoints and time of making corresponding checks) is saved in non-volatile memory (EEPROM), where it can be stored until the device is connected to computer.

The code-keys of checkpoint identification (Dallas Semiconductor) do not require power supply and also do not require installation. The checkpoint identification keys are attached at necessary place with a special holder. Sizes of checkpoint identification keys are $\varnothing 17.35 \times 5.89$ mm.

Program software allows programming the rules of passing route, but after receiving the data from data readers it allows to analyze adequacy of the guards activities; compose reports and print the reports or send by E-mail if necessary.

The user interface is in Latvian and operates under Win9x/2000/NT/XP. The language of user interface can be changed in accordance with special order.

The fact of date reading by ICK is confirmed with sound and light signals.

The information of the same ICK can be written in the data-reader repeatedly if the next reading takes place no sooner than after one minute. The memory volume of the data-reader is designed for registering 1700 events. A special cable is used for data transmitting to PC. Date reader sizes do not exceed 26x40x160mm.

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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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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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