

Institute of Solid State Physics University of Latvia

# **ANNUAL REPORT**

2008



Riga 2009

#### Annual Report 2008, Institute of Solid State Physics, University of Latvia.

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#### INTRODUCTION

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

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

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

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

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

#### The research of the ISSP includes:

- 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 perfomed in 2002. The second Meeting of International Supervisory board took place at April 3, 2007. Below is a short excerpt citation from the evaluation report: "... the overall development of ISSP has been good with excellent quality of research as evidenced by publications, active participation in international projects etc..."

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff.** At present there are 258 employees working at the Institute, 31 of 146 members of the research staff hold Dr.habil.degrees, 75 hold Dr. or PhD. At the end of 2008 there were 21 PhD students and 46 undergraduate and graduate students in physics and optometry programmes working at the ISSP.

#### Table 1

#### **ORGANIZATIONAL STUCTURE OF THE ISSP IN 2008 International Supervisory Board Council of Institute** Dr.phys. L.Trinklere Director Dr.habil.phys. A. Sternberg **RESEARCH DIVISIONS** ADMINISTRATION AND AND LABORATORIES SERVICES **Department of Crystal Physics** Vicedirector for Research Dr.phys P.Kulis Dr.habil.phys. I.Muzikante **Department of Disordered Materials** Vicedirector for Education **Physics** Dr.habil.phys. A.Krumins Dr.habil. phys .D.Millers **Department of Ferroelectrics** Vicedirector for Innovation Dr.phys V.Zauls Dr.phys. J.Teteris **Department of Semiconductor Materials Finance and Accounting** Dr.phys A.Lusis A.Jozepa **Department of Radiation Physics Personell office** Dr. habil. phys. J.Berzins D.Popele Lab. of Theoretical Physics and Mechanical Workshop **Computer Modelling** J.Katkevics Dr. habil.phys. J.Kotomin Lab. of Optical Recording Utilities Dr.phys J.Teteris R.Siatkovskis Lab. of Wide Band Gap Materials Energetics Dr. habil. phys. B.Berzina J.Ruhmanis Lab. of Surface Physics Library Dr.phys.F.Muktepavela L.Rihtere Lab. of Visual Perception Dr. habil. phys. I.Lacis Lab. of Organic Materials Dr.habil.phys. I.Muzikante Lab. of Electronic Engineering Dr. A.Kristins Lab. of Didactic Systems Dr.phys. J.Kuzmin

# 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.

Table 3

# **International Advisory Board of the Institute**

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

The annual report summarizes the research activities of the ISSP in 2008. The staff of the Institute has succeed in 31 **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 297.4 thous. Ls (ca. 403 thous. EUR).

In 2005 a the new Law of Science was passed by Parliament of Latvia. According to this law the state **budgetary financing in Latvia** for science has to **increase yearly per 0.15% from GDP** up to reaching a 1% value. The budgetary increase was focused on scientific infrastructure financing and launching of National Research Programmes (NRP). One of the scientific priorities in Latvia is **materialscience**. ISSP became coordinating institution for the Materials NRP and collaborates as well in the NRP "Energetics" attracting 727,0 thous. Ls budget in 2008. The infrastructure financing for ISSP in 2007 was 957,4 thous. Ls. and it was partly used also for the salaries of the scientific and maintenance staff of the Institute. (Table 4). 7 projects the total amont of 1 691,1 thous. Ls supported by the EU Structural funds have been realised in the Institute: 5 applied science projects, 1 project for purchasing of modern research equipment, and 1 project for reconstruction.

No	Author	Award
1.	Dr.habil.phys.	Full Member of Latvian Academy of Science
	I.Muzikante	
2.	Dr.habil.phys. I.Lacis	The "Grindex" and Latvian Academy of Science
		award
3.	Mg.phys. I.Aulika	L'Oreal prize for woman scientists
4.	Dr.phys. V.Kashchejevs	Author of the best scientific achievment (from
		Latvian Academie of Science)
5.	Mg.E.Laizane	The L. and M.Jansons award in physics for young
		scientists

#### Main awards, received at 2008:

At the end of 2008, more than 50 students, master's candidates and doctoral candidates worked in 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 2008 three conferences have been organised at the Institute:

- 24<sup>th</sup> Scientific Conference of the Institute of Solid State Physics, University of Latvia, February 20 22, 2008;
- Annual International Baltic Sea Region conference "Functional materials and nanotechnologies", April 1 4, 2008;
- The 6<sup>th</sup> International Conference "Advanced Optical Materials and Devices", August 24 – 27, 2008, Riga, Latvia (in cooperation with University of Latvia)

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Structural funds from EU
2000	478.8 + 77	238.3	36.9	146.3	43	
2001	617.3	238.8	64.5	116.5	183	
2002	612.8	239.9	90.0	133.0	131	
2003	764.6	245.7	172.3	152.5	179	
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 2 3 6,5	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

INCOME OF ISSP, THOUSAND Ls, FROM 1993 – 2008

\*) - investment for building reconstruction



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

- F-Bridge 76.8 thous. EUR
- Catherine 8.7 thous.EUR
- Green Rose 18.6 thous. EUR
- MIND 27.1 thous. EUR
- 4 EURATOM projects 209.3 thous. EUR
- one INTAS project 3.4 thous. EUR
- Mary Curie reintegration grant 45.0 thous. EUR

The International funding were increased to 291.8 thous. Ls in 2008. (Table 4)

#### Main achievments in 2008:

1. 83 SCI papers published by the staff of Institute.

2. Purchasing and installation of modern technological and research equipment (469.7 thous. LVL by EU Structural funds) (Appendix 2)

3. Reconstruction of workshop building of the Institute as well as the ventillation system (985.0 thous. LVL by Structural funds).

4 23 B.sc. thesis and 4 M.Sc. thesis in physics were defended under the supervision of our scientists (Table 5)

5. I.Aulika, O.Balcers, A.Fedotovs and R.Paeglis were acquired degree of doctor of physics (PhD) University of Latvia (Table 5)

Table 5

# PhD, Master of Science (M.Sc.) and Bachelors of Science (B.Sc.) Thesis prepared at the Institute in 2008

No	Author	Tittle	Supervisor
1.	I.Aulika	Optical depth profile and phase	Dr.phys.V.Zauls
		transition investigation of	
		NaNbO <sub>3</sub> and Pb(Zr,Ti)O <sub>3</sub> thin	
		films	
2.	O.Balcers	Phototermal properties of	Dr.phys.J.Teteris
		amorphous chalcogenide thin	
		films	
3.	A.Fedotovs	EPR of radiation defects in	Dr.habil.phys.U.Rogulis
		fluoride crystals and oxyfluoride	
		glass ceramics	
4.	R.Paeglis	Measurement of the kinematics of	Dr.habil.phys.I.Lacis
		they eye in describing cognitive	
		processes	
5.	J.Mastrikov	First-principles calculations of	Dr.J.Maier, Germany
		LaMnO <sub>3</sub> surface reactivity	

#### PhD thesis

#### M.Sc. thesis

No	Author	Tittle	Supervisor
1.	A.Andrejevs	Effects of space-time geometry on	
		selected microphysics problems	Dr.habil.phys.J.Tambergs
2.	E.Laizāne	Optical patterning of azobenzene	Dr.habil.phys.I.Muzikante
		containing polymer films	
3.	G.Mārciņš	Development principles of AlGaN	Dr.habil.phys. I.Tale
		solid solution thin film structures in	
		MOCVD synthesis	
4.	A.Vembris	Nonlinear optical efficiency and	Dr.phys. M.Rutkis
		stability investigation of the	
		polymer materials doped with	
		indandion derivatives	

**B.Sc. thesis** 

No	Author	Tittle	Supervisor
1.	J.Aleksejeva	Holographic recording in organic	Dr.phys. J.Teteris
		and inorganic compound by UV	
		laser	
2.	A.Apals	Research of water splitting process	Dr.phys. J.Kleperis
		in high frequency electric and	
2	I Plums	Investigation of structural changes	Dr phys G Childraidza
5.	J.DIUIIIS	in proton conducting polymer	Di.phys.O.Chikvaidze
		membranes using spectroscopic	
		methods	
4.	D.Bruvers	Determination of proton	Dr.phys.J.Kleperis
		conductivity in polymer	
		membranes	
5.	I.Dirba	Research of possibility to use	Dr.phys.J.Kleperis
		water electrolysis gases as fuel in	
6	I Caulto	Internal combustion engine	Manhua A Shanakavakia
0.	J.GIUDE	erbium jons in ovyfluoride glass	wig.phys. A.Shafakovskis
		and glass-ceramics	
7.	A.Jakimovics	Structure of Odd-Odd Nucleons	
		188Re in the framework of the	Dr.habil.phys.J.Tambergs
		Rotor plus two – quasiparticles	
		model	
8.	D.Kasjane	Spectral characteristics of	Dr.phys.L.Trinklere
		nanostructured AIN and related	
0	Е Изина	materials	Drahua IVIanaria
9.	E.Kullis	effectivity of solar heating system	DI.phys. J.Kiepens
10.	A.Mozers	Spectral characteristics of the III	Dr.habil.phys.I.Tale
		grup nitride thin films	f f f f f f f f f f f f f f f f f f f
11.	P.Nazarovs	Raman spectroscopy of ZnWO <sub>4</sub> -	Dr.phys.A.Kuzmins
		NiWO <sub>4</sub> system	
12	I Detersone	Class fibre surface modification	Dr. nhva W. Ealitia
12.	A. Dotrubing	Broportion of somiconductor	Dr.phys. P. Delekova
15.	A.reu unins	nanocrystals produced by a laser	DI.phys.B.Folakovs
		ablation	
14.	L.Shirmane	Luminiscence characteristics of	Dr.phys.V.Pankratovs
		nanocristalline yttrium-	1 5
		aluminium garnet	
15.	J.Timoshenko	Application of wavelet transform	Dr.phys.A.Kuzmins
		to Extended X-ray Absorption	
16	<b>T T T T T</b>	Fine Structure spectra analysis	D 1 1 1 1 1 1 1 D 1
10.	L. v aldere	Structure of defects in nano-size	Dr.naoii.pnys.U.Rogulis
17	M Chubarovs	Pure and doned III group nitrides	Dr hahil phys I Tale
1/.		thin films electrical properties	
18.	U.Gertners	Direct holographic recording of	Dr.phys. J.Teteris
		surface – relief grating on	1 5
		amourphous chalcogenide films	

19.	M.Kozlovskis	Water splitting with rotation and magnetic field influence	Dr.phys. J.Kleperis
20.	R.Lisovskis	Changes of the structure and micromechanical properties in LiF crystals induced by swift <sup>132</sup> Xe ions	Dr.phys.I.Manika
21.	E.Rancans	Determination of bonded hydrogen amount in the AB <sub>5</sub> type composite materials	Dr.phys.L.Grinberga
22.	R.Taukulis	Interferometer for nanometric displacement sensing	Dr.phys. V.Zauls
23.	R.Zabels	Zn – ZnO Nanocomposite coatings and structure modification during annealing in Zn-Zn-O	Dr.phys.F.Muktepavela

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

Prof. Dr. A.Krumins

# **CRYSTALS PHYSICS**

#### Head of Department Dr. phys. P. Kulis

#### **Research Area and Main Problems**

- 1. Recombination mechanisms of the electronic excitations in new optical binary and ternary compounds the project is aimed to investigate the exact mechanisms of annihilation, localization and recombination of the electronic excitations and their relationships in new binary and ternary inorganic compounds (nominally pure and doped with some active impurities).
- 2. 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.
- 3. 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 syntesized usig 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 NaYF<sub>4</sub>:Er, LaF<sub>3</sub>:Er and in chemically synthesized oxyfluorides.
- 4. 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 fotonic devices in joint stock company "Alfa".
- 5. The main goals of EURATOM project are investigation and characterization of the impurity content in fusion plasmas and reactor hot wall. 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 evaporated metal ions and the charge exchange emission during ionization of evaporated metal ions.

#### **Scientific Staff**

- 1. Dr. phys. L.Dimitrocenko
- 2. Dr. phys. A. Fedotovs
- 3. Dr. phys. P. Kulis
- 4. Dr. phys. B. Polyakov
- 5. Dr. habil. phys., asoc. prof. U. Rogulis

- 6. Dr. habil. phys. M. Springis
- 7. Prof., Dr. habil. phys. I. Tale
- 8. Dr. phys. E. Tamanis
- 9. Dr. phys. J. Trokss
- 10. Dr. phys. A. Veispals
- 11. Mg. E. Elsts
- 12. Mg. phys. J. Jansons

#### **Technical Staff**

J. Straumens

#### **PhD Students**

- 1. J. Butikova
- 2. A. Gulans
- 3. A. Sarakovskis

#### Students

- 1. J. Aizezers
- 2. Dz. Berzins
- 3. M. Cubarovs
- 4. G. Doke
- 5. M. Ezerins
- 6. J. Grube
- 7. G. Marcins
- 8. A. Petruhins
- 9. L. Vaidere

#### Scientific visits abroad

- 1. Dr. habil. phys. I. Tale, Italia, Rome 4 days;
- 2. Dr. habil. phys. I. Tale, Germany, Rostock, Julih, 5 days;
- 3. Dr. habil. phys. I. Tale, England, London, Cullham, 2 days;
- 4. Dr. phys. L. Dimitročenko, Šveice, Montrex, konference IWN-2008, 6 days;
- 5. Dr. habil. phys. U. Rogulis, Aracaju-SE-Brasil, 7 days;
- 6. Dr. phys. A. Fedotovs, Aracaju-SE-Brasil, 7 days;
- 7. Asist. E.Elsts, University of Antverpen, Belgium, 3 months;

# Cooperation

#### Latvia

Joint stock company "Alfa"

#### **Czech Republic**

Institute of Physics, Academy of Science of the Czech Republic Prague, Czech Republic (Dr. J. Rosa, Dr. M. Nikl).

#### 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" Achen, Germany
- 4. Max Plank Institute of Plasma Physics, Garching, Germany

#### Portugal

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

# Main results

#### INTRINSIC AND IMPURITY DEFECT LUMINESCENCE IN GaN-AIGaN ALLOY THIN FILMS

L. Dimitrocenko, J. Grube, P. Kulis, G. Marcins, B.Polyakov, A. Sarakovskis, M. Springis, I. Tale

Functional monocrystalline heterostructures of pure and Si-doped AlGaN alloys have been grown by metal organic chemical vapor deposition. Photoluminescence

spectroscopy of free electron – hole recombination at low temperature states that Sidoping enhances the concentration of both the cation vacancy and the complex Sivacancy centers as acceptors in donor – acceptor pairs. Fine structure of the luminescence spectrum is caused by both the intentionally doped donors and the compositional disorder of acceptors. The doped interface exists between layers with different composition.

#### AIGaN-InGaN-GaN NEAR ULTRAVIOLET LIGHT EMITTING DIODE

L. Dimitrocenko, J. Grube, P. Kulis, G. Marcins, B. Polyakov, A. Sarakovskis, M. Springis, I. Tale

A 382-nm InGaN/AlGaN light-emitting diode (LED) was made on a sapphire substrate by metal-organic vapour phase deposition (MOCVD) technique. Growing of the undoped and Si-doped GaN and  $Al_xGa_{1-x}N$  monocrystalline layers with a surface roughness of < 1 nm required for making light emitting devices has been carried out. To enhance the LED emission efficiency, a modified symmetric composition of an active single quantum well (SQW) structure was proposed. In addition to the conventional p-doped AlGaN:Mg electron overflow blocking barrier, an n-doped AlGaN:Si SQW barrier layer was formed in the structure that was meant to act as an additional electron tunnelling barrier.

#### EPR OF INTRINSIC RADIATION DEFECTS IN LiYF4 CRYSTAL

A. Fedotovs, U. Rogulis, L. Dimitrocenko

Electron paramagnetic resonance (EPR) spectra of a nominally pure LiYF<sub>4</sub> crystal were investigated after X-ray irradiation at room temperature (RT). The orientation of its optical axis c has been determined by means of optical polarization and the angular dependencies of the EPR spectra were measured in ab and ac planes. The obtained results showed the presence of a radiation-induced defect which is stable at RT. The broad EPR band of this defect in the X-microwave range is found to be structureless at RT. Basing on the estimated g-values, we suggest that the EPR spectra of the observed radiation defect could belong to an electron trap center. The structure of the spectrum could be resolved by measurements at 77 K. The spectra exhibit strong angular dependence, which is explained by the g-anisotropy and hyperfine interaction of the unpaired electron spin with two neighbouring fluorine nuclei.

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

#### A. Fedotovs, U. Rogulis, A. Sharakovskis, L. Dimitrocenko

We studied oxyfluoride composites based on a lithium silicate and borate glasses with fluorides, obtained at the ISSP of LU. EPR spectra were measured before and after X-ray irradiation at room temperature and at liquid nitrogen temperature. Fluoride crystallites within samples were created by means of thermal treatment at specific temperatures. EPR spectra of radiation defects in fluoride single crystals (LiF, LiBaF<sub>3</sub> and others) often showed well-pronounced hyperfine structure (hfs) caused by interaction with neighboring flourine nuclei. Radiation induced defects in oxyfluoride glass ceramics, in which crystallites have not yet created, shows no explicit hfs of fluorine nuclei. However in glass ceramics, which already contains fluoride crystallites, the hfs characteristic to fluorine nuclei appears in the EPR spectra.

#### STRUCTURE SENSITIVE INVESTIGATIONS ON LUMINESCENT CENTRES IN Mn-ACTIVATED LiBaF<sub>3</sub> DOSIMETERS

B. Henke<sup>\*</sup>, U. Rogulis, S. Schweizer<sup>\*</sup>

The structure sensitive investigations were done at the University of Paderborn by detecting the microwave-induced changes in the integral photoluminescence (PL) of LiBaF<sub>3</sub>:Mn single crystal for wavelengths longer than 550 nm. The investigations were carried out applying a microwave of 25 GHz (K-band) at a temperature of 1.5 K. The analysis of the angular dependent PL-EPR spectra, recorded for different orientations of the magnetic field, yielded that the 600 nm luminescence band is due to an excited triplet state (S = 1) of an manganese-related complex.

<sup>\*</sup>Department of Physics, University of Paderborn, Paderborn, Germany

#### TEMPERATURE EFFECTS IN UP-CONVERSION PROCESSES OF ERBIUM – YTTERBIUM DOPED OXYFLUORIDE SILICATE GLASS

#### J. Grube, A. Sarakovskis, L. Dimitrocenko, M. Springis

 $Er^{3+}$  - Yb<sup>3+</sup> doped oxyfluoride glass has been synthesized and investigated. It was found that the up-conversion luminescence spectrum of the sample excited by 980 nm laser diode is highly dependent on the temperature of the sample. Using fluorescence intensity ratio technique the green up-conversion emissions at 525 nm and 550 nm were studied in details in the temperature range 120 K - 600 K. The potential applicability of the obtained results in the field of the temperature sensing is discussed.

#### TIME-RESOLVED SPEKTROSCOPY OF UP-CONVERSION PROCESSES IN Er DOPED NaYF4 SILICATE GLASS CERAMICS

A. Sarakovskis, J. Grube, L. Dimitrocenko, M. Springis

Among a huge variety of up-converting materials (PbF<sub>2</sub>, CaF<sub>2</sub>, LaF<sub>3</sub> etc.), NaYF<sub>4</sub> doped with rare-earth ions is one of the most prospective ones. It can be explained by its low maximum phonon energy, which makes the probabilities of non-radiative transitions much lower than those for other crystals. Unfortunately NaYF<sub>4</sub> can not be obtained as a bulk crystal that minimizes its chances to be used for commercial purposes.

The aim of the current research was to study the energy relaxation mechanisms during up-conversion processes by means of spectral and time-resolved measurements both in glass and glass ceramics containing NaYF<sub>4</sub>:Er. For this purpose the transparent oxyfluoride silicate glass was synthesized. After the thermal treatment of the precursor glass oxyfluoride ceramics containing NaYF<sub>4</sub>:Er was obtained.

The well-known luminescence bands centred at 550 nm and 670 nm corresponding to optical transition in  $\text{Er}^{3+}$  ion have been observed in both the glass and glass ceramics samples under 450 nm and 980 nm excitation. The luminescence decay times of the green and red bands measured at 20 K for the glass differ from those measured for the glass ceramics; moreover a slow intensity rise prior to the decay of the red band is observed for the glass ceramics sample when measured at RT.

The obtained results allow us to consider that both excited state absorption and energy transfer mechanisms are involved in the creation of the luminescence, however their contribution at various energy relaxation stages appears to be different.

# UP-CONVERSION LUMINESCENCE STUDIES ON Er<sup>3+</sup>, Yb<sup>3+</sup> AND Tm<sup>3+</sup> DOPED OXYFLUORIDE GLASS AND GLASS CERAMICS

#### A. Sarakovskis, J. Grube, L. Dimitrocenko, S. Fomins, and M. Springis

In the past years much attention has been paid to the studies of up-conversion processes in the rare-earth doped phosphors related to the emission of higher-energy photons (VIS and UV) when excited by lower-energy photons (usually IR). The up-conversion process could be used in a wide range of applications like white light simulation, improvement of solar battery efficiency etc.

In this work  $Er^{3+}$ ,  $Yb^{3+}$  and  $Tm^{3+}$  doped oxyfluoride glass and glass ceramics containing fluoride crystallites were synthesized. Under IR excitation various luminescence bands corresponding to optical transitions in activator ions ( $Er^{3+}$  and  $Tm^{3+}$ ) were observed in the blue, green and red spectral regions. The relative intensities of the bands were found to be highly dependent on the doping levels of the activators, which might be attractive for white light simulation devices.

Based on the stationary and time-resolved luminescence measurements for the glass and glass ceramics different energy transfer mechanisms between rare-earth activators are discussed and possible application of the material in the high color and spatial resolution devices are considered.

#### Scientific publications

- 1. B. Henke, U. Rogulis, S. Schweizer, *Structure sensitive investigations on luminescence centres in Mn-activated LiBaF*<sub>3</sub> dosimeters, Radiation Measurements, 2008, vol. 43, pp. 319-322.
- L.Dimitrocenko, J. Grube, P. Kulis, G. Marcins, B. Polyakov, A. Sarakovskis, M. Springis, I. Tale, *AlGaN-InGaN-GaN near ultraviolet light emitting diode*, -Latvian Journal of Physics and Technical Sciences, 2008, vol.45, Nr.4, pp. 25-32.
- J. Grube, A. Sarakovskis, L. Dimitrocenko, M. Springis. *Temperature effects in up-conversion processes of erbium ytterbium doped oxyfluoride silicate glass*, Latvian Journal of Physics and Technical Sciences, 2008, vol.45, Nr.6, pp. 47-54.

#### **Books (in Latvian)**

- 1. J. Jansons. *Fotonu skaitīšana un tās lietojums* 2008., http://www.cfi.lv/resource/show/373
- 2. J. Jansons. Latvijas Universitātes Fizikas institūts (1919–1944) un tā sagatavotie fiziķi LU Apgāds, 2008., 220 lpp.

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

- 1. J. Jansons, *Fiziķis un pedagogs Andrejs Bumbērs (1887–1959) –* "Zvaigžņotā Debess", 2008. gada pavasaris (199), 27. 28. lpp.
- J. Jansons. Profesors Boriss Bružs (1897–1987) "Zvaigžņotā Debess", 2008. gada vasara (200), 24. – 26. lpp.
- 3. J. Jansons. *LU fizikas docents Arnolds Liberts (1888–1938) 120* "Zvaigžņotā Debess", 2008. gada rudens (201), 27. – 28. lpp.

4. J. Jansons. *Fizikas profesors Fridrihs Treijs (1887–1965) –* "Zvaigžņotā Debess", 2008./09. ziema (202), 25. – 26. lpp.

#### **Lectures on Conferences**

### 16<sup>th</sup> International Conference on Defects in Insulating Materials ICDIM2008, Aracaju-SE-Brasil

- 1. U. Rogulis, R.C. Baetzold, J.-M. Spaeth, *Luminescence-detected EPR of oxygenvacancy complexes in CaF*<sub>2</sub>, - Abstract of the 16<sup>th</sup> International Conference on Defects in Insulating Materials ICDIM2008, Aracaju-SE-Brasil, 2008, A031.
- A. Fedotovs, U. Rogulis, A. Sarakovskis, L. Dimitrocenko, *EPR of radiation defcts in Lithium-oxyfluoride glass-ceramics*, Abstract of the 16<sup>th</sup> International Conference on Defects in Insulating Materials ICDIM2008, Aracaju-SE-Brasil, 2008, A053.

# 24th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 20-22, 2008

- J. Grube, A. Sarakovskis, L. Dimitrocenko, M. Springis, *Temperature effects in up-conversion processes for erbium ytterbium doped oxyfluoride silicate glass*, - Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 14.
- A. Sakovskis, L. Dimitrocenko, J. Grube, M. Springis, Spectral and timeresolved studies of up-conversion luminescence in glass ceramics containing NaYF<sub>4</sub>: Er nanocrystals, - Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 15.
- 3. A. Fedotovs, U. Rogulis, A. Šarakovskis, L. Dimitročenko, *EPR of radiation defects in fluoride crystsals and oxyfluoride glass ceramics,* Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 16.
- I. Tāle, L. Dimitročenko, J. Grūbe, P. Kūlis, G. Mārciņš, B. Poļakovs, A. Šarakovskis, M. Spriņģis, *Eksitonu un piemaisījumu centru luminescence AlGaN sakausējumos*, - Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 23.
- L. Dimitročenko, B. Poļakovs, I. Tale, G. Mārciņš, GaN/AlGaN/ AlN pārklājumu iegūšanas metodika UV gaismas diožu struktūru veidošanai, - Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 24.
- O. Lielausis, A. Miķelsons, E. Platacis, A. Romanchuks, I. Tale, A. Šarakovskis, Development of a multi-jet gallium limiter for installation on the Tokomak Isttok, - Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 28 lpp.
- 7. J. Butikova, A. Šarakovskis, I. Tale, *Laser ablation spectroscopy of the first wall materials of ASDEX upgrade tokomak*, Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 29 lpp.
- 8. J. Jansons, Manuscript of the book "Physics Iinstitute of Latvia University (1919-1944) and its graduates, Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p. 43.
- B. Poļakovs, A. Petruhins, I. Tale, *Vacuum chamber for pulsed laser deposition*,
  Abstracts of the 24<sup>th</sup> Scientific Conference, 2008, p 70.

# International Baltic Sea Region conference "Functional materials and nanotechnologies", Riga, 2008

1. L. Dimitricenko, J. Grube, P. Kulis, G. Marcins, B. Polyakov, M. Springis, I. Tale, *Exciton and impurity Mg and Si luminescence in AlGaN alloys*, - Abstracts

of the International Baltic Sea Region conference "Functional materials and nanotechnologies", Riga, 2008, p.36, (oral presentation)

- 2. B.Polyakov, A.Petruhins, J.Butikova, A.Kuzmin, I.Tale, *Some aspects of pulsed laser deposition of Si nanocrystalline films*, Abstracts of the International International Baltic Sea Region conference "Functional materials and nanotechnologies", Riga, April 1-4, 2008. Abstract, p.50 (oral presentation).
- 3. A. Sarakovskis, J. Grube, L. Dimitrocenko, M. Springis, *Time-resolved spektroscopy of up-conversion processes in Er doped NaYF*<sub>4</sub> silicate glass ceramics, Abstracts of the International Baltic Sea Region conference "Functional materials and nanotechnologies", Riga, 2008, p.102, (poster presentation)
- 4. A. Petruhins, B. Polyakov, K. Smits, L. Grigorjeva, M. Springis, P. Kulis, I. Tale, *Pulsed laser deposition of ZnO and ZnO:Al thin films,* Abstracts of the International Baltic Sea Region conference "Functional materials and nanotechnologies", Rīga, April 1-4, 2008. Abstract, p.159 (poster presentation).
- 5. J. Butikova, A. Sharakovskis, I. Tale, *Laser-induced ablation spectroscopy for Deuterium detection in plasma facing components*, Abstracts of the International Baltic Sea Region conference "Functional materials and nanotechnologies", Riga, 2008, p.170, (poster presentation).

# 6<sup>th</sup> International Conference"Advanced Optical Materials and Devices", Riga, 2008,

- L. Dimitricenko, J. Grube, P. Kulis, G. Marcins, B. Polyakov, M. Springis, I. Tale, *Formation of deepAcceptor centres in AlGaN alloys*, - Abstracts of the 6<sup>th</sup> International Conference"Advanced Optical Materials and Devices", Riga, 2008, p.26, (oral presentation).
- 2. A. Sarakovskis, J. Grube, L. Dimitrocenko, S. Fomins, and M. Springis, Upconversion luminescence studies on Er<sup>3+</sup>, Yb<sup>3+</sup> and Tm<sup>3+</sup> doped oxyfluoride glass and glass ceramics, - Abstracts of the 6<sup>th</sup> International Conference"Advanced Optical Materials and Devices", Riga, 2008, p.51, (poster presentation).
- 3. J. Grube, A. Sarakovskis, L. Dimitrocenko, and M. Springis, *Spectral and timeresolved luminescence studies on oxyfluoride glass and glass ceramics containing LaF<sub>3</sub>:Er<sup>3+</sup>*, - Abstracts of the 6<sup>th</sup> International Conference"Advanced Optical Materials and Devices", Riga, 2008, p.54, (poster presentation).

# **DEPARTMENT OF DISORDED MATERIAL PHYSICS**

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

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

#### **Research area and Main Problems**

*Main problems*. Electronic processes, defect states and doping effects in simple and complex oxides in different forms: single crystals, nanocrystals, nanostructured ceramics, thin films, glasses, optical fibers. The main materials under studies: ZnO, ZrO<sub>2</sub>, YAG and YAP, ZnWO<sub>4</sub> and other tungstates, materials for persistent luminescence applications, pure and doped SiO<sub>2</sub> – based glasses for high transparency optics or optical fibers, crystalline SiO<sub>2</sub> 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,  $10^{12}$  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<sup>-1</sup> and 22000-7000 cm<sup>-1</sup> spectral regions).

Vacuum ultraviolet spectroscopy: McPherson 234/302 200mm monochromator with  $D_2$  lamp with MgF<sub>2</sub>-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	Defect studies Group	Laboratory of
radiation physics		Solid state optics
	Dr.habil.phys. A.Silins	
Dr.habil.phys.S.Chernov	Dr.habil.phys. L.Skuja	Dr.habil.phys.A.Trukhin
Dr.habil.phys. L.Grigorjeva		Dr.phys.K.Trukhins
Dr.habil.phys. D.Millers	Students	
Dr.phys. V.Pankratov	L.Tiluga	
Technical staff		
Eng. A.Sitdikov		
Eng. E.Arhipova		
Ph.D students		
K.Smits		
M.Shorokhov		
Students		
L.Bukonte		
L.Shirmane		

#### **Scientific Visits Abroad**

- 1. Dr.habil.phys.L.Grigorjeva, Estonia (14 days)
- 2. Dr.habil.phys. D.Millers, Poland (7 days)
- 3. Dr.phys. V.Pankratov (6 months)
- 4. K.Smits, Brazil (7 days)
- 5. K.Smits, Poland (7 days)
- 6. Dr.habil.phys.L.Grigorjeva, Poland (7 days)
- 7. Dr.habil.phys.L.Grigorjeva, France (6 days)
- 8. Dr.habil.phys.L.Grigorjeva, Poland (6 days)
- 9. Dr.habil.phys. D.Millers, Poland (6 days)
- 10. Dr.habil.phys. L.Skuja, Japan (2 months)
- 11. L.Shirmane, Germany (10 days)
- 12. Dr.habil.phys.L.Grigorjeva, Greece (6 days)
- 13. Dr.habil.phys. L. Skuja , France (6 days)
- 14. Dr.habil.phys. 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) Institute of Atomic Physics and Spectroscopy, University of Latvia (Prof.

J.Spigulis, Dr. A.Skudra)

#### USA

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

#### Estonia

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

#### Russia

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

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

#### Poland

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

#### Germany

Institute of Inorganic Chemistry University of Karlsrune (TH), (Prof.C.Feldman) **Denmark** 

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

#### Italy

University of Palermo (Prof. R. Boscaino, Dr. M. Cannas, Dr. S. Agnello) Japan

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

#### Scientific publications

- V.Pankratov, L.Grigorjeva, S.Chernov, T.Chudoba, W.Lojkowski. Luminescence properties and energy transfer processes in nanosized cerium doped YAG. IEEE Transact.on Nucl.Sci. 2008, vol.55, No.3, p. 1509-1513.
- 2. 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.
- 3. V.Skvorcova, N.Mironova, L.Grigorjeva, D. Millers, K.Smits. Transient and color centers in neutron irradiated MgO. Nucl.Instr. and Methods in Phys. Res.B (NIMB) vol.266, 2008, pp.2941-2944.
- 4. K.Smits, L.Grigorjeva, D.Millers, J.D.Fidelus, W.Lojkowski. Radiative decay of electronic excitations in ZrO<sub>2</sub> nanocrystals and macroscopic single crystals. IEEE Transactions on Nuclear Sci., v.55, No.3, 2008, p.1523-1526.
- L. Grigorjeva, D. Millers, J. Grabis, C.J.Monty, A.Kalinko, K. Smits, V.Pankratov and W.Łojkowski. Luminescence properties of ZnO nanocrystals and ceramics. IEEE Transctions on Nuclear Sci, vol.55, No.3, 2008, p.1551-1555.
- 6. 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.
- L. Skuja, K. Kajihara, M.Hirano, H.Hosono. Hydrogen-related radiation defects in SiO<sub>2</sub> - based glasses. Nuclear Instruments and Methods in Physics Research Section B. v.266, No12-13, p.2971-75 (2008).
- K. Kajihara, T. Miura, H. Kamioka, A.Aiba, M. Uramoto, Y. Morimoto, M. Hirano, L. Skuja, H. Hosono, Diffusion and reactions of interstitial oxygen species in amorphous SiO<sub>2</sub>: A review. J.Non-Crystalline Solids v.354, p.224-232(2008).
- 9. K. Kajihara, M. Hirano, L. Skuja, H. Hosono, Intrinsic defect formation in amorphous SiO<sub>2</sub> by electronic excitation: Bond dissociation versus Frenkel mechanisms, Phys. Rev. B78, p.094201(1-8) (2008).

#### **Lectures in Conferences**

# International Baltic Sea Region Conference "Functional materials and nanotechnologies 2008 (FM&NT)" April 1-4, Riga, Latvia.

1. L.Grigorjeva, D.Millers, K.Smits, W.Lojkowski, T.Chudoba, J.Fidelus, K.Bienkowski, J.Grabis, C.J.Monty. Luminescence of ZnO ceramics. Book of abstract, p.30.

2. K.Smits, D.Millers, L.Grigorjeva, A.Opalinska, W.Lojkowski. The site selective luminescence of  $Eu^{3+}$  in  $ZrO_2$  nanocrystals. Ibid, p.31.

3. V.Pankratov, L.Grigorjeva, L.Shirmane, W.Lojkowski, T.Chudoba. Perculiarities of luminescence properties of cerium doped YAG nanocrystals. Ibid, p.53.

4.J .D.Fidelus, L.Zych, K.Smits, D.Millers, L.Grigorjeva, K.Haqberko, W.Lojkowski. Advanced nanoporous zirconia ceramics for luminescent oxygen sensors. Ibid, p.55.

5. A.I.Popov, G.J.McIntyre, J.Zimmermann, V.Pankratov, C.Wilkinson, H.von Seggern. Evaluation of luminescent properties of neutron image plates. Ibid, p.90.

6. V.Pankratov, A.I.Popov, S.Chernov, C.Feldmann. Time-resolved luminescence of LaPO<sub>4</sub>:Ce, Tb nanophosphor. Ibid, p.92.

7. B.Polyakov, A.Petruhins, K.Smits, L.Grigorjeva, M.Springis, P.Kulis, I.Tale. Pulsed laser deposition of ZnO and ZnO:Al thin films. Ibid, p.159.

8. F.Muktepavela, G.Bakradze, L.Grigorjeva, R.Zabels, A.Gerbreders, E.Tamanis, A.Presz. Effect of the annealing on structure and properties of ZnO films obtained by mechanoactivated oxidation. Ibid, p.172.

9. A.Presz, W.Lojkowski, J.D.Fidelus, L.Grigorjeva, F.Muktepavela, J.Grabis, C.J.Monty. Visualization of ZnO nanostructures by scanning electron microscopy. Ibid, p.173.

10. L.Skuja, K.Kajihara, M.Hirano, H.Hosono, A.Silins, Spectroscopic signatures of hydrogen in oxygen deficiency - related centers in amorphous SiO<sub>2</sub>, ibid, Poster Po90.

# LU CFI 24<sup>th</sup> Scientific Conference

1.A.Kalinko, A.Cimmermane, L.Grigorjeva, G.Mežinkis, K.Smits. The luminescence of ZnO embedded in PVOH polimer matrix. Abstracts, p.17.

2. M.Šorohov, L.Grigorjeva, D.Millers. Low temperature luminescence of the TlBr crystals: growth methods dependence. Ibid, p.18.

3. K.Smits, D.Millers, L.Grigorjeva, J.D.Fidelus, W.Lojkowski. Eu<sup>3+</sup> luminescence of ZrO<sub>2</sub> nanocrystals. Idid, p.20.

#### International Conference Defects in Insulating Materials (ICIDIM2008), 24-29 August, Aracaju, Brazil

1. K.Smits, D.Millers, L.Grigorjeva, J.D.Fidelus, W.Lojkowski. Defects and charge transferin ZrO<sub>2</sub>. Abstracts, A178. Aviable on CD.

2. L.Skuja, K.Kajihara, M.Hirano, H.Hosono. Vacuum-UV range optical absorption on oxygen dandling bonds in amorphous SiO<sub>2</sub>. Ibid, A183.

15<sup>th</sup> International conference on Luminescence and Optical Spectroscopy of Condensed Matter. 7-11 July, 2008, Lion, France

1. L.Grigorjeva, D.Millers, V.Pankratov, K.Smits, C.J.Monty, J.D.Fidelus. The luminescence in ZnO, ZnO:Ce and ZnO:Gd powders. Book of Abstracts, p.158.

# The second International Workshop on Advanced Spectroscopy and Optical Materials, 13-17 July, 2008, Gdansk, Poland.

1. L.Grigorjeva, D.Millers, K.Smits, V.Pankratov, W.Lojkowski, J.Fidelus, K.Bienkowski, C.J.Monty. Excitonic luminescence of ZnO nanopowders and ceramics. Book of Abstracts, p.2-P-4.

2. D.Millers, L.Grigorjeva, K.Smits, A.Opalinska, W.Lojkowski. Photo- and cathodoluminescence of ZrO<sub>2</sub>:Eu nanocrystals Ibid, p.5-P-1.

# The 6<sup>th</sup> International Conference "Advanced Optical Materials and Devices" 24-27 Aug., 2008, Riga, Latvia.

1. M.Knite, L.Bukonte, V.Tupureina, L.Grigorjeva, D.Millers, K.Smits, J.Grabis. Fast luminescence of ZnO embedded into polimer matrices. Abstracts, O5-7.

# European Materials Research Society (E-MRS) Fall Meeting. 15<sup>th</sup>-19<sup>th</sup> September, 2008, Warsaw, Poland.

1. J.Kouam, J.D.Fidelus,L.Grigorjeva, A.Kuzmin, F.Sandiumenge, L.Balcells, M.S.Martin-Gonzalez, C.J.Monty. Nanostructural characterization and nagnetic properties of pure and Fe, Co or Mn-doped TiO<sub>2</sub> nanopowders prepared by Solar Physical Vapor Deposition (SPVD). Book of Abstracts, p.117.

2. J.Fidelus, L.Zych, D.Millers, K.Smits, L.Grigorjeva, W.Lojkowski, K.Gaberko. Advanced nanoporous yttria-stabilized zirconia ceramics for luminescence oxygen sensors. Ibid, p.204.

3. L.Grigorjeva, D.Millers, K.Smits, W.Lojkowski, J.Fidelus, k.Bienkowski, T.Chudoba, C.Monty. ZnO ceramic sintering and luminescence properties. Ibid, p.219.

4. D.Millers, L.Grigorjeva, K.Smits, J.Fidelus, A.Opalinska, W.Lojkowski. Excitation transfer in zirconia nanocrystals and ceramics. Ibid, p.219.

5. K.Smits, D.Millers, L.Grigorjeva, A.Sarakovskis, A.Opalinska, J.Fidelus, W.Lojkowski. Eu luminescence in zirconia nanocrystals. Ibid, p.220.

# 2<sup>nd</sup> International Symposium on Transparent Conductive Oxides. 26-28 Oct., 2008, Crete, Greece.

1. L.Grigorjeva, D.Millers, K.Smits, J.Fidelus, W.Lojkowski, T.Chudoba, K.Bienkowski, C.J.Monty. Time-resolved luminescence spectra of ZnO nanopowders and ceramics. Abstract, P-5.

2. F.Muktepavela, G.Bakradze, L.Grigorjeva, R.Zabels, E.Tamanis. Properties of ZnO coatings obtained by mechanoactivated oxidation. Ibid, P-130.

# 7<sup>th</sup> International Symposium on SiO<sub>2</sub>, advanced dielectrics and related devices, June 30- July 2, St. Etiennne, France.

1. L.Skuja, K. Kajihara, M.Hirano, H.Hosono. Hydrogen hyperfine interactions in E'type centers in synthetic silica glass, Abstracts, p.15.

2. A.N.Trukhin, J. Teteris, A. Fedotovs, D. L. Griscom, G. Buscarino. Photosensitivity of SiO<sub>2</sub>-Al and SiO<sub>2</sub>-Na glasses under ArF (193 nm) laser, Abstracts, p.17.

3. A.N.Truhin. Luminescence of polymorph crystalline and glassy SiO<sub>2</sub>, GeO<sub>2</sub>. Abstracts, p.65

# SOLID STATE OPTICS LABORATORY

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

#### **Research area and Main Problems**

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

#### Scientific staff

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

#### **Scientific Visits Abroad**

- Professor, Dr. hab. Phys. A. Trukhin, Symposium SiO<sub>2</sub> Advanced Dielectrics and Related Devices, Centre de Congrès de Saint-Etienne (France), June 30 - July 2, 2008
- 2. Dr. Phil., Dr. Phys. K.Truhins, USA, Postdoctoral position at University of Illinois at Chicago, Chicago, Illinois, USA

# Cooperation

#### Russia

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)

#### Germany

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

#### USA

Glass 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. Naionale 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

#### RECOMBINATION LUMINESCENCE OF OXYGEN-DEFICIENT CENTERS IN SILICA

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The luminescence of pure dry silica glasses prepared by PCVD and KS-4V methods was studied under ArF laser pulses in range of temperatures 10-300 K. The PCVD samples were of two kinds: one is amorphous, as received at temperatures below glass-forming temperature  $T_g$  and second was fusion-affected sample. The only observed luminescence was luminescence of oxygen deficient centers (ODC) with spectrum corresponding to twofold-coordinated silicon modified with surrounding and excited in recombination process. There is a correspondence in properties between KS-4V silica and fused PCVD silica. Amorphous PCVD silica has no luminescence at that condition. So, fusion process stimulates formation of ODCs. The decay kinetics possesses fast and slow components and the slow component of the ODC blue band is faster and of the UV band is slower than for lone twofold coordinated silicon agreeing with recombination process of luminescence excitation. The model of processes is presented as charge separation under excitation with creation of a nearest self-trapped hole and electron trapped on the twofold-coordinated silicon modified by surrounding.

#### SELF-TRAPPED EXCITON SINGLET – TRIPLET SPLITTING IN THE CRYSTALS WITH α-QUARTZ STRUCTURE: SiO<sub>2</sub>, SiO<sub>2</sub>-Ge, GeO<sub>2</sub>, AIPO<sub>4</sub> AND GaPO<sub>4</sub>

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A fast component of the self-trapped exciton (STE) luminescence was discovered in the crystals with  $\alpha$ -quartz structure: SiO<sub>2</sub>, SiO<sub>2</sub>-Ge, GeO<sub>2</sub>, AlPO<sub>4</sub> and GaPO<sub>4</sub>, manifesting the singlet – singlet transitions of STE. Comparison of time resolved PL spectra of triplet – singlet transition and fast singlet – singlet transitions allows estimate singlet – triplet splitting of STE in pure SiO<sub>2</sub>  $\alpha$ -quartz crystal by value 0.2 eV. In the cases of others crystals the singlet – triplet splitting there is smaller than 0.2 eV. Small singlet – triplet intervals is witnessing that electrons of the STE are not confined in one atom's area.

#### PHOTOLUMINESCENCE EXCITED BY ArF AND KrF LASERS AND OPTICAL ABSORPTION OF STISHOVITE MONO-CRYSTAL

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Two photoluminescence bands were found in silicon dioxide stishovite mono-crystal sample under ArF (193 nm) and KrF (248 nm) excitation. The blue band is situated at 3.17±0.02 eV in the case of ArF and at 3±0.2 in the case of KrF. The UV band is at 4.5±0.05 eV in the case of ArF and at 4±0.05 eV in the case of KrF. The position of the UV band compared with experiment of x-ray excited luminescence, where it is 4.6±0.05 eV with FWHM 0.8±0.05 eV (Solid State Communications, 127 (2003) 415). The blue band possesses slow decay kinetics with time constant  $16\pm 2 \mu s$  and UV band is fast on the level of 2±0.5 ns. Thermal quenching of both bands is started for T higher than 150 K. The activation energies are similar for intensity and time constant, and are equal 0.23±0.01 eV; 0.13±0.01 eV for blue and UV band correspondingly with equal values of frequency factor 2.10<sup>11</sup> s<sup>-1</sup>. Optical absorption contains several bands at 4.5 eV, at 5.5 eV, at 7 eV and strong band starting from 7 eV adjoining intrinsic absorption threshold above 8.75 eV. Excitation at 7.86 eV (F<sub>2</sub> laser) does not provide luminescence. The nature of luminescence excited in the transparency range of stishovite is ascribed to a defect presumably created by previous irradiation of the crystal. Similarity of the stishovite luminescence with that of oxygen-deficient silica glass and induced by radiation luminescence of a-quartz crystal allow conclude similar nature of centers in those materials.

#### Scientific publications

- A.N.Trukhin ,K.M.Golant ,Y.Maksimov ,M.Kink, R.Kink, Recombination luminescence of oxygen-decient centers in silica, Journal of Non-Crystalline Solids 354 (2008) 244-248.
- A N Trukhin, Self-trapped exciton singlet-triplet splitting in crystals with α-quartz structure: SiO<sub>2</sub>, SiO<sub>2</sub>-Ge, GeO<sub>2</sub>, AlPO<sub>4</sub> and GaPO<sub>4</sub>, 2008 J. Phys.: Condens. Matter 20 125217 (5pp).
- 3. A.N. Trukhin ,T.I.Dyuzheva ,L.M.Lityagina, N.A. Bendeliani, Photoluminescence excited by ArF and KrF lasers and optical absorption of stishovite mono-crystal J.Phys.: Condens. Matter 20 (2008) 175206 (5pp).

#### **Presentation at conferences**

- 1. A N Trukhin, Self-trapped exciton singlet–triplet splitting in crystals with  $\alpha$ -quartz structure: SiO<sub>2</sub>, SiO<sub>2</sub>–Ge, GeO<sub>2</sub>, AlPO<sub>4</sub> and GaPO<sub>4</sub>, 24. CFI LU Zinātniskās konferences referātu tēzes, Rīga, Latvija, 20.-22. Februāris 2008, 13.lpp.
- 2. A.N. Trukhin, J.Teteris, A.Fedotov, Photosensitivity of SiO<sub>2</sub>-Al and SiO<sub>2</sub>-Na glasses under ArF (193 nm) and F<sub>2</sub> (157 nm) lasers, book of abstract of Intern. Baltic Sea region conference "Functional materials and nanotechnologies 2008, Institute of Solid State Physics, University of Latvia, Riga, Latvia, p. 35.
- 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, Book of Abstracts: 7 Symposium SiO2 Advanced Dielectrics and Related Devices, Centre de Congrès de Saint-Etienne (France), June 30 - July 2, 2008, p.17
- 4. A.N. Trukhin, Luminescence of polymorph crystalline and glassy SiO2, GeO2, Book of Abstracts: 7 Symposium SiO2 Advanced Dielectrics and Related Devices, Centre de Congrès de Saint-Etienne (France), June 30 July 2, 2008, p.65-66.

# **DEPARTMENT OF FERROELECTRICS**

#### Head of Department Dr. phys. V. Zauls

#### **Research Area**

The Division of Ferroelectric Physics is involved in 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 scaning microscopy with EDX option, full range of dielectric impedance and hysteresis measurement tools, optical studies with emphasis on ellipsometry and reflectometry. Recently more attention has been directed towards environmentaly friendly lead-free ferroelectrics and materials for energy applications.

#### Main research topics in 2008

- Theoretical modelling of the structural phase transitions in ferroelectric materials with microscopic scale features determined by a connection between classical and quantum physics.
- Synthesis of ferroelectric ceramics including wide range of traditional compositions; lead free niobates; transparent PLZT ceramics; production of customized targets for Pulsed Laser Deposition (PLD).
- Development of ferroelectric materials for future thermonuclear reactor diagnostics applications.
- Investigation of surface microstructure and composition of ceramics and thin films by optical microscopy, SEM, and EDX.
- Nanoscale piezoresponse, AFM imaging, and patterning of ferroelectric and relaxor thin films.
- o Dielectric impedance spectroscopy and characterization of functional materials.
- Investigation of physical properties gradients, thickness and interface effects in the crossection of thin films and multilayer coatings studied by optical reflectometry and ellipsometry
- Optical measurements and materials for vision science; studies of eye aberration dynamics by high-speed Hartmann-Shack aberrometer; applications of PLZT ceramic and polymer dispersed liquid crystal (PDLC) passive and active optical elements for bio-optical experiments and medicine.

#### 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. Marite Kalnberga
- 16. Mg. chem. Anna Kalvane
- 17. Mg. phys. Karlis Kundzins

#### Visitors from Abroad

#### Technical staff

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

#### PhD students

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

#### **Graduate Students**

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

**Prof. A. Kholkin**, Departmet of Ceramic and Glass Engineering, Research Unit on Ceramic Materials, University of Aveiro, Portugal.

**Dr. Qi Zhang**, Materials Department, Microsystems and Nanotechnology Centre, Cranfield University, UK.

#### Scientific Visits Abroad

#### Mg. Maija Antonova

1. Symposium "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius, Lithuania, June 15-19, 2008.

#### Dr. phys. Ilze Aulika

- 1. LUSSI, Blois, France, January 21-24, 2008.
- 2. Institute of Physics, Prague, Czech Republic, February 21-26, 2008.
- 3. Symposium "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius, Lithuania, June 15-17, 2008.
- 4. Jozefa Stefana Institute, Ljubljana, Slovenia, June 18-21, 2008.
- 5. International Conference "Electroceramics XI", Manchester, UK, August 31 September 05, 2008.
- 6. Institute of Physics, Prague, Czech Republic, and L.O.T.-Oriel GmbH & Co seminar, Darmstat, Germany, October 20 November 1, 2008.

#### Dr. phys. Karlis Bormanis

- 1. 18th Conference on Ferroelectric Physics, VKS-18, Sanct-Petersburg, Russia, June 9-14, 2008.
- 2. Symposium "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius, Lithuania, June 15-19, 2008.
- 3. 9<sup>th</sup> European Conference on Applications of Polar Dielectrics, ECAPD'9, Roma, Italy, August 26-29, 2008.

#### Dr. sc. ing. Maruta Dambekalne

- 1. Symposium "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius, Lithuania, June 15-19, 2008.
- 2. International Conference "Electroceramics XI", Manchester, UK, August 31 September 05, 2008.

#### Dr. phys. Eriks Klotins

- 1. Fundamental Physics of Ferroelectrics 2008, Colonial Williamsburg, VA, February 10-13, 2008.
- 2. Russia/CIS/Baltic/Japan Symposium on Ferroelectricity RCBJSF-9, Vilnius, Lithuania, June 15-19, 2008.
- 3. International Conference in Statistical Physics 2008, Kolympary Chania, Greece, July 14-18 2008.
- 4. International Conference "Frontiers of Quantum and Mesoscopic Thermodynamics", Prague, Czech Republic, July 28 August 2, 2008.

#### Mg. phys. Maris Livins

1. Symposium "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius, Lithuania, June 15-19, 2008.

#### Dr. phys. Anatoly Mishnev

1. Seminar "X-ray reflectometry & Texture Analysis", company PANalytical, Almelo, Netherlands, June 8-14, 2008.

#### Mg. ing. Ilze Smeltere

1. Jozef Stefan Institute, University of Ljubljana, Slovenia, June 18-21, 2008.

2. LUSSI Blois, France, January 21-24, 2008.

#### Dr. habil. phys. Andris Sternberg

- 1. 18th Conference on Ferroelectric Physics, VKS-18, Sanct-Petersburg, Russia, June 9-14, 2008.
- 2. Symposium "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius, Lithuania, June 15-19, 2008.

#### Dr. phys. Vismants Zauls

- 1. LUSSI, Blois, France, 21.-24.01.2008.
- 2. Conference "The 8<sup>th</sup> Russia/CIS/Baltic/Japan Symposium on Ferroelectricity", Vilnius (Lithuania), 15.-17.06.2008.
- 3. Jozef Stefan Institute, Ljubljana, Slovenia, 18.-21.06.2008.
- 4. Conference "Electroceramics XI", Manchester (UK), 31.08.-05.09.2008.
- 5. L.O.T.-Oriel GmbH & Co seminar, Darmstat, Germany, 20.10.-1.11.2008.

# Cooperation

#### Latvia

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

#### Austria

1. Faculty of Physics, University of Vienna (Prof. A. Fuith).

2. Atomic Institute of Austrian Universities, Technical University Vienna (Prof. H.W. Weber).

#### Belorussia

1. Institute of Solid State Physics and Semiconductors, National Academy of Science, Minsk (Prof. N.M. Olekhnovich).

#### **Czech Republic**

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

#### Denmark

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

#### Finland

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

#### Japan

- 1. Shonan Institute of Technology (Prof. S. Sugihara).
- 2. Shizuoka Institute of Science and Technology (Prof. T. Ogawa).

#### Lithuania

1. Vilnius University, Vilnius (Prof. J. Banys).

#### Poland

1. Institute of Physics, Krakow Pedagogical University, Krakow

(Prof., Dr.Phys. hab. Cz.Kus, Dr. B.Garbarz – Glos, Prof., Dr.Phys.hab. J.Suchanich).

#### Portugal

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

#### Russia

- 1. Ural State University, Ekaterinburg (Prof. V. Shur).
- 2. Volgograd State Architectural and Engineering 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).
- 6. Dagestan State University (S.A. Sadikov).
- 7. Laboratory of Adaptive Optics, Moscow State University (A.Larichev, N.Iroshnikov).

#### Slovenia

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

#### Spain

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

#### **Main results**

#### SYNTHESIS AND CHARACTERIZATION OF Sb-SUBSTITUTED (K<sub>0.5</sub>Na<sub>0.5</sub>)NbO<sub>3</sub> PIEZOELECTRIC CERAMICS

M.Dambekalne, M.Antonova, M.Livinsh, A.Kalvane, A.Mishnov, I.Smeltere, R.Krutokhvostov, K.Bormanis, and A.Sternberg

In the present work lead-free piezoelectric ceramics (K<sub>05</sub>Na<sub>0.5</sub>)NbO<sub>3</sub> were prepared by addition of 0.5 mol%MnO<sub>2</sub> as a sintering aid, and effect of Sb<sup>5+</sup> substitution for Nb<sup>5+</sup> on the Curie temperature, structure, dielectric and piezoelectric properties was studied. KNN and the KNNSb<sub>x</sub>+0.5MnO<sub>2</sub> (x = 0, 0.02, 0.04, 0.05, 0.06, 0.07 and 0.10) ceramics were sintered from 1050° to 1170°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 of undoped KNN was assumed 1160°C for 4 h. At this temperature the density of ceramics reached 4.26 g/cm<sup>3</sup> (94.5% of TD) and sintering shrinkage was 19.0%. After adding 0.5 mol.% MnO<sub>2</sub> the optimal sintering temperature of KNN ceramic rapidly decreases to 1100°C and sintering density reaches 4.35 g/cm<sup>3</sup> (96.5%TD). The optimal sintering tempe-rature of Sb substituted KNN ceramics occurs within 1110° - 1140°C range of temperature and sintering density reaches 4.40g/cm<sup>3</sup> (97.6% of TD). It must be noted that the density was very sensitive to the variation of sintering temperature in a narrow range, which decreased when the sintering temperature was only  $10^{\circ} - 20^{\circ}$ C lower or higher than the optimal one. It can be observed, that the Sb substitution has no significant effect on the densification of the ceramics, unlike Sb, the sintering aid MnO<sub>2</sub> improves the densification effectively. The co-effects of MnO<sub>2</sub> doping and Sb substitution lead to significant improvements in dielectric and piezoelectric properties of KNN.

The co-effects of MnO<sub>2</sub> doping and Sb<sup>5+</sup> substitution lead to significant improvement in dielectric and piezoelectric properties:  $\varepsilon$  at the T<sub>c</sub> increased from 6000 (KNN) to 12400 (x=0.04), d<sub>33</sub> = 92 ÷ 192pC/N, k<sub>p</sub> = 0.32 ÷ 0.46, k<sub>t</sub> = 0.34 ÷ 0.48.



SEM HV: 3.00 kV WD: 13.8030 mm  $10 \mu \text{m}$ SEM of KNN at  $1160^{\circ}$ C.

SEM of KNN+0.5MnO<sub>2</sub> (x = 0) at  $1100^{0}$ C.



SEM of  $KNNSb_x$  (x = 0.06) (without MnO<sub>2</sub>) at 1140<sup>o</sup>C.

SEM of KNNSb<sub>x</sub>+0.5MnO<sub>2</sub> (x = 0.06) at 1130<sup>o</sup>C.



Temperature dependence of the dielectric permittivity  $\varepsilon$  (Fig.a) and losses tand (Fig.b) for (K<sub>0.5</sub>Na<sub>0.5</sub>)NbO<sub>3</sub> and (K<sub>0.5</sub>Na<sub>0.5</sub>)Nb<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub> + 0.5mol%MnO<sub>2</sub> ceramics, where x = 0 ÷ 0.10 at 1 kHz.



Temperature dependence of phase transitions of  $(K_{0.5}Na_{0.5})Nb_{1-x}Sb_xO_3 +$ 0.5mol%MnO<sub>2</sub> ceramics, where  $x = 0 \div$ 0.10: orthorthombic to tetragonalferroelectric (T<sub>O-T</sub>) and ferroelectrictetragonal to paraelectric-cubic (T<sub>c</sub>).



Variations of piezoelectric properties ( $d_{33}$ ,  $k_p$  and  $k_t$ ) with x ( $K_{0.5}Na_{0.5}$ )Nb<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub> + 0.5mol%MnO<sub>2</sub> ceramics.

#### OPTICAL GRADIENT OF THE TRAPEZIUM-SHAPED NaNbO<sub>3</sub> THIN FILMS STUDIED BY SPECTROSCOPIC ELLIPSOMETRY

#### I. Aulika, A. Dejneka\*, V. Zauls, and K. Kundzins

Thickness gradient NaNbO<sub>3</sub> (NN) thin films (Fig. 1.) were made by the pulsed laser ablation technique on Si/SiO<sub>2</sub>/Ti/Pt/SrRuO<sub>3</sub> substrate to study the variation of the optical properties with the sample thickness.

Ellipsometric studies of the optical gradient of NaNbO<sub>3</sub> thin films were performed in the photon energy range of 1.24 - 4.96 eV. Effective values of the complex refractive index and thickness non-uniformity, roughness and depth profile of the real part of the refractive index *n* were evaluated.

An exponential growth of the refractive index as the function of thickness was established (Fig. 2b). With increase of the thickness, n close to the bottom of the film decrease, but closer to the top of the film increase. This explains why effective values of the host material of NN are almost constant with the thickness (Fig. 2a). With increase of the thickness



**Fig. 1.** Illustrative pictures of the multilayer structure of the NN thin film. In direction from the bottom to the top: Silicon Si, Silicon dioxide SiO<sub>2</sub>, titanium Ti, platinum Pt, strontium ruthenium oxide SrRuO<sub>3</sub>, NN thin film with different thickness (graded color of the film illustrates depth profile of the refractive index) and a top layer of the surface roughness.

the value of the exponent has a tendency to increase, while the variation range of the refractive index reaches its maximum value around 200 nm and then decreases (Fig. 2c). The real reason of such behavior is under further investigation now, but we suppose that it could be caused by stress and strain distribution in gradient structure.

\* Institute of Physics, Academy of Science, Czech Republic



**Fig. 2.** Dispersion of the effective refractive index of the NN at the different thicknesses (a) (nm) and thickness non-uniformity (%). Depth profile of the refractive index n as faction of the film thickness (b). Value of the exponent and variation range of n versus thickness (c).

#### PHASE TRANSITIONS IN THE PLZT x/85/15 SOLID SOLUTIONS

E. Birks, I. Aulika, M. Antonova, A, Fuith\*, A. Sternbergs

Transparent lanthanum doped lead zirconate titanate  $Pb(La_xZr_{1-y}Ti_y)O_3$  (PLZT x/85/15, x = 1, 2, 4, 5, 6 and 8, y = 15) ceramics were produced from PLZTx powder, synthesized using peroxohydroxopolymer (PHP) method, by a two-stage hot-pressing sintering process. The role of La in  $Pb_{1-x}La_x(Zr_{1-y}Ti_y)O_3$  solid solutions were investigated by thermal expansion and thermo-elastic measurements.

The thermal dependence of elastic modulus has a different behaviour at La concentration range below and above 4 % (Fig. 1a). The rather abrupt drop of elastic modulus (Fig. 1b) if temperature is approaching phase transition from high temperature side with following smooth increase below phase transition temperature for compositions with  $x \le 4$  corresponds to behaviour, derived from thermodynamic description of 1<sup>st</sup> order FE phase transition and is related to electrostrictive coupling of polarisation with mechanic deformation. It should be noted that such thermal dependence of elastic modulus is observed also for composition x = 4, where the low temperature phase apparently is AFE. Therefore the two sublattice thermodynamic description could be more appropriate for description of elastic properties in x/85/15 solid solutions with La concentrations up to 4 %. At higher La concentrations thermal dependence of elastic modulus at phase



Fig. 1. Thermal expansion (a) and thermal dependence of elastic modulus (b) of PLZT x/85/15 compositions with a) x = 1, 2, and b) x = 4, 5, 6, and 8.

transition gradually transfers to a quite symmetric minimum and apparently reflects relevant decrease of jump thermal expansion. The influence of La on nature of dielectric permitivity in x/85/15 comparing with PLZT of lower Zr/Ti ratio is described by more pronounced decreasing of stability of ferroelectric phase if concentration of La increases. In concentration range from x = 4 the polar microregions coexist with macroscopic antiferroelectric phase. Diffused maximum of dielectric permittivity, observed above x = 4, is described by thermal behaviour of noninteracting polar microregions.

\* Faculty of Physics, University of Vienna, Austria

#### SCATTERING AND DEPOLARIZATION IN A POLYMER DISPERSED LIQUID CRYSTAL CELL

Juan M. Bueno<sup>\*</sup>, Maris Ozolinsh and Gatis Ikaunieks

An imaging polarimeter in transmission has been used to explore the effects of scatter and depolarization induced by a polymer dispersed liquid crystal cell. The experiment was carried out for three visible wavelengths. Both a directional and a scattered component can be distinguished in the light transmitted by this material. Whereas the directional component increased with voltage, the scattered portion decreased. This was a common behaviour for all three wavelengths. The polarimetric analysis revealed that the degree of polarization was also affected by changes in the voltage applied to the cell. Depolarization effects in the scattered component were usually high and decreased with voltage. However those associated with the directional part were low for high voltages and also increased when reducing the voltage.

<sup>\*</sup>Laboratorio de Óptica (Dpto. Física), Universidad de Murcia, Spain

#### PHOTOINDUCED AsSeS THIN FILM PHASE PLATES AS ADAPTIVE OPTICS MIRRORS FOR EYE ABERRATION CORRECTION

S.Fomins, M.Reinfelde, A.Larichev<sup>\*</sup>, N.Iroshnikov<sup>\*</sup>, A.Gerbreders, M.Ozolinsh

Amorphous chalcogenide thin films are an excellent material for holographic recordings. AsSeS thin film coating is a usefull optical material for it's thickness to be easly corrected with the use of exposure to light and consecutive chemical etching. Following properties allow to treat the surface of AsSeS chalcogenide films and to use them in adaptive optics systems for correction of the optical wavefront. Hereby, we characterize AsSeS film properties to be used for correction of optical aberrations of the human eye. The thickness of the film is characterized.

<sup>\*</sup>Laboratory of Adaptive Optics, Moscow State University, Russia

#### FERROELECTRIC LIQUID CRYSTAL GLASSES FOR AMBLYOPIA RESEARCH

Sergejs Fomins, Maris Ozolinsh, Gunta Krumina, and Varis Karitans

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 0.0002 s. FLC filters can be used as the optical shutters for machine vision purposes, also in vision research. On the basis of FLC filters we have developed ferroelectric glasses, allowing temporal separation 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 an appliance for dynamic visual system training to promote the functionality of the worse-seeing eye. For fast switching the filters are powered by a 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 shutters open-close state are controlled through the PC parallel port. The main application of the system is use for amblyopia research and training.

#### INTRINSIC LOCALIZED EXCITATIONS IN NONLINEAR LATTICES: CLUES TO THE NATURE OF POLAR NANOREGIONS

#### E. Klotins

The study is addressed to a topical problem of self-localization in a class of complex oxides categorized as ferroelectric relaxors. Basically, their anomalous and technologically important features are associated with the dynamics of microscopic scale polar regions supported by somewhat artificial metastable entities. A unified approach to the spontaneous emergence and stability of the polar nanoregions is assigned to intrinsic localized excitations in Hamiltonian lattices with nonlinearity and nonGibbsian statistics as necessary and sufficient ingredients of the theory.

The concern is extension of the pioneering mathematically driven results in toy lattices [S. Flach and A. Gorbach, Physics Reports 467, 1-116 (2008)] toward the

systems with dipole-dipole interactions and other specific features supporting the localized excitations in ferroelectric materials.

The working definition capturing long time stability, as well as the fact that localized excitations are triggered at a variety of initial conditions arrive from statistical explanation essentially different from conventional grounds [B. Rumpf, Phys Rev. E 69, 016618 (2004)].

Going from toy Hamiltonians toward the first-principles effective ones the lattice dynamics is represented by conservation of energy in localized excitations. Figure 2 illustrates time development of energy in elementary lattice  $i \in [1,31]$  starting with a targeted initial state in sites  $i \in [11,21]$ . Due the nonlinearity of the problem the energy remains constant, spatially localized at sites  $i \in [11,21]$  so constituting the existence proof of localized excitation.



Fig.1. Illustrative diagram of localization transition distinguished by entropy as a function of total energy  $E_{<}$  and particle number  $A_{<}$  captures essential features of ferroelectric relaxors. The two colors divide the Gibbsian (pink online) from the nonGibbsian (red/yellow online) behavior. Within the negative total energy and positive thermodynamic temperature there is no localization. Otherwise, the temperature is negative at positive total energy and the linear mode is getting unstable.


Fig 2 Spatially localized, time-periodic and long lived excitation in Hamiltonian system with quartic local and dipole-dipole type intersite potentials. Time (in arbitrary units) covers five periods of optical mode.

Assignment polar nanoregions as having the status of intrinsic localized excitations shed a light on their emergence, slow relaxation, and energy/entropy balance. The problems in progress includes linear (in)stability and superimposing lattice dynamics with emergence of symmetry breaking and nonzero dipole moments.

Further developments could help the essence of aforementioned problems to be revealed.

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- 3. Ilze Aulika, Alexandr Dejneka, Vismants Zauls, and Karlis Kundzins. Optical Properties of BST/PZT Nanocomposite Superlattices Studied by Spectroscopic ellipsometry. Abstract book, p. 61.
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- 7. E. Klotins. Critical Mode Coupled to the Heath Bath and Implications of ab initio Thermodynamics. Abstract book, p. 98 (invited).
- 8. M. Palatnikov, O. Shcherbina, N. Sidorov, K. Bormanis. Domain Structure Of Lithium Niobate Single Cystals Containing Lanthanide Admixtures. Abstract book, p. 154.
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- 1. Maris Ozolinsh, Michéle Colomb, and Gatis Ikaunieks. Light Scattering and Visual Performance. Abstracts, p. 46.
- 2. G. Krumina, G. Ikaunieks, and M. Ozolinsh. The Perception of Isoluminant Coloured Stimuli of Amblyopic Eye and Defocused Eye. Abstracts, p. 47.
- 3. A. Sarakovskis, J. Grube, L. Dimitrocenko, S. Fomins, and M. Springis. Up-Conversion Luminescence Studies on Er<sup>3+</sup>, Yb<sup>3+</sup> and Tm<sup>3+</sup> Doped Oxyfluoride Glass and Glass Ceramics. Abstracts, p. 51
- 4. P. Chufyrev, N. Sidorov, M. Palatnikov, and K. Bormanis. Manifestation of Structural Features in Raman Spectra of LiNbO<sub>3</sub> Single Crystals. Abstracts, p. 71.
- 5. S. Fomins, M. Ozolinsh, G. Krumina, and V. Karitans. Ferroelectric Liquid Crystal Glasses for Vision Research. Abstracts, p. 88.
- 6. Gatis Ikaunieks, and Maris Ozolinsh. Factors Affecting Intraocular Light Scattering from Different Color Straylight Sources. Abstracts, p. 89.
- 7. V. Karitans, M. Ozolinsh, and G. Kuprisha. Electronic Eye Occluder with Time-Counting and Reflection Control. Abstracts, p. 90.
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- Jan Macutkevic, Saulius Rudys, Juras Banys, Ramunas Adomavicius, Gintaras Valusis, Arunas Krotkus, Robertas Grigalaitis, Andris Sternberg, and Karlis Bormanis. Soft Mode Behavior in (1-x)PMN-xPSN Ceramics. Abstracts and CD proceedings, N-034-P.

# 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 Xray absorption, EXAFS), electrical and electrochemical impedances, AFM, TGA/DTA, etc
- Solid state ionics:
  - electro-, photo-, thermo-, chemo- or gaso-chromic phenomena in transition metal oxides
  - structural changes due to ion intercalation
  - lattice dynamics and structural and electronic phase transitions
  - solid state reactions at interfaces electrode solid electrolyte
  - gases and ions sensing phenomena and detection technologies
- Functional coatings and multi layer electrochemical systems
- Hydrogen absorption phenomena in metals, semiconductors and insulators
- Development of hydrogen generation equipment and new nano structured materials for hydrogen storage
- New measurement technologies and instruments with artificial intellect (incl., eNose)
- Development methods and techniques for quality and reliability testing for lead -free joints of PCB

# Scientific staff

- 1. Dr.phys. P.Cikmacs
- 2. Dr.chem. G. Bajars
- 3. Dr.phys. V.Eglitis
- 4. Dr.phys. J.Gabrusenoks
- 5. Dr.phys. L.Grīnberga
- 6. Dr.phys. R.Kalendarjovs
- 7. Dr.phys. U.Kanders
- 8. Dr.phys. J.Kleperis

- 9. Dr.phys. J.Klavins
- 10. Dr.phys A.Kuzmins
- 11. Dr.phys. A.Lusis
- 12. Dr.phys. E.Pentjuss
- 13. Dr.hab.phys. J.Purans
- 14. Dr.phys. V.Ogorodņiks
- 15. Dr.chem. G.Vaivars
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# 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, Faculty of Medicine, Riga, Latvia;
- 3. Riga Technical University (RTU) Institute of Biomaterials and Biomechanics (Dr. I.Lasenko)
- 4. Riga Technical University Institute of Inorganic Chemistry (Dr. J. Grabis, Dr. I.Zalite, Dr. A. Dindune).
- 5. Latvian Academy of Science Institute of Physical Energetics (Prof. N.Zeltins)
- 6. Latvian Electroindustry Business Innovation Centre (LEBIC).
- 7. Riga City Council Environmental Department.

# Estonia

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

# France

CRMC-N, Universite de la Mediterranee (Aix-Marseille II) (Marseille, France) - Prof. Y.Mathey, Eng. D. Pailharey, Prof. D. Tonneau.

# China

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

# **Czech Republic**

Institute of Physics of the Academy of Sciences (Prague, Czech Republic)– Dr.O.Šipr.

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2. Tuebingen University – U. Weimar, N. Papamichail

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

# Norway

Institute for Energy Technology, Kjeller

# Poland

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# 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

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

NOSE2 – EC Network of Excellence on Artificial Olfactory Sensing (Partners from ISSP: Dr.J.Kleperis, Dr.A.Lusis).

# Main results

# DEVELOPMENT OF NANOSTRUCTURED AND FUNCTIONAL MATERIALS

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

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

Analysis of the symmetry of lattice vibrations of WOCl<sub>4</sub>, WO<sub>2</sub>Cl<sub>2</sub> and WO<sub>3</sub> has been carried out in the work. Symmetry and form of vibrations which correspond to lattice deformation changing to a lower symmetry have been determined. Vibrations involving oxygen and chlorine atom have been identified. Symmetry of vibrations and their activity in IR and Raman spectra has been determined. The results of calculation have been compared with Raman spectra.

**Development of leaching technology and sonochemistry for nanostructuring and funtionalization technical silicate glass fibers**. The main research activities are related to study influence of ultrasound on leaching kinetics of glass fibers and pores structure. The leaching of groups of atoms or ions from multi component non-crystalline solids in acid electrolytes is one of technologies for making materials with defined nanostructures for design of new functional composites. The materials for functionalization are used technical silicate glass fibers from A/S VSŠ: E and K glasses fibers. E glass is based on calcium alumoborosilicates and K glass is based on sodium alumosilicates. 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 influences of ultrasound on leaching process versus temperature and time have been studied. The leaching process is changing a surface morphology of glass fibers as well as internal nanostructure of glass fibers by forming pores. In paper will be presented results of investigations about influence of

- ultrasound on leaching kinetics of glass fibers and pores structure,
- ultrasound and leaching temperature and time on glass fibers and pores structure,
- physical and chemical treatment of leached glass fiber on the adsorptiondesorption properties,
- mass loses of fibers.

The mass loses of glass fibers are important characteristic for understanding leaching mechanism and for analyzing influence of leaching products on fiber properties. The mass loses, e.g., for **E** glass fibers leached in 1N H<sub>2</sub>SO<sub>4</sub> solution 30 minutes at 90±2  $^{0}$ C with and without US are 31% un 19% accordingly. The ultrasound in temperature range 42-92  $^{0}$ C enlarges mass losses by 11-12% and changes the pore structure. The pore size 2-15 nm with specific 0,1-300 m<sup>2</sup>/g for leached fibers have been obtained. The shrinking of glass fibers leached at 80  $^{0}$ C with and without ultrasound are 13% and 11% accordingly.



The ultrasound shifted pores distribution to micropores direction and reduced volume of mesopore.

# LOCAL STRUCTURE STUDIES BY EXAFS WITH FEMTOMETER ACCURACY

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

The dependence of the dynamical properties of crystals on the isotopic composition is of primary importance. The force constants depend on atomic species and crystal structure.

The zero-point amplitude of atomic vibrations is however influenced also by the nuclear masses, the lighter isotopes undergoing larger oscillations than the heavier ones. As a consequence of anharmonicity, the difference in zero-point amplitude of motion reflects on a difference of interatomic equilibrium distances and lattice parameters. In the case of germanium, the expected relative change in the lattice parameter between <sup>70</sup>Ge and <sup>76</sup>Ge is as small as  $\Delta a/a \approx 5 \times 10^{-5}$ . Note that these effects, of genuine quantum origin, progressively disappear when temperature increases.

An investigation of the isotopic effect on the amplitudes of nearest-neighbours relative vibrations (parallel mean square relative displacement (MSRD)) and on the nearest-neighbours average distance in powdered samples of <sup>70</sup>Ge and <sup>76</sup>Ge has been performed by extended x-ray absorption fine structure (EXAFS) spectroscopy.

Two highly isotopically enriched Ge samples with the degrees of enrichment 98.2% for  $^{70}$ Ge and 99.9% for  $^{76}$ Ge have been produced at the Kurchatov Institute (Russia), and their Ge K-edge EXAFS spectra have been recorded with high accuracy from 20 to 300 K at beamline BM29.

The difference of the MSRD values for two isotopes has been clearly evidenced (Figure 1) and is in good agreement with a behaviour expected from the Einstein model based on the single force constant  $k_0=8.496(40) \text{ eV/Å}^2$  and two characteristic frequencies: 7.70(2) THz for <sup>70</sup>Ge and 7.39(2) THz for <sup>76</sup>Ge.

The effect of isotopic mass has been revealed also in thermal expansion (Figure 2). The zero-point values of the nearest-neighbours average distance measured by EXAFS are consistent with the values of distance between average positions measured by Bragg diffraction, once the effects of vibrations perpendicular to the bond are taken into account. The possibility of detecting relative distance variations smaller than 10 femtometers by means of a conventional transmission EXAFS apparatus and a standard procedure of data analysis has been demonstrated.



Fig. 1: Difference of the EXAFS MSRDs as a function of temperature for the two isotopes <sup>70</sup>Ge and <sup>76</sup>Ge. The solid line shows the difference between two Einstein models.



Fig. 2: Difference of the nearest-neighbors average interatomic distance in <sup>76</sup>Ge and <sup>70</sup>Ge, determined from EXAFS analysis (diamonds), compared with the difference of distances between average positions determined from x-ray backscattering (circles).

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

J. Kleperis, L. Grīnberga, G. Vaivars\*, G. Chikvaidze, G. Bajārs, J. Hodakovska, M. Vanags, V. Ņemcevs, A. Purviņš<sup>1</sup>, O. Krievs<sup>1</sup>, L. Ribickis<sup>1</sup>, E. Rancāns<sup>2</sup>, J. Blūms<sup>2</sup>, D. Bruvers<sup>2</sup>, E. Kums<sup>2</sup>, M. Kozlovskis<sup>2</sup>, I. Dirba<sup>2</sup>, J. Zalāns<sup>3</sup>, J. Vinklers<sup>3</sup>, I.Klepere<sup>4</sup> Institute of Solid State Physics of University of Latvia; \*In collaboration with University of the Western Cape, Institute of Advanced Material Chemistry, Cape Town, South Africa;

*I* – *Riga Technical University, Institute of Industrial Electronics and Energetics;* 

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

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

4 – Student from Biological Faculty of University of Latvia

**Research of hydrogen absorption/desorption phenomena in new composite materials for hydrogen storage.** A Sievert type instrument was purchased thanks to the State research program in material sciences. This instrument determines the amount of gas sorbed by measuring pressure changes in a reservoir of known volume and temperature. By knowing the initial and final pressure and volume of a sample chamber the quantity of gas absorbed or desorbed by the different samples like metals, ceramics and polymers, is calculated. There can be performed pressure-composition isotherm (PCT) and cycle life measurements where the tolerance of the sample to various atmospheres can be determined. The PCTPro-2000 uses advanced software for automation of the experimental measurements. An experimental range of pressure lies between 0.01 and 200 bars and temperatures in a sample chamber can be set up from cryogenic to 400°C. A new instrument is operated by Hydrogen material laboratory. An approbation of PCTPro-2000 and the first measurements of absorbed and desorbed amount of hydrogen of hydrides and composites were made using palladium samples.



*Figure 1.* Hydrogen absorption/desorption curve of palladium powder sample measured at RT with PCT Pro-2000 instrument.

Water electrolysis using DC power modified with short time pulses. Water electrolysis in Hydrogen Economy is considered as the source of "green" hydrogen when energy (light & electricity) is taken from renewables (sun, wind, hydropower, biomass etc.). Therefore it is important to make electrolysis process as efficient as possible. Commercial electrolysers based on alkali electrolyte waste noticeable energy in heat due ohmic losses in highly conductive electrolyte. We used clean water based electrolysis cell with electrodes of special configuration and surface coatings, and high frequency and high voltage power. Deionized and degassed water is excellent dielectric (water molecules are very polar (has  $\varepsilon_r = 80.1$  at 20 °C), therefore the cell made as cylindrical capacitor (an inner cylinder with radius *a* enclosed by an outer cylinder with radius *b*, both with length *L*) has capacitance  $C = \frac{2 \cdot \pi \cdot \varepsilon_r \cdot \varepsilon_0 \cdot L}{\ln\left(\frac{b}{r}\right)}$ . Making circuit from

capacitance (electrolysis cell) and coil with changeable inductance  $\Delta L$ , the resonance

frequency is  $f = \frac{1}{2\pi \cdot \sqrt{\Delta L \cdot C}}$ . We applied mono-polar AC voltage to power this circuit

and tried to find resonant frequency, when the power consumed by electrolysis cell will be minimal. Interesting step-charging effect was noticed when limited number of current pulses was applied to circuit.

Different tests were made using AC voltage with amplitude from 10 mV to 5 kV. From impedance measurements the resonant frequency was determined at 31 kHz, but it changes with amplitude of applied voltage. At higher potentials peculiar phenomena of water atomization was observed in space between electrode plates.

**Usage of gases from water electrolysis as fuel in internal combustion engines.** The number of cars is increasing year by year by tens millions. Largest producers in the world are Japan, Germany, China and United States of America. Only in 2006 there were manufactured 49,886,549 cars. There are around one billion traffic units on roads today in the entire world, and <sup>3</sup>/<sub>4</sub> from them are older 8-10 years. The fuel consumption is larger for older vehicles, and exhausts contain more harmful gases and particles (nitrogen oxides, carbon monoxide, hydrocarbons and soot or particles). The researchers of ISSP UL and company "Hydro Energo Ltd" developed additional unit for cars - air refining system HE2 for internal combustion engines, reducing

concentration of harmful exhaust gases and decreasing fuel consumption. Analysis is made for factors influencing an efficiency of electrolysis unit built in this system. Optimization of self built electrolyser is performed accordingly technical demands of standard gasoline car. Firsts test showed fuel economy (Table 1), but further experiments necessary to test an influence of addition of water electrolysis gases to fuel – how the composition of exhausts will change.

1,8L gasoline engine with Mono Jetronic fuel injection system		
Measurements	Without HE2	With HE2
CO concentration, vol %	2,41	0,60
CH <sub>x</sub> concentration, ppm	155	93
Fuel consumption: liters/100km	8,2	6,2

Table 1. Tests results of vehicle without and with air refining system built in motor.

The diffusion of water and methanol and thermal changes in proton conducting membranes. The polymer electrolyte membrane fuel cells (PEMFC) are used as new power sources for automotive and portable devices. Nafion<sup>®</sup> is mostly used membrane in PEMFCs nowadays. Although this membranes show high proton conductivity and good chemical stability, its high cost makes them problematic for commercial purposes. Besides, both automotive and stationary applications require membranes, able to operate at higher temperatures and having the lower methanol permeability. In collaboration with Institute of Advanced Material Chemistry of University of Western Cape (South Africa), new SPEEK based membranes were made and tested as proton conducting polymers.



*Figure 2*. Diffusion crossover of methanol in self-made SPEEK and commercial Nafion proton exchange membranes measured by FTIR-ATR spectroscopy.

Fourier Transform Infrared and Attenuated Total Reflectance (FTIR-ATR) spectroscopy was used to measure the diffusion and sorption of both methanol and water in Nafion<sup>®</sup>, Fumasep<sup>®</sup>, Fumapem<sup>®</sup> and self-made SPEEK polymer membranes. Spectra were recorded in transmission and ATR modes using the Bruker Equinox55 FTIR spectrometer (400–6000 cm<sup>-1</sup>, resolution 1 cm<sup>-1</sup>). The methanol and water concentration in membranes as well as the effective mutual diffusion coefficient was determined. It was observed that self-made SPEEK membranes shown reasonable decrease of the methanol crossover as compared to commercial membranes (Figure 2). Spectra of membranes measured at higher temperatures indicated that the modified SPEEK membranes preserve their structure at temperatures higher then 130°C.

**Research of temperature distribution on the surface of steel coated with different light absorbing layers.** People needs for energy are growing, but nature resources such as oil, gas, coal are not inexhaustible. It is important to acquire alternative energy resources; and one of them is solar energy. We can use solar energy in two ways – with solar photovoltaic elements to produce electric energy and with solar thermal collectors to produce hot water or air. Usually copper plate is used for absorber of solar collector, but that makes collector expensive. An aim of this work is to replace the copper with stainless steel in solar collector and to test the efficiency of possible cheaper collector.



*Figure 3.* Heat absorption research of steel plate with light absorbing coating for efficient solar absorbers.

To increase efficiency of steel collector, different coatings were tested and compared. Most efficient coating was made from acetylene burning in air atmosphere at 450 °C, and Raman spectra of this layer showed that partly oriented carbon nanotubes can be formed (Figure 3). Next task is to improve carbon coating technology by increasing part of oriented carbon nanotubes, as well as an adhesion of coating to steel substrate.

## APPLICATION TECHNOLOGIES OF AN ELECTRONIC NOSE AND INSTRUMENTS FOR AIR QUALITY CONTROL

V. Ogorodniks, N. Jurks<sup>1</sup>, I. Taivans<sup>1</sup>, A. Osite<sup>2</sup>, A. Viksna<sup>2</sup>, S. Jankovska<sup>3</sup>, J. Kleperis<sup>4</sup> Institute of Solid State Physics of University of Latvia; 1 - Medical Faculty of University of Latvia; 2 - Chemical Faculty of University of Latvia; 3 - Geography and Earth Science Faculty of University of Latvia; 4 - In collaboration with Department of Environment, Riga City CouncilDiagnostic of lung's diseases patients with the electronic nose.

The aim of this investigation was to identify odours characteristic for lung cancer of lung disease patients by comparing breath patterns of specific lung's diseases, and by comparing patients before surgical operation (removal of a sick part of a the lung) and after.



*Figure 1.* Scatter plot of canonical scores for breath samples from healthy people and patients with lung cancer and other lung diseases (asthma, COPD, pneumonia and past operation - removed lung cancer).

From the results obtained from number of patients the online diagnostics method will be developed to screen the typical lung's diseases guided by comparison odours in data base. Important tasks will be the development of the conception of instrument for online diagnostics of expired breath and to find most suitable types of sensors to be used in screening procedures. The results with gas chromatograph indicated some characteristic peaks of specific volatile organic compounds found only for most of patients with lung cancer. To date, it is unknown which volatile compounds are responsible for the response of sensors of e-nose. We assume that sensors are responding to combined effects of microbial metabolites and volatile cellular compounds in breath of patients. The most important results are received in the discriminate analysis. It was shown that lung cancer can be easy discriminated from another lung's diseases, using short breath sampling times and short analysis time (shorter than 1 minute) – see Figure 1. Volatiles from cancer are giving largest part in the responses of different sensors in e-nose. Further development of this approach is necessary to develop the new screening and monitoring methods.

Research of air quality in Riga. Air quality levels in larger cities are elevated due to a combination of high vehicle emission densities, large coherent urban areas, and often poor dispersion conditions due to street canyons. In street canyons, which are common in central parts of European cities, the dispersion is restricted by the building geometry causing higher pollution. At the same time urban areas have high population density and the population exposure to air pollution poses a significant health risk. Traffic air pollution is the major source of degradation of air quality in larger cities. Human exposure to traffic air pollution in major cities poses a significant public health risk as numerous studies have shown that exposure to air pollution increases risks of developing cancer, respiratory and allergy diseases, and aggravates the condition of people suffering from respiratory or heart diseases. Pollutants of concern are particles, nitrogen dioxide and somewhere ozone. Evaluation of air quality monitoring data has revealed that air quality limit values and target values for PM10 and NO<sub>2</sub> are currently exceeded in the large number of European cities, Riga including. In this situation the municipalities had to develop an Action Program for the reduction of air pollution. Accordingly to Regulations of the Latvian Cabinet of Ministers № 588 On Air Quality (2003), municipality of Riga developed Action Program with number of actions stipulating the direct measures to improve air quality. Analysis is made on results of different activities – is air pollution in city centre decreasing

### **RESOURCE SCIENCE AND SUSTAINABLE DEVELOPMENT**

# G. Bajārs, A. Lūsis, Ē. Pentjušs

Participation of ISSP in two EC financed projects "GreenRoSE" and "EcoDesign" as well as in activities organized by Ministries of Economics and Environment (for example, investigation contract EM 2006/11: "Handbook for implementation of RoHS directive in Latvian E&E industry"), from one side, and from other side - EU concept of Sustainable Development and Lisbon strategy give us possibility to continue new research area related to resources science.

Now one of basic issues of knowledge based economy is sustainable development. We need technologies and products with zero impact on environment, e.g. clean technologies and products with minimal material and energy consumption. The civilization faces-off with resource problems, first of all with energy resources. Now the civilization faces before challenge what we have to do. The material science and solidstate ionics close related to such technologies, for example, technologies of electrochemical energy generation and accumulation. We have to create new area of knowledge based on natural sciences (physics, chemistry and biology) named resource science (resource physics, resource chemistry and resource biology).

The first steps to build up some framework as driving force is EU directives (RoHS and EuP–EcoDesign) and activities of implementation of them.

# 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. Available services for quality and reliability testing:

### Tests for lead-free materials applied in PCB assemblies

- 1. Chemical test methods
- 2. Mechanical test methods
- 3. Flammability

4. Miscellaneous for analysis of RoHS Directive restricted elements and materials *Tests for PCB with lead-free finishes* 

1. Visual and dimensional examination

- 2. Surface conditions tests
- 3. Mechanical test methods\*
- 4. Electrical tests
- 5. Environmental tests

*Tests for lead free components for SMT and THT* 

- 1. Visual and dimensional examination
- 2. Surface conditions tests

*Tests for PCB assemblies* 

1. Visual and dimensional examination

2. Miscellaneous test (Analysis of metallographic cross-section of solder joints; pull test)

Prepared and published (in Latvian) guidelines about RoHS and handbook for SMEs on internet: <u>http://www.em.gov.lv/em/images/modules/items/item\_file\_13148\_1.doc</u>

http://www.letera.lv/pic/rohs\_direktīva.doc

## EFFECTS OF EXTERNAL ENERGETIC FACTORS ON TRITIUM RELEASE FROM THE EXOTIC 8-3/13 NEUTRON-IRRADIATED BERYLLIUM PEBBLES

J. Tīliks\*, A. Vītiņš, G. Ķizāne\*, V. Tīlika\*, E. Kolodinska\*, S. Kalēja\*, B. Leščinskis\*;

\* - Laboratory of Radiation Chemistry of Solids, Institute of Chemical Physics, University of Latvia, Kronvalda bulvāris 4, LV-1010 Riga, Latvia

Tritium release from samples of 9-13 mg of the EXOTIC 8-3/13 neutronirradiated beryllium pebbles under the separate and simultaneous action of temperature 490-770 K, 5 MeV fast-electron radiation 14 MGy·h<sup>-1</sup> for 3 h and magnetic field (MF) of 1.7 T was investigated. Annealing of Be samples about 9-13 mg was performed in a continuous flow of the purge gas He + 0.1% H<sub>2</sub> of the rate 14-15 L/h without and in MF of 1.7 T and/or 5 MeV fast-electron radiation of the dose rate P=14 MGy·h<sup>-1</sup> in a special rig (Fig. 2).



Fig. 2. Scheme and photo of the rig for tritium release experiments under separate or simultaneous action of temperature up to 850 °C, 5 MeV fast-electron radiation of the dose rate  $P=14 \text{ MGy}\cdot\text{h}^{-1}$  and magnetic field of 1.7 T.

The pebbles were found to be very dissimilar with respect to their total tritium content – 2.5-9 MBq·g<sup>-1</sup>. The batch contained also some coarse agglomerates of the pebbles containing 10-19 MBq·g<sup>-1</sup> of tritium having also a high tritium release. For the pebbles having the total tritium 2.5-5.3 MBq·g<sup>-1</sup>, the electron radiation for 3 h caused the fractional tritium release 17-26 % (B=0) and 21-29 % (B=1.7 T), the temperature of the pebbles being <550 K (Fig. 3a). The annealing of the pebbles at the temperature ramp at 5 K/min to 553 K and at 553 K for 3 h caused the fractional tritium release 10-19 % (B=0) and 14 % (B=1.7 T). For the pebbles having the total tritium 3.6-5.8 MBq·g<sup>-1</sup>, the annealing of the pebbles at the temperature ramp at 5 K/min to 770 K and at 770 K for 1 h caused the fractional tritium release 17-24 % (B=0) and 25 % (B=1.7 T), but with the

simultaneous additional action of the electron radiation for 3 h the fractional tritium release was 24-42% (B=0) and 32-37% (B=1.7 T) (Fig. 3b).



**Fig. 3.** Values of the fractional release of tritium from the samples of the EXOTIC 8-3/13 Be pebbles having the initial total tritium activity 2.5-5.3  $MBq\cdot g^{-1}$  (a) and 3.6-8.6  $MBq\cdot g^{-1}$  (b) at the temperature  $\leq 553$  K for 3 h (a) and 770 K for 1 h (b) without or with electron radiation of P=14 MGy·h<sup>-1</sup> for 3 h and without or with MF of 1.7 T. Values of the initial total tritium activity (MBq·g<sup>-1</sup>) are given as labels to the data points.

### **Scientific Publications**

- 1. L.Grinberga, J.Kleperis, G.Bajars, G.Vaivars, A.Lusis (2008) Estimation of hydrogen transport mechanisms in composite materials. *Solid State Ionics, Vol.179,2009, Issues 1-6,* pp. 42-45.
- J. Purans, N.D. Afify, G. Dalba, R. Grisenti, S. De Panfilis, A. Kuzmin, V.I. Ozhogin, F. Rocca, A. Sanson, S.I. Tiutiunnikov and P. Fornasini. Isotopic effect in extended x-ray-absorption fine structure of germanium, *Phys. Rev. Lett.* 100 (2008) 055901:1-4.
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# **Participation in Conferences**

# 1. Annual 24rd Conference of Institute of Solid State Physics of University of Latvia, February 20-22, 2008, Riga, Latvia:

- 1) J. Blums, G. Chikvaidze, G. Vaivars, Peculiarities in the optical and vibrational spectra of polymeric membranes.
- 2) D. Bruvers, J. Kleperis, L. Grinberga, G. Vaivars. Conductivity measurement methodology and results of proton conducting membranes.
- 3) J. Hodakovska, Polymer membranes for fuel cells synthesis and properties.
- 4) M. Vanags, V. Nemcevs, J. Kleperis, Water electrolysis with high voltage and high frequency method.
- 5) L. Grinberga, Hydrogen safety aspects in a laboratory and daily life. Annual 24rd Conference of
- 6) J. Zalans, J. Vinklers, J. Kleperis, B. Skele, Practical demonstration of membrane electrode assembly MEA and attainable power.

- 7) A. Apals, M. Vanags, Influence of magnetic field to water electrolysis in cell with cylindrical electrodes.
- 8) V. Ogorodnik, J. Kleperis, Use of sensor controls with expanded opportunities for diagnostics of social and environmental problems.

# 2. International Baltic Sea Region Conference "Functional materials and nanotechnologies" FM&NT-2008, Riga, April 1-4, 2008:

1) L. Grinberga, J. Kleperis, E. Rancans, preparation and properties of nanocomposite metal hydride battery electrodes.

2) G. Vaivars, Sivapregasen Naidoo, Qiling Ying, V. Linkov, Low temperature quaternary catalyst synthesis used for methanol and hydrogen oxidation on MWCNT.

3) L. Khotseng, S. Feng, G. Vaivars, Nickel nanostructures synthesized using template method.

4) H. Luo, G. Vaivars, R. Mohamed, V. Linkov, Cross – linked PEEK – WC proton exchange membranes for fuel cell.

5) G. Chikvaidze, G. Vaivars, H. Luo, J. Kleperis, FTIR-ATR study of protonnation and thermal changes in commercial and home-made membranes.

6) J. Kleperis, L. Grinberga, G. Chikvaidze, J. Gabrusenoks, A. Lusis, J. Klavins, Hydrogen built-up peculiarities based on metal hydride and inorganic carrier nanoparticles.

## 3. International conference Eco-Balt 2008, May 15-16, Riga:

- 1) J. Kleperis, Riga's First Action Plan To Improve Air Quality (2004-2008) Comparison With Actions Plans Of European Cities.;
- 2) M. Vanags, J. Kleperis, Water splitting into hydrogen and oxygen using water dielectric properties;
- 3) S. Jankovska, I. Steinberga, J. Kleperis, Particulate Matter Monitoring Results In Typical Street Canyon (Riga Case Study;.
- 4) L. Grinberga, J. Kleperis. Safety Aspects In Hydrogen Economics.
- 5) <u>G.Bajārs</u>, A.Vīksna (2008) Green chemistry study course at the University of Latvia (oral).

# 4. 5th Baltic Conference on Electrochemistry (BEC-5) Tartu, Estonia, April 30 – May 3, 2008

- 1) L. Grinberga, J. Kleperis G. Vaivars, Different additives and binders in the cathode fr NiMH batteries
- 2) M. Vanags, G. Bajars, J. Kleperis, A. Lusis. Influence of high voltage AC and magnetic field on water electrolysis.
- 3) J. Hodakovska, H. Luo, G. Vaivars, G. Chikvaidze, J. Kleperis. Characterization of sulfonated poly(ether ether ketone) polymer membranes for fuel cells.
- 1. IX Meeting "Fundamental problems of Solid State Ionics", June 24. 27, 2008, Chernogolovka (Russia):
  - 1) J.Hodakovska, J.Kleperis, L.Grinberga, G. Vaivars "Conductivity measurement of mixed polymer membranes for fuel cells";
  - 2) G. Chikvaidze, G. Vaivars, H. Luo, J. Kleperis, FTIR-ATR study of the diffusion of water and methanol and thermal changes in convention and home-made polymer membranes;

- 3) G. Vaivars, Development of Nanostructured materials for Hydrogen Economy devices;
- 4) L. Grinberga, J. Kleperis, Safety conditions for hydrogen systems.

# 6. International Seminar on Materials for Hydrogen Energy, devoted to European Regional Fund Project No. VPD1/ERAF/CFLA/05/APK/2.5.1./000066/033 "New materials and electronics for hydrogen energy systems", Sigulda (Latvia), March 27-28, 2008:

- 1) G. Vaivars, Strategy of development of materials for hydrogen energy.
- 2) L. Khotseng, Hydrogen and Fuel cell development in South Africa.
- 3) Luo Hongze, Membranes for fuel cells and electrolysers,
- 4) G. Bajars, Eco design and energy.
- 5) G. Chikvaidze, Vibration spectroscopy in application to hydrogen materials.
- 6) I. Purvins, I. Steiks, Direct current converter for fuel cell system.
- 7) E. Rancans, Properties of metal hydride electrodes in dependence from impurities and additives.
- 8) Dirba, Addition of water electrolysis gases to gasoline in an internal combustion engines.

# 7. International conference on Engineering Education in Sustainable Development, Graz, Austria, September 22-24, 2008:

G.Bajars, A.Lusis, A.Ubelis (2008) Integration of ecodesign course in design studies at the University of Latvia. Abstracts of Engineering Education in Sustainable Development 2008 Conference, Graz, Austria, p.49. (oral)

## 8. Invited talk at the Ångström Laboratory, Uppsala, Sweden, December 03, 2008:

J. Purans "EXAFS studies of local structure with *femtometer accuracy : Present* Status and Future Perspectives" (oral presentation).

# 9. Invited talk at the Max-Plank Institute of Solid State Research, Sttutgart, March 26, 2008:

J.Purans " EXAFS studies with femtometer accuracy of isotopic effects and local structure of solid solutions: Present Status and Future Perspectives" (oral presentation).

# LABORATORY OF DIDACTIC SYSTEM

# Head of Laboratory – Prof., Dr.phys. J.Kuzmin

## **Research Area and Main Problems**

Research field of the Laboratory is related to

• investigation of possibilities to use internet technology to create new methods of eeducation;

• development, application and education on cluster computing.

# **Scientific Staff**

- 1. Prof., Dr.phys. J.Kuzmin
- 2. Dr.phys. A.Kuzmin

### Students

- 1. Nikolais Jovlevs
- 2. Mārcis Galiņš

### Didactic Laboratory activities at the University of Latvia

- 1. LU PPF "Operational Systems" lectures, Prof. J.Kuzmin.
- 2. LU PPF "System Approach I and II" lectures, Prof. J.Kuzmin.
- 3. LU PPF "Modern Educational Environments" lectures, Prof. J.Kuzmin.
- 4. LU PPF "Introduction to programming languages" lectures, Prof. J.Kuzmin.
- 5. LU PPF "Knowledge testing Systems" lectures, Prof. J.Kuzmin.

### **Scientific Visits Abroad**

- 1. Prof. J.Kuzmin, USPU, Ural State University, Yekaterinburg, Russia
- 2. Dr. A.Kuzmin, IFN-CNR, Institute for Photonics and Nanotechnologies, Section "CeFSA", Trento, Italy

# Cooperation

### Latvia

- 1. LU Faculty of Education and Psychology (Prof. A.Geske, lect. L.Kuzmina)
- 2. Latvian schools

Italy

1. IFN-CNR CeFSA (Trento, Italy) - Dr. F. Rocca.

Russia

1. Ural State Pedagogical University (dean of Informatics Faculty, M.Lapionok)

# **Main Results**

During the year 2008, the Didactic System Laboratory was specialised in the investigation of the internet technologies for the implementation of the online real-time teaching system and in the further development of the Latvian SuperCluster (LASC) system. Main results are described briefly below.

• Internet technology in the e-Education applications.

First part of investigations was devoted to problem of real-time online teaching in telepresence form. Main purpose of these activities was concerned with didactical online experiments to clarify positive and negative features of online teaching technology. The second part of investigations was devoted to possibilities of Second Life systems readiness for online lectures. All work was done in cooperation with Ural State Pedagogical University (USPU).

All results of online experiments summarized in four pros & cons groups: online education material preparation, online professors activities, online students activities and student-professor online interaction. Evaluation of present state systems like Second Life permits to make conclusion about practical unreadiness of such systems for typical educational tasks.

#### • Developments of the Latvian SuperCluster (LASC) system.

Further developments of the LASC system has been performed during the last year. LASC is a Beowulf-like Linux cluster project, developed at the ISSP starting from 2002.

The cluster is running the RedHat Linux operating system and consists presently of 28 heterogeneous (Pentium III/XEON/Opteron) nodes: one front-end (master) node used as a file server, and 27 computational nodes. The nodes are interconnected by two local area networks (LANs) operated through four 24-ports Gigabit Ethernet switches. The first LAN is used for file exchange and communication purposes, whereas the second LAN is dedicated for data exchange during parallel computations. The resources available to the users are 110 CPUs, having the theoretical peak performance of about 219 GFLOPS, 220 GB RAM memory and 10.3 TB total hard disk space.



The detailed information on the cluster configuration, its resources, and different useful documentation/links are available at the LASC website (http://www.cfi.lu.lv/lasc/). The website provides also with real-time status monitoring of the LASC activity by the Ganglia monitoring system. As an example, the LASC average load, CPU, memory and network utilization during last year are shown in figures below:



The experience gained during development of the LASC system is presently used within the lecture course "Introduction to Cluster Computing" at LU PPF.

# **Scientific Publications**

- 1. Y. Kuzmin, Pros and cons of e-education. Proceedings of the V International scientific conference «Innovation technologies in the higher education pedagogics» October, 27th, 2008, lpp.21-34.
- 2. Y. Kuzmin, Educational possibilities of Internet system such as "Second Life". Proceedings of the V International scientific conference «Innovation technologies in the higher education pedagogics» October, 27th, 2008, lpp.35-43.
- Yu. Kuzmin, M.Lapenok. Use of Distant Learning Technologies in Students' Special Preparation of Computer Science Department. Proceedings of Fourth International Conference on Contemporary Issues in Higher Education. September 3-6, Izrael 2007. 186-193.pg.
- 4. J. Kuzmins, Kuzmina L. Dialogu materiāls WebCT vidē. Izglītības vadība. LU Zin.Raksti. 709.sējums, Rīga, 2007, lpp. 78-83.
- 5. J. Kuzmins, Dialogu kursu ģenerators AMATA Izglītības vadība. LU Zin.Raksti. 709.sējums, Rīga, 2007, lpp. 84-91.

# **Participation in Conferences**

- 1. Y. Kuzmin, Pros and cons of e-education. V International scientific conference «Innovation technologies in the higher education pedagogics» October, 27th, 2008.
- 2. Y. Kuzmin, Educational possibilities of Internet system such as "Second Life". V International scientific conference «Innovation technologies in the higher education pedagogics», October, 27th, 2008.

# 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 five 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;
- stochastization of magnetic field lines in magnetized fusion plasma;
- gyrotron development for thermonuclear reactors .

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

### Scientific staff

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

# Scientific visits abroad

- Dr. hab. E. Kotomin, Max Planck Institute for Solid State Research, Stuttgart, Germany (9 months), Northwestern University, Evanston, USA (1 month), The Eurasian University, Astana, Kazakhstan (2 weeks)
- Dr. hab.V. Kuzovkov, Uuniversity of Freiburg, Germany (1 week)
- Dr. O. Dumbrajs, Fukui University, Japan (3 months), Max Planck Institut für Plasmaphysik, Garching, Germany (3 months).
- Dr. R. Eglitis, Rutgers University, USA (5 months)
- Dr. V. Kashcheyevs, University of Cambridge, Cambridge, UK (1 week).
- Dr. S. Piskunov, University of Duisburg-Essen (10 months), LNF Frascati, Italy (1 week)
- Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (3 months), National Laboratory of Frascati, Italy (10 days), Deutsches Elektronen-Synchrotron DESY Hamburg, Germany (10 days)

# PhD students

12. D. Bocharov

13. A. Gopejenko

- Dr. D. Gryaznov, EC Institute of Transuranium Elements, Karlsruhe, Germany (10 months), Max Planck Institute for Solid State Physics, Stuttgart, Germany (1 month).
- Yu. Mastrikov, Max Planck Institute for Solid State Research, Stuttgart, Germany (11 months).
- Yu. Zhukovskii, Northwestern University, Evanston, USA (2 months), Max Planck Institute for Solid State Research, Stuttgart, Germany (3 weeks), Institute for Materials Research I, Karlsruhe (3 weeks), St. Petersburg State University, Russia (3 weeks), National Laboratory of Frascati, Italy (2 weeks).
- A. Gopejenko, Forschungszentrum Karlsruhe, Institut für Materialforschung I, Karlsruhe, Germany (5 months).

# 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. ESRF, Grenoble (Dr. A.Rogalev)	
Germany	4. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. van Uffelen).	
	5. Institut für Materialforschung I Forschungszentrum Karlsruhe (Dr. A.	
	Möslang)	
	6. Universität Duisburg-Essen (Prof. Dr. E. Spohr)	
	7. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)	
	8. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm)	
	9. Physikalisch-Technische Bundesanstalt, Braunschweig (Dr. Bernd Kästner).	
	10. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A.Kotlov)	
	11. Institut für Hochleistungsimpuls & Mikrowellentechnik, Karlsruhe (Dr. B.	
	Piosczyk)	
	Universität Ulm, Germany (Dr. T. Jacob)	
Greece	13. School of Electrical and Computer Engineering, National Technical	
	University of Athens, Zographou (Dr. Y. Kominis)	
Israel	14. Ben Gurion University of the Negev, Ber Sheeva (Profs. A. Aharony and D.	
	Fuks)	
Italy	15. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr.M.Cestelli-Guidi)	
Japan	16. FIR Center, University of Fukui (Prof. T. Idehara)	
Lithuania	18. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)	
Romania	19. University of Craiova (Dr. D. Constantinescu)	
Russia	20. St. Petersburg University (Prof. R.A. Evarestov)	
Spain	21. University of Barcelona (Prof. F. Illas)	
	22. Imperial College London (Prof. R.W. Grimes)	
UK	24. University College London (Profs. A.M. Stoneham and A. Shluger)	
	25. Cavendish Laboratory, University of Cambridge (M.R. Buitelaar)	
Ukraine	26. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)	
	27. Northwestern University, Evanston, Illinois (Prof. D.E. Ellis)	
USA		
	28. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr M.Kukla)	
	Rutgers University (Prof. D. Vanderbilt)	

# **Main Results**

## MODELING OF PHASE SEPARATION IN Au-Ni SURFACE ALLOY

### G. Zvejnieks

# E.E. Tornau (Semiconductor Physics Institute, Vilnius, Lithuania)

Detailed microscopic mathematical model of alloy phase separation can open new ways to optimize the Au/Ni surface catalyst. We proposed the kinetic Monte Carlo simulations of biatomic Au<sub>0.3</sub>Ni<sub>0.7</sub> surface alloy separation in Au/Ni(111) system by taking into account CO adsorption and nickel carbonyl formation reaction. We estimated Au-Au, Ni-Ni and Au-Ni pair interaction constants (v(Au-Au)=-0.08 eV, v(Ni-Ni)=-0.39 and v(Au-Ni)=-0.25) using *ab initio* calculations and find that they satisfy the inequality  $|v(Au-Au)|+|v(Ni-Ni)| \le 2|v(Au-Ni)|$ . This condition ensures an increased Au concentration on step edge after alloy relaxation. In different limiting cases we have studied: (i) Step flow rate dependence on Au-CO interaction which is one of the main factors (along with CO pressure and reaction rate) governing the process of nickel carbonyl formation. (ii) Step flow rate increase with CO coverage, c<sub>CO</sub>, which qualitatively agrees with the experiment only for c<sub>CO</sub>  $\le 0.45$  monolayer. (iv) We demonstrated both CO influence on reaction process and Au domain formation.

### ANDERSON LOCALIZATION: 2-D SYSTEM IN AN EXTERNAL MAGNETIC FIELD AND THE GENERALIZED DIFFUSION APPROACH

V. Kuzovkov W. von Niessen (*TU Braunschweig, Germany*)

The analytical approach developed by us for the calculation of the phase diagram for the Anderson localization via disorder is generalized to the case of a strong magnetic field when q subbands (q=1,2,3) arise. It is shown that in a line with the generally accepted point of view, each subband is characterized by a critical point with a divergent localization length  $\xi=1/\gamma(E,\sigma)$  which reveals anomaly in energy (*E*) and disorder ( $\sigma$ ) parameters. These critical points belong to the phase coexistence area which cannot be interpreted by means of numerical investigations. The reason for this is a logical incompleteness of the algorithm used for analysis of a computer modelling for finite systems in the parameter range where the finite-size scaling is no longer valid.



**Figure 1** Phase diagram for q = 1 (a), q = 2 (b) and q = 3 (c).



**Figure 2** Surface plot  $\gamma(E, \sigma)$  for q = 1 (a), q = 2 (b) and q = 3 (c).

# FIRST-PRINCIPLES CALCULATIONS OF PURE AND DEFECTIVE PEROVSKITE SURFACES

E.A. Kotomin, Yu. Zhukovskii, R.I. Eglitis, S. Piskunov, A. Gopeyenko, E. Heifets (*Max Planck Institute, Germany*)
E. Spohr (*Universität Duisburg-Essen, Germany*)
T. Jacob (*Universität Ulm, Germany*)
D. E. Ellis (*Northwestern University, USA*)
D. Vanderbilt (*Rutgers University, USA*)

A wide class of ternary oxides – ABO<sub>3</sub>-type perovskites – continues to attract a considerable attention as materials for catalytic and electrochemical applications, e.g. solid oxide fuel cells (SOFC), ceramic membranes for gas separation, actuators, sensors, *etc.*. For example, some of these oxides are catalytically active in the oxidation of CO and reduction of NO in automobile exhaust reduction. Mixed oxides with the ABO<sub>3</sub> 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.

In a close collaboration with prof. D.Vanderbilt (Rutgers University, USA), we performed *ab initio* calculations of a surface relaxation and rumpling for CaTiO<sub>3</sub>, SrTiO<sub>3</sub> and PbZrO<sub>3</sub> (001) as well as CaTiO<sub>3</sub> and SrTiO<sub>3</sub> (011) surfaces. The calculations are based on hybrid B3LYP exchange-correlation functionals. In the case of CaTiO<sub>3</sub>, the surface rumpling is much larger for the CaO-terminated than for the TiO<sub>2</sub>-terminated (001) surface, whereas different terminations of the CaTiO<sub>3</sub> (011) surface lead to very different surface energies. Our calculations indicate a considerable increase in the Ti-O bond covalency near the TiO-terminated SrTiO<sub>3</sub> (011) surface with respect to the bulk, which is much larger than that for the (001) surface.

In a close cooperation with Prof. D. Ellis (Northwestern University, USA), using the hybrid DFT-LCAO approach as implemented into the *CRYSTAL* code, we performed calculations of surface O vacancies with trapped electrons (known as the *F* centers) in three key perovskite crystals:  $SrTiO_3$ ,  $PbTiO_3$  and  $PbZrO_3$ . 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.

In a close cooperation with Prof. Spohr (Universität Duisburg-Essen, Germany), Dr. Heifets (Max Planck Institute, Germany), and Dr. Jacob (Universität Ulm, Germany), we have performed detailed calculations of the atomic, electronic structure and thermodynamic stability of  $La_{1-x}Sr_xMnO_3$  (LSM) solid solutions and its parent compound  $LaMnO_3$  (LMO). Due to its high electrochemical performance, thermal and chemical stability, and



Fig. 1. Sections of thermodynamic stability diagram for LSM (001) surface structures for O<sub>2</sub> partial pressure ( $p = 0.2p_0$ ) and temperatures of (a) 300 K (room temperature), (b) 1100 K (SOFC operational temperature), and (c) 1500 K (sintering temperature). The region, where LSM (x = 1/8) is stable, is the hatched area between LaMnO<sub>3</sub>, La<sub>2</sub>O<sub>3</sub>, Mn<sub>2</sub>O<sub>3</sub>, and SrO precipitation lines. The numbers from 1 to 8 in the circles indicate precipitation lines for (1) La, (2) Mn, (3) Sr, (4) La<sub>2</sub>O<sub>3</sub>, (5) Mn<sub>2</sub>O<sub>3</sub>, (6) SrO, (7) LaMnO<sub>3</sub>, and (8) SrMnO<sub>3</sub>. Hollow arrows indicate the sides from respective precipitation lines where the precipitation occurs. Insets show magnified areas with the region of LSM stability (a hatched quadrangle).

compatibility with yttria-stabilized zirconia (YSZ) electrolyte, LSM (x  $\approx 0.2$ ) has been actively used as a mixed ionic-electronic conducting electrode in high-temperature SOFC. Understanding the mechanism of reaction of oxygen reduction on the surface of LSM nanofilms deposited on oxide electrolytes demands thorough theoretical analysis at the atomistic level. In this study, first-principles calculations by means of a hybrid density-functional theory are used to describe La(Sr)O- and MnO<sub>2</sub>-terminated surfaces of both cubic LMO and LSM. Surfaces containing oxygen vacancies are also considered. Calculated thermodynamic stability diagrams (Fig. 1) predict that Sr-rich La(Sr)O-terminated LSM(001) become stable under conditions close to precipitation of SrMnO<sub>3</sub>. On the other hand, both La(Sr)O- and MnO<sub>2</sub>-terminated LSM(001) are stable at room temperature, while only La(Sr)O-terminated LSM(001) is predicted to be stable under SOFC operation conditions (temperature-gas pressure). We predict a significant decrease in the O vacancy formation energy at higher temperatures which leads to a high vacancy concentration which permits efficient SOFC operation. The neutral oxygen vacancy attracts only ~0.6e and ~0.2e on La(Sr)O- and MnO<sub>2</sub>-terminated LSM (001), respectively. Thus, the vacancies are positively charged, they strongly polarize surrounding atoms and serve as potential adsorption

### POINT DEFECTS AND REACTIVITY OF ABO3 PEROVSKITES

E.A. Kotomin, Yu. Zhukovskii, Yu. Mastrikov, S. Piskunov, A. Gopeyenko, R.A. Evarestov, V. Alexandrov (*St. Petersburg University, Russia*) D.E. Ellis (*Northwestern University, Evanston, USA*)
R. Merkle, V.Alexandrov, E.Heifets and J. Maier (*Max Planck Institute for Solid State Research, Stuttgart, Germany*)

We performed a series of first-principles (*ab initio*) calculations of defects in ABO<sub>3</sub>type perovskites which is important for many high tech applications. In particular, in close collaboration with Max Planck Institute, Stuttgart we performed *ab initio* DFT plane-wave supercell calculations of the atomic and molecular oxygen adsorption and diffusion on the LaMnO<sub>3</sub> (001) surface which serves as a model material for a cathode of solid oxide fuel cells (SOFC). The calculations show that the dissociative adsorption of O<sub>2</sub> molecules from the gas phase is energetically favorable on surface Mn ions even on a defect-free surface.

The surface migration energy for adsorbed O ions is found to be quite high, 1.60 eV. We predict that the adsorbed O atoms could penetrate into electrode first plane when much more mobile surface oxygen vacancies (migration energy of 0.69 eV) approach the O ions strongly bound to the surface Mn ions. Formation of the O vacancy nearby O atom adsorbed atop surface Mn ion leads to an increase of the O-Mn binding energy by 0.74 eV whereas the drop of this adsorbed O atom into a vacancy posesses no energy barrier. As Fig.1 demonstrates the *ab initio* thermodynamics predicts that under typical SOFC operation temperatures (~1200 K) the MnO<sub>2</sub> (001) surface with adsorbed O atoms is the most stable in a very wide range of oxygen gas pressures (above  $10^{-2}$  atm). Second, in collaboration with Northwestern University, USA we performed ab initio calculations of Cu electrode growth on BaTiO<sub>3</sub> surfaces which important for micro-, nanoelectronic applications. In order to compare Cu adhesion upon two kinds of perfect cubic (001) oxide surfaces: (i) TiO<sub>2</sub>- and BaO-terminated substrates of partly covalent BaTiO<sub>3</sub> and (ii) highly ionic MgO substrate, we have performed DFT-LCAO calculations using a hybrid B3PW Hamiltonian. 2D symmetrical slabs used here contain seven BaTiO<sub>3</sub> and five MgO substrate layers covered on both sides by submonolayers of ordered Cu atoms. The Cu periodic coverage density atop the surface oxygen anions was varied from



Fig.1. The stability diagram of different LaMnO<sub>3</sub> surfaces vs  $O_2$  gas pressure (10<sup>-m</sup> atm.) and temperature. Numbers in cicles indicate precipitation of metals and binary oxides.

1/8 to 1/2 monolayer. Copper bonding on the BaTiO<sub>3</sub>(001) surface has been found to be *noticeably stronger* than that on ionic MgO(001). Cu adatoms attract the electron density from BaO-terminated and donate it towards TiO<sub>2</sub>-terminated BaTiO<sub>3</sub>(001) substrates, respectively, by an amount that is about threefold larger than for a Cu/MgO(001) interface.

We performed also the hybrid LCAO calculations of  $Fe^{4+}$  impurities substituting host  $Ti^{4+}$  ions in the bulk and on the surface of  $SrTiO_3$  varying iron concentration. The calculated local atomic deformation is in a good agreement with the EXAFS experimental data. We predict iron impurity segregation to the (001) surface which can contribute to the space charge effect and affect properties of internal interfaces and grain boundaries in ceramic samples.

We modelled also the external Li atom storage in nanocomposites known as the interfacial mechanism. This study is aimed to increase capacity and efficiency of Li batteries widely used in home electronics. To understand the mechanistic details of the experimentally observed lithium storage anomaly, we have performed comparative *ab initio* calculations on the atomic and electronic structure of the non-polar Cu/LiF(001) and model Li/LiF(001) interfaces. As we have shown the Cu/LiF(001) interface permits an insertion of only one monolayer of extra Li atoms, unlike Li bilayer in the case of Ti/Li<sub>2</sub>O(111). Diffusion of the excess Li along the interface is found to be accelerated owing to the splitting of the individual pathways for Li<sup>+</sup> and e<sup>-</sup>, which explains a high rate performance observed experimentally at low potential. We also compared theoretical estimate and experimental capacity results in the Cu/LiF nanocomposite. The results of first-principles simulations on both orthorhombic and monoclinic phases

The results of first-principles simulations on both orthorhombic and monoclinic phases of CaFeO<sub>3</sub> perovskite crystal were analysed. The obtained atomic structure is consistent with x-ray diffraction data. The transition from a metallic orthorhombic to a narrow-gap semiconducting monoclinic phase is ascribed to the larger distortion of the Fe–O–Fe bond angle in the latter case. Calculations of Raman and optic active phonon modes at the  $\Gamma$  point of the Brillouin zone are performed and discussed. The isotopic substitution technique is applied to analyze the vibration modes obtained. The found charge/spin disproportionation is analyzed and compared with available experimental estimates.

Lastly, point defects affect considerably properties of ABO<sub>3</sub>-type perovskite-based devices. One of the main defects is oxygen vacancy. In order to study its properties, we combined the hybrid DFT-LCAO approach with 135 atom supercell calculations of O vacancies with trapped electrons (known as the *F* centers) in three cubic perovskite crystals: SrTiO<sub>3</sub>, PbTiO<sub>3</sub> and PbZrO<sub>3</sub>. The local lattice relaxation, charge redistribution and defect energy levels in the optical gap were compared. We demonstrated how difference in chemical composition of host materials leads to quite different defect properties. The results obtained for three types of defective cubic ABO<sub>3</sub> perovskites show a strong defect property dependence on a chemical nature of A and B atoms: the same *F* centers could be deep defects in PbZrO<sub>3</sub> and shallow in SrTiO<sub>3</sub> and SrTiO<sub>3</sub>.

### FUNDAMENTAL AND APPLIED NANOELECTRONIC PUMPS

### V. Kashcheyevs

M.R. Buitelaar (*Cavendish Laboratory*, *University of Cambridge*, *UK*) B. Kästner (*Physikalisch-Technische Bundesanstalt*, *Braunschweig*, *Germany*)

electron pumps, based of periodic Ouantum modulation of quantum dot parameters, is a rapidly developing class of nanoelectronic devices. applications Fundamental involve probing of excitation spectrum electron and quantum information processing while the main applied interest is the development of a quantum current standard.

In collaboration with the experimental group at University of Cambridge (Dr. Markk Buitelaar ,Cambridge, UK), we have identified signatures of a artificial molecule states in carbon-nanotube based adiabatic pump [3], see the figure. This work has been recognized as one of the **top 10 science achievements in Latvia in 2008** by the Latvian Academy of Sciences (the annual 'Top 10' covers all branches of science, from medicine to lettonica to physics). In collaboration with the experimental group at Physikalisch-Technische Bundesanstalt



(Dr. Bernd Kästner, Braunschweig, Germany) we have continued work on a novel nonadiabtic architecture for a quantized source of current (quantized pumping) [1,2]. Application of magnetic field has allowed to achieve the highest accuracy of current quantization to date. We continue theoretical work towards optimizing this architecture towards metrological accuracy (100 parts per billion).

### HYSTERESIS IN MODE COMPETITION IN HIGH POWER 170 GHZ GYROTRON FOR ITER

## O. Dumbrajs T. Idehara (*University of Fukui, Japan*)

Gyrotrons are microwave sources whose operation is based on the stimulated cyclotron radiation of electrons oscillating in a static magnetic field. Gyrotron devices are now able to generate several orders of magnitude as much power at millimeter wavelength as classical microwave tubes, and can operate at frequencies higher than are conveniently available from other types of tubes. Gyrotron oscillators can have a wide application, including technological processes, atmospheric sensing, ozone conservation, artificial ionospheric mirror, extra-high resolution electron spin resonance spectroscopy, nuclear magnetic resonance spectroscopy, new medical technology spectroscopy, etc. However, the main application of powerful gyrotrons is electron cyclotron resonance plasma heating in tokamaks and stellarators and the noninductive current drive in tokamaks.

The study of one very interesting phenomenon—hysteresis—is relatively limited, although perfect understanding of hysteresis is important in connection with mode competition, frequency tuning, voltage overshooting, amplitude modulation of the signal, etc. In gyrotrons hysteresis is the phenomenon that causes the amplitude of oscillations to lag behind the magnetic field and the voltage, so that operation regions of modes for rising and falling magnetic field and voltage are not the same.

In the present work, we generalize our single mode hysteresis calculations to multimode case with particular emphasis on mode competition in 170 GHz gyrotrons for ITER and calculate mode map in the plane "frequency mismatch – dimensionless current" for the operating mode. The theory is illustrated by a number of specific examples.

# HYSTERESIS IN SAWTOOTH CRASH IN ASDEX UPGRADE TOKAMAK

O. Dumbrajs

### V. Igochine, H. Zohm and ASDEX Upgrade Team (MPI für Plasmaphysik, Euratom-Association, D-85748 Garching, Germany)

A hysteresis model is used to describe experimental data on sawtooth crash in ASDEX Upgrade tokamak. The model is based on hysteresis which arises due to the fact that the value of the current density gradient (approximated, for the H-mode discharges studied here, by the temperature gradient) at the q = 1 surface required to turn on the instability is greater than the gradient required to maintain the instability once it is turned on. The value of the hysteresis parameter can be chosen such that the model reproduces correctly the two time scales of the sawtooth crash in ASDEX Upgrade tokamak: the slow rise time (~7 ms) and the rapid crash time (~50  $\mu$ s).



Hysteresis in sawtooth crash. Temperature gradient (red curve) rises until the instability threshold at 3.6 keV/m. At this moment  $t = t_1$  the instability is turned on by switching the function Q (green curve, arbitrary units) to  $\chi_{max}$ . The central temperature (black

curve) begins to decrease and diffusion coefficient (blue curve, arbitrary units) begins to increase. During further evolution due to hysteresis the function Q is switched back to  $\chi_{\min}$  not at  $t = t_2$  when temperature gradient passes again the instability threshold, but at  $t = t_3$  when temperature gradient becomes equal to  $\beta k = 1.8 keV/m$ .

### AB INITIO MODELLING OF ADVANCED NUCLEAR FUEL OXIDATION

E.A. Kotomin, Yu. Zhukovskii, Yu. Mastrikov, D. Gryaznov, D. Bocharov, R.A. Evarestov, A.V. Bandura, M.V. Losev (*Department of Quantum Chemistry, St. Petersburg State University, St. Petersburg, Russia*) P. Van Uffelen (*Institute of Transuranium Elements, Karlsruhe, Germany*),

In close collaboration with the *Institute for Transuranium Elements, Karlsruhe*, we have continued first-principles calculations of UN fuels. Uranium mononitride attract a considerable attention as promising nuclear fuel materials for future Generation IV reactors. In order to predict nuclear fuel performance under different operating conditions and then during a prolonged time in repository for a spent fuel, it is necessary to understand and predict material physico-chemical properties.

Theoretical studies of uranium compounds are especially difficult due to a relativistic character of electron motion in the U atom core and strong electron-electron correlation. Moreover, UN is characterized by a mixed metal-covalent chemical bonding.

UN samples typically contain considerable amount of O impurities, which greatly affect fuel properties. Therefore, it is necessary to understand mechanism of oxygen adsorption as well as further oxidation of uranium nitride.



Fig. 1. The difference electron density maps  $\Delta \rho(r)$  (the total density of the interface minus the densities of substrate and adsorbate with optimized interfacial geometry) for the O adatoms atop the surface: (left) N anions and (right) U cations on the UN(001) surface obtained using results of calculations. Solid (red) and dashed (blue) isolines correspond to positive and negative electron density, respectively. Isodensity increment is 0.003 e Å<sup>-3</sup>.

The results of PW DFT calculations of the lattice constant, bulk modulus, cohesive energy, charge distribution, band structure and density of states (DOS) for UN pure bulk and surface are analysed. The DFT plane wave (PW) calculations on a pure

UN bulk and surface as well as oxygen atomic absorption on defect-free UN surface were compared with the corresponding LCAO DFT calculations performed by Prof. R.A. Evarestov group (*Faculty of Chemistry, St. Petersburg State University*). The results acquired for oxygen interaction with UN surfaces demonstrate a strong chemisorption typical for metallic surfaces. An analysis of the difference electron charge redistributions for both configurations of  $O_{ads}$  (Fig. above) confirms that the O adatom forms a strong chemical bonding with the surface U cation which could be considered as one-site complex. In the case of O adatom atop the surface N anion this is rather multicenter adsorption complex involving four adjacent surface U ions. A comparison of the DFT GGA with LCAO calculations shows their excellent agreement.

DFT PW calculations show also that O impurities are able to penetrate easily into the UN in bulk and oxidize the fuel which agrees well the results of experimental studies. The oxygen incorporation into (pre-existing) N vacancy is energetically more favorable than that into the tetrahedral interstitial position. However, it is energetically favorable even to create N vacancy and place O atom therein.

Based on the GGA calculations, we demonstrated that  $O_2$  molecules oriented parallel to the UN substrate can dissociate either (*i*) spontaneously, when the molecule center lies above the surface hollow site or atop N ion, or (*ii*) with the activation barrier, when a molecule sits atop the surface U ion. This explains fast UN oxidation in air. A study of He impurities are in progress.

# SIMULATION OF YTTRIUM AND OXYGEN SOLUTE ATOMS IN FCC FE LATTICE IN SUPPORT OF ODS STEEL DEVELOPMENT

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Reduced activation steels strengthened by yttria precipitates are considered as promising structural materials for future fusion- and advanced fission-reactors. In particular, application of oxide dispersion strengthened (ODS) steels for fusion reactor blanket structure allows increasing its operation temperature by ~100°C. Both size and spatial distributions of oxide precipitates significantly affect mechanical properties and radiation resistance of ODS steels. However, the mechanism of ODS nanoparticle formation is still not well understood. Some recent experiments indicate that at least part of yttrium oxide particles might be dissolved in the steel matrix during mechanical alloying. If so, yttrium dissolved above its equilibrium solubility limit will precipitate during hot isostatic pressing of mechanically alloyed powder. Slow diffusion of large substitutional yttrium atoms is probably a limiting factor for yttrium oxide particle growth. Diffusion of interstitial oxygen is much faster and, therefore, can not delay the growth of precipitate. In this paper we consider an Y-vacancy pair as a simplest diffusing yttrium-containing complex.

In collaboration with *Institute for Materials Research I, Research Center Karlsruhe*, we have performed a series of large-scale first principles calculations on perfect  $\gamma$ -Fe lattice as well as that containing a single Fe atom vacancy, O and Y impurity atoms. In our model iron matrix is represented by a face-centered cubic  $\gamma$ -Fe lattice, which is stable at typical hot isostatic pressing temperatures. Our calculations performed for the 4×4×4  $\gamma$ -Fe supercell have shown that oxygen atoms reside on either O (six nearest Fe neighbors) or T (four nearest Fe neighbors) interstitial positions (the latter has been found to be ~0.1-0.2 eV less favorable than the former) which quantitatively confirm results of theoretical simulations on oxygen atom absorbed inside the fcc Al lattice. The excessive electronic charge accepted by oxygen impurity in O center of  $\gamma$ -Fe lattice achieves ~1.4 e (cf. 1.8 e for the same position of O atom in fcc Al lattice). The oxygen
insertion results in a considerable expansion of the two first coordination shells around an impurity atom (~9 and 1.75%, respectively, in octahedral interstitial). A barrier of O migration between the nearest O and T centers (1.62 eV) has been found in a good qualitative agreement with the corresponding experimental values (1.72-1.75 eV, according to different studies).Our calculations have shown that there is a considerable binding between yttrium atom and vacancy at some distances (Figures 1a and 1b). This allows us to determine the pair-wise energies necessary for further kinetic Monte Carlo simulations, aimed at understanding the yttrium oxide precipitation process.





Figure 1a. Configuration of the Y and Fe-vacancy pair at 1NN position before relaxation

Figure 1b. Configuration of the Y and Fe-vacancy pair at 1NN position after relaxation

### MICROSTRUCTURE OF Ag<sub>2</sub>BI<sub>4</sub> (B =Hg, Cd) SUPERIONICS STUDIED BY SEM, IMPEDANCE SPECTROSCOPY AND FRACTAL DIMENSION ANALYSIS

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Two silver ion conducting solid electrolytes, Ag<sub>2</sub>HgI<sub>4</sub> and Ag<sub>2</sub>CdI<sub>4</sub>, representing a wide class of AgI-based halogenide superionics have been the subjects of study by means of electrical impedance spectroscopy, SEM, porosity measurements and fractal dimension analysis. Even though both materials have been obtained by the same method under strictly identical conditions they were found to exhibit certain differences at the microstructural level. Thus, by the direct measurements of porosity and density it was found that the grain boundaries are better developed in silver mercuric iodide. On the assumption that pore geometry in the materials under study displays fractal character it was shown that the fractal dimension of the pore contours is larger in the case of Ag<sub>2</sub>HgI<sub>4</sub>. These results are in agreement with electrical studies which indicated that the

grain boundary capacitance in  $Ag_2CdI_4$  is two orders of magnitude smaller than that of the silver mercuric iodide.

#### AB INITIO SIMULATIONS ON THE ATOMIC AND ELECTRONIC STRUCTURE OF REGULAR AND DEFECTIVE SINGLE-WALLED BN NANOTUBES AND NANOARCHES

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To simulate the perfect single-walled (SW) boron nitride (BN) nanotubes (NTs) and nanoarches (NAs) of armchair- and zigzag-type chiralities as well as uniform diameter we have constructed their 1D-periodic models, in the framework of collaboration with the LNF INFN, Frascati, and Politecnico di Torino, Italy. In the NAs of both chiralities, the half-NTs have been extended by two fragments of parallel nanoribbons joint to their edges. The nanotubes and nanoarches have been calculated using formalism of the localized Gaussian-type atomic functions as implemented in the CRYSTAL-06 code. For ab initio calculations, we have applied the DFT Hamiltonians containing either PWGGA or hybrid (DFT+HF) B3PW exchange-correlation functionals. We have compared the calculated both structural and electronic properties of BN NTs and NAs with those for h-BN and c-BN bulk. After calculation of Hessian matrix for the optimized structures of BN bulk (both phases) and nanotubes (both chiralities) using the CRYSTAL code we have estimated their normal phonon modes within the harmonic approximation. Applying both atomistic and continuum models we have calculated the elastic energies and moduli for SW BN nanoarches. Their careful study is necessary not only for reliable comparison with the corresponding experimental data but also for proper description and even prediction for some of them (firstly, the phonon and elastic structure of BN nanotubes and nanoarches). Recent experimental IR measurements on h-BN and BN NT samples qualitatively confirmed the spectra predicted in this study. The hybrid B3PW method is found to be more reliable for the simulation of the whole spectrum of properties for BN bulk and nanostructures.

Using the hybrid B3PW method for *ab initio* calculations in collaboration with the *LNF INFN, Frascati,* we have also simulated the relaxed structure, the electron charge re-distribution and the energetics of neutral nitrogen vacancy (F center) as well as  $C_N$  and  $O_N$  substitutes in BN nanotubes. All three types of point defects cause an appearance of the energy levels inside the BN NT band gap (Fig. 1) accompanied by relaxation of the nearest atomic spheres closest to the point defect and electronic charge redistribution around it. Energetically, formation of carbon and oxygen substitutes in BN NTs is more preferable than that for N vacancy.  $C_N$  point defects serve as electron acceptors making BN nanotube a *p*-type semiconductor. Oxygen substitutes are typical electron donors in BN NT and in the case of its *zz*-chirality they show a metallic behavior. We also can conclude that different nature of chemical bonding in nanotubes of III group metal nitrides can result in a noticeable difference between their properties, especially in presence of defects.



Figure 1. Aside views of periodic fragments of ~8.5 Å thick 1D BN NTs containing single defects (*F* center,  $C_N$  and  $O_N$ ) distributed along axes of nanotube upon: a) *ac*-NT (6,6) with supercell periodicity 16.2 Å and b) *zz*-NT (10,0) with supercell periodicity 17.3 Å. Large light-gray balls show single defects (*F* centers,  $C_N$ ,  $O_N$ ) whereas light turquoise balls correspond to B atoms and N atoms are shown by dark blue.



Figure 2. Band structures of BN NTs containing a single defect *per* supercell: *F* center upon *ac*-NT (a) and *zz*-NT (b);  $C_N$  upon *ac*-NT (c) and *zz*-NT (d);  $O_N$  upon *ac*-NT (e) and *zz*-NT (f). Arrows show the defect bands whereas zero level in all the energy scales is chosen at the top VB.

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### **Presentations at Conferences**

# I. International Workshop "Fundamental Physics of Ferroelectrics", (Williamsburg, VA, USA, February, 2008).

1. R.I. Eglitis and D. Vanderbilt "*Ab initio* calculations of BaTiO<sub>3</sub>, PbTiO<sub>3</sub>, SrTiO<sub>3</sub> (001) and (011) surface structures". Abstracts: p. 70-71.

# II. International workshop "Interaction and Interference in Nanoscopic Transport" (Dresden, Germany, February, 2008).

2. V. Kashcheyevs, C. Karrasch, T. Hecht, and V. Meden, "From single particle to correlation-dominated criticality in a level-crossing transition". Abstracts: Po. 22.

# III. 24<sup>th</sup> ISSP Conference (Riga, Latvia, February, 2008).

3. A. Gopejenko, Yu.F Zhukovskii, P.V. Vladimirov, and E.A. Kotomin, "*Ab initio* calculations of O and Y impurities in Fe *fcc* lattice". Abstracts: p. 4.

4. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, R.A. Evarestov, E.A. Kotomin, "Structure and properties of UN nuclear fuels: quantum chemistry approach". Abstracts: p. 6.

5. O. Dumbrajs, "Gyrotrons for ITER". Abstracts: p. 27.

# *IV.* 72<sup>nd</sup> Annual Meeting of German Physical Society (Berlin, Germany, February 2008).

6. S. Piskunov, E. Spohr, and T. Jacob, "Electronic structure and thermodynamic stability of cubic  $La_{1-x}Sr_xMnO_3$  (001) surfaces: First principles calculations by means of hybrid density-functional theory". Abstracts: p. 592-593.

# V. Nuclear Cross-Over (NXO) workshop on nuclear fuels (Tokyo, Japan, February, 2008)

7. E.A. Kotomin, Yu.A. Mastrikov, and Yu.F Zhukovskii, "First-principles modeling of nuclear fuels".

# VI. Solvay workshop dedicated to memory of Radu Balescu (Brussels, Belgium, March, 2008)

8. O. Dumbrajs, "Stochastic processes in gyrotrons".

*VII. American Physical Society March Meeting (New Orleans, USA, March, 2008)* 9. R.I. Eglitis and D. Vanderbilt, "*Ab initio* calculations of BaTiO<sub>3</sub>, PbTiO<sub>3</sub>, and SrTiO<sub>3</sub> (001) and (011) surfaces". Abstracts: p. 347.

# VIII. International Baltic Sea Region conference "Functional materials and nanotechnologies 2008" (Riga, Latvia, April, 2008).

10. E.A. Kotomin, Yu.A. Mastrikov, Yu.F. Zhukovskii, S. Piskunov, and J. Maier, "First-principles modelling of perovskite surface reactivity". Abstracts: p. 19.

11. Yu.F. Zhukovskii, S. Piskunov, B. Berzina, L. Trinkler, and S. Bellucci, "Atomic

and electronic structure of single-walled BN nanotubes containing nitrogen vacancies". Abstracts: p. 25.

12. A.I. Popov, G.J. McIntyre, C. Wilkinson, "Photostimulable storage phosphors and image-plate development for neutron imaging". Abstracts: p. 32.

13. D. Bocharov, Yu. Zhukovskii, R.A. Evarestov, E.A. Kotomin, and A. Bandura, "Atomic and molecular oxygen adsorption on the UN (001) surface". Abstracts: p. 87.

14. V. Alexandrov, R.A. Evarestov, E.A. Kotomin, A. Kuzmin, J. Purans, M. Vracar, R. Merkle, J. Maier, "Theoretical and structural studies of charge ordering in CaFeO<sub>3</sub> and SrFeO<sub>3</sub>". Abstracts: p. 88.

15. A.I. Popov, G.J. McIntyre, J. Zimmermann, V. Pankratov, C. Wilkinson, and H.von Seggern. "Evaluation of luminescent properties of neutron image plates". Abstracts: p. 90.

16. A.I. Popov, P.V. Savchyn, V.T. Adamiv, Ya.V. Burak, and I.M. Teslyuk, "Influence of doping on the luminescence properties of the lithium tetraborate single crystals". Abstracts: p. 91.

17. V. Pankratov, A.I. Popov, S. Chernov, and C. Feldmann, "Time-resolved luminescence of LaPO<sub>4</sub>: Ce, Tb nanophosphor". Abstracts: p. 92.

18. A.I. Popov, P.V. Savchyn, M. Cestelli Guidi, I.D. Karbovnyk, S.V. Myagkota, M. Piccinini, A.S. Voloshinovskii, "Influence of CsPbCl<sub>3</sub> nanocrystals dispersed in Rb  $_{0.8}$ Cs $_{0.2}$ Cl matrix on its vibration parameters". Abstracts: p. 160.

19. V. Kashcheyevs, "Fitting carbon nanotubes into confined geometries: energy balance of single-walled bundles versus multiwalled configurations". Abstracts: p. 165.

20. V.N. Kuzovkov and W.von Niessen, "Anderson localization: Random walk approach". Abstracts: p. 166.

21. Yu.Shunin, S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, "Modelling of fundamental properties for interconnects between Ni film and carbon nanotubes". Abstracts: p. 167.

22. S. Piskunov, E. Spohr, T. Jacob, E. Heifets, E.A. Kotomin, and D.E. Ellis, "Thermodynamic stability of La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> surfaces: calculations by means of hybrid density functional theory". Abstracts: p. 181.

# IX. The 6<sup>th</sup> International Conference ''Information Technologies and Management'', IT&M'2008 (Riga, Latvia, April, 2008).

23. D. Bocharov, Yu.F. Zhukovskii, and E.A. Kotomin, "Spontaneous dissociation of  $O_2$  molecules at oxygen adsorption on the UN(001) surface". Abstracts: p. 14.

24. A. Gopeyenko, Yu.F. Zhukovskii, P.V. Vladimirov, and E.A. Kotomin, "*Ab initio* Calculations of oxygen and yttrium impurities in *fcc* Fe". Abstracts: p. 23.

25. Yu.F. Zhukovskii, V. Kashcheyevs, S. Piskunov, Yu.N. Shunin, and E.A. Kotomin, "Carbon nanotubes and nano-interconnects as basic elements for the next-generation nano-electronic devices". Abstracts: p. 25.

# X. Baltic conference on Electrochemistry (Tartu, Estonia, April-May, 2008).

26. E.A. Kotomin, J. Maier, Yu.A. Mastrikov, and Yu.F. Zhukovskii, "First-principles calculations of the solid oxide fuel cells and interfacial storage in Li batteries". Abstracts: I-7

*XI.* 213<sup>th</sup> Meeting of American Electrochemical Socienty (Phoenix, USA, May, 2008). 27. E.A. Kotomin, Yu.A. Mastrikov, E. Heifets, R. Merkle, J. Fleig, J. Maier, A. Gordon, and J.Felsteiner, "First-principles modeling of SOFC cathode".

28. E.A. Kotomin, Yu.F. Zhukovskii, P. Balaya, and J. Maier, "Enhanced interfacial lithium storage in nanocomposites of transition metals with LiF or Li<sub>2</sub>O: experimental studies and theoretical simulations".

# XII. Workshop on Nano-Materials and Nano-Technologies for Electrical and Electronic Engineering, n-MATE-2008 (Salerno, Italy, June, 2008).

29. Yu.F. Zhukovskii, "Atomic and electronic structure of carbon nanotubes and their bundles".

# XIII. 9<sup>th</sup> International Symposium on Ferroelectricity, RCBJSF-9 (Vilnius, Lithuania, June, 2008).

30. Yu.F. Zhukovkii, E.A. Kotomin, S. Piskunov, and Yu.A. Mastrikov, "The effect of oxygen vacancies on the atomic and electronic structure of cubic ABO<sub>3</sub> perovskite bulk and the (001) surface: *Ab initio* calculations". Abstracts: p. 33.

# XIV. International conference "Advances in Atomic and Molecular Physics 2008" (Ratnieki, Latvia, June, 2008).

31. V. Kashcheyevs, B. Kastner, and M. Buitelaar, "Low-frequency excitation of quantum dots: charge pumping in nanocircuits".

# XV. 2008 IEEE International Conference on Plasma Science (Karlsruhe, Germany, June, 2008).

32. O. Dumbrajs and T. Idehara, "Hysteresis in mode competition in high power 170 GHz gyrotron for ITER".

# XVI. International Workshop "Computational Challenges and Tools for Nanotubes" CCTN08 (Montpellier, France, June, 2008).

33. V. Kashcheyevs, S. Piskunov, and Yu.F. Zhukovskii, "Modeling of electronic properties of CNT bundles and interconnects". Abstracts: p. 9.

# XVII. 9<sup>th</sup> International Conference on the Science and Application of Nanotubes, NT08 (Montpellier, France, June-July, 2008).

34. Yu.F. Zhukovskii, Yu.N. Shunin, S. Piskunov, and E.A. Kotomin, "First principles simulations of interconnects between CNTs and Ni(111) film". Abstracts: p. 284.

# XVIII. 7<sup>th</sup> International Workshop "Strong Microwaves: Sources and Applications" (Nizhny Novgorod, Russia, July-August, 2008).

35. O. Dumbrajs, M.Yu. Glyavin, T. Idehara, Z.C. Ioannidis, V.I. Khizhnyak, A.G. Luchinin, M.V. Morozkin, T. Saito, and I.G. Tigelis, "Continuously tunable coaxial gyrotrons".

36. B. Piosczyk, S. Alberti, F. Albajar, K. Avramidis, P. Benin, T. Bonicelli, S. Cirant, O. Dumbrajs, D. Fasel, J. Flamm, G. Gantenbein, T. Goodman, J.-P. Hogge, S. Illy, S.

Jawla, J. Jin, S. Kern, C. Lievin, I. Pagonakis, O. Prinz, T. Rzesnicki, M. Thumm, and M.Q. Tran, "Status of the European 2 MW, 170 GHz coaxial cavity gyrotron for ITER".

# XIX. The 6<sup>th</sup> International Conference ''Advanced Optical Materials and Devices'' (Riga, Latvia, August, 2008).

37. V. Kashcheyevs, "Transport-probed spectroscopy: from phonon-assisted tunnelling to adiabatic charge pumping". Abstracts: PI-09.

38. V. Pankratov, A.I. Popov, S. Chernov, C. Feldmann, "Synthesis and Characterization of LaPO<sub>4</sub>:Ce,Tb nanophosphors". Abstract 1P-10.

39. D. Bocharov, A. Kuzmin, J. Purans, and Yu.F. Zhukovskii, "Quantum chemistry studies of the O K-edge X-ray absorption in WO<sub>3</sub> and AWO<sub>3</sub>". Abstracts: 3P-05.

# XX. International workshop in honour of Prof. Cesare Pisani (Torino, Italy, September, 2008).

40. E.A. Kotomin, Yu.F. Zhukovskii, S. Piskunov, and D.Ellis, "Hybrid DFT calculations of the F centers in cubic ABO<sub>3</sub> perovskites".

41. V. Alexandrov, E.A. Kotomin, R.A. Evarestov, and J. Maier, "Ab initio study of bulk and surface iron defects in SrTiO<sub>3</sub>".

# XXI. 33<sup>rd</sup> International Conference on Infrared, Millimeter, and Teraherz Waves (California, USA, September, 2008).

42. O. Dumbrajs, Y. Kominis, and G.S. Nusinovich, "Gyrotron dynamics in the process of mode switching in gyrotrons".

43. S. Kern, A. Avramides, M.H. Beringer, O. Dumbrajs, and Y.H. Liu, "Gyrotron mode competition calculations: investigations on the choice of numerical parameters".

# XXII. EMC 2008 Europe: "Next-generation Nanointerconnects" (Hamburg, Germany, September, 2008).

44. S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, "Electronic properties of Ni(111)/CNT nanointerconnects: Modeling from first principles".

# XXIII. 25<sup>th</sup> International Symposium on Fusion Technology, (Rostock, Germany, September, 2008).

45. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Moslang, "Simulation of yttrium oxide particle formation in iron in support of ODS steel development". Abstracts: p. 226.

### XXIV. Festkorper mit Speicherfunktion (Energie, Information, Stoffe), 14. Vortragstagung der FG Festkorperchemie und Materialforschung (Bayreuth, Germany, September, 2008).

46. E.A. Kotomin, Yu.F.Zhukovskii, and J.Maier, "Atomistic modelling of a new mechanism for a Li storage in batteries". Abstracts: A61, p.13 (also published in Z.Anorg. Allg. Chem., vol. 634, p.2055 (2008)).

# XXV. 7<sup>th</sup> International Workshop ''Materials Models and Simulations for Nuclear Fuels'' (Karlsruhe, Germany, September, 2008).

47. D. Gryaznov, E. Heifets, and E.A. Kotomin, "VASP calculations for perfect and defective actinide nitrides and oxides".

48. D. Bocharov, Yu.F. Zhukovskii, and E.A. Kotomin, "Interaction of the oxygen molecule with the UN(001) surface: *Ab initio* modeling".

49. S.N. Rashkeev, E.A. Kotomin, Y.A. Mastrikov, and P. van Uffelen, "First principles modelling of defect migration in uranium nitride and transuranus prediction of fuel performance".

50. D. Gryaznov, and D. Fuks, "Ab initio thermodynamics of (U,Zr)N solid solutions".

51. P. van Uffelen, and E.A. Kotomin, "Using first principle calculations for nitride fuels in a fuel performance code".

# XXVI. 9<sup>th</sup> International Workshop Nanoscience & Nanotechnology (Frascati, Italy, October, 2008).

52. Yu.N. Shunin, Yu.F. Zhukovskii, and S. Bellucci, "Simulations of properties of CNT/Ni(111) interconnects using the effective media approach". Abstracts: P. 32-34.

53. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin, and S. Bellucci. "2D periodic models of Ni(111)/CNT interconnects (bundles): ab initio calculations". Abstracts: p. 35-37.

54. V. Kashcheyevs and M. Buitelaar, "Adiabatic pumping put to test: modeling of low-frequency electron transport through carbon nanotubes". Abstracts: p. 38.

*XXVII.* 22<sup>nd</sup> *IAEA Fusion Energy Conference (Geneva, Switzerland, October, 2008).* 55. V. Igochine, O. Dumbrajs, H. Zohm, and G. Papp, "The role of stochastization in fast MHD phenomena on ASDEX Upgrade".

# XXVIII. Intrenational Workshop on Fundamentals of Li Based Batteries (Schloss Ringberg, Germany, November, 2008).

56. E.A. Kotomin, Yu.F.Zhukovskii, and J.Maier, "First principles modelling of interfacial mechanism for Li storage in nanocomposites".

# XXIX. 14<sup>th</sup> International Conference on Thin Films & Reactive Sputter Deposition 2008 (Gent, Belgium, November, 2008).

57. G. Zvejnieks and E.E. Tornau, "Modeling of phase separation in Au-Ni surface alloy".

# XXX. International workshop ''Towards Reality in Nanoscale Materials'08'' (Levi, Finland, December, 2008).

58. V. Kashcheyevs, "Models for charge localization and adiabatic redistribution in carbon nanotubes".

### XXXI. 2008 Fall MRS Meeting (Boston, MA, USA, December 2008).

59. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin, and D.E. Ellis, "Comparison of the atomic and electronic structure of single *F*-centers in cubic PbZrO<sub>3</sub>, PbTiO<sub>3</sub>, and SrTiO<sub>3</sub> perovskites". Abstracts: C.9.1.

60. S. Piskunov, E. Spohr, T. Jacob, E. Heifets, E.A. Kotomin, and D.E. Ellis, "Thermodynamic stability and electronic structure of LaMnO<sub>3</sub> and La<sub>0.875</sub>Sr<sub>0.125</sub>MnO<sub>3</sub> (001) surfaces: first-principles calculations by means of a hybrid density-functional theory". Abstracts: PP.9.32.

# 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 lithoghraphy for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed. The methods for fabrication of subwavelength-gratings and surface-relief features with nanometer scale have been developed.

#### **Scientific Staff**

- 1. Dr. M.Reinfelde
- 2. Dr. J.Teteris
- 3. Dr. O.Balcers
- 4. Dr. K.Jefimovs

#### **Technical Staff**

- 1. J.Gurovs
- 2. D.Popele

### **PhD Students**

A.Gerbreders E.Sledevskis

#### 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 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).

### **Main Results**

#### SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

#### M.Reinfelde and J.Teteris

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

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

The recording of the subwavelength gratings with a period of 0.15  $\mu$ 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  $\Lambda = \lambda_0/2$  n sin $\theta$ , where  $\lambda_0$  is the wavelength of laser light in vacuum, n is refractive index of the resist and  $\theta$  is the half-angle between the laser beams inside the resist. The right angle prisms with n= 1.8 - 2.6 were used to increase the value of  $\theta$ . The grating period and profile after chemical etching was measured by AFM. The transmission, reflection and polarization properties of the obtained gratings were studied.

#### AMORPHOUS CHALCOGENIDE THIN FILMS IN OPTICAL RECORDING TECHNOLOGIES

#### J.Teteris

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

The main functional principles and practical application of amorphous chalcogenide photoresists for production of the embossed *rainbow* holograms and holographic optical elements are discused. The laser interference lithography is used as a low-cost method for the exposure of large surfaces with regular patterns like subwavelength-gratings and microsieves. The regular features with the sizes of about 50

nm and less can be fabricated by this method. The Bragg reflection gratings were recorded and studied in amorphous  $As_2S_3$  and As-S-Se films. Amorphous chalcogenide thin films are thought to be one of the potential materials for all-optical integrated circuits for the optical communication systems due to their excellent infrared transparency, large nonlinear refractive index, and low phonon energies. The possibility to use the amorphous chalcogenide films as a media for holographic recording, processing and storage of information with high density is discussed.

#### IMMERSION HOLOGRAPHIC LITHOGRAPHY IN AMORPHOUS CHALCOGENIDE THIN FILMS

J.Teteris, J.Aleksejeva and M.Reinfelde

The recording of the surface-relief and refractive index modulated gratings with a period of  $0.15 - 1.0 \,\mu\text{m}$  was performed by solid immersion holographic method. The grating period for two intersecting light beams in a coupling prism with refractive index n can be expressed as  $\Lambda = \lambda_0/2$  n sin $\theta$ , where  $\lambda_0$  is the wavelength of laser light in vacuum, n is refractive index of the prism and  $\theta$  is the half-angle between the laser beams inside the prism. The right angle prisms with n = 1.5 - 2.6 were used. Amorphous As-S-Se based photoresist with refractive index  $n_1=3.2$  at 0.488  $\mu$ m was used for the recording of surface-relief gratings. After recording, wet etching of the photoresist was performed to obtain a surface-relief grating. The grating period and profile were measured by AFM. If the recording was performed in air (n=1) and the angle between the beams was equal to  $90^{\circ}$ , a grating with a period of 0.345 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<sub>2</sub>S<sub>3</sub> amorphous films were studied. The angular selectivity of holographic recording in amorphous chalcogenide thin films has been improved significantly by a decrease of grating period.

#### SURFACE RELIEF FORMATION DURING HOLOGRAPHIC RECORDING

#### U.Gertners and J.Teteris

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

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

#### NANOSTUCTURED SURFACES FOR OPTICAL ANTIREFLECTION

#### J.Aleksejeva and J.Teteris

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

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

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

#### OPTICAL RECORDING IN SPIROPYRAN AND POLYMER COMPOSITE FILMS

#### A. Gerbreder and J. Teteris

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

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

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

### **Scientific Publications**

- A.Bulanovs, V.Gerbreders, E.Sledevskis, V.Pashkevich and J.Teteris, Investigation of As<sub>2</sub>S<sub>3</sub>-Al films for dot-matrix holographic recording. *Proc.SPIE*, vol.**7142** (2008) 714211.
- 2. E.Sledevskis, Vj.Gerbreders, V.Kolbjonoks, J.Teteris and A.Gulbis, Second harmonic generation in selenium thin films. *Proc.SPIE*, vol.**7142** (2008) 71420F.

- 3. A.Gerbreders, J.Teteris and V.Kolobjonoks. Holographic recording in polymer composites of organic photochromes and chalcogenides. *Proc.SPIE*, vol.**7142** (2008) 714212.
- 4. A. Ozols, M. Reinfelde, Dm. Saharov, K. Kundzins, V. Kampars, V. Kokars "Holgraphic recording of surface relief gratings in tolyle-baserd azobenzene oligomers" *Thin Solid Films* **516** (2008) 8887–8892.
- 5. Andris Ozols and Mara Reinfelde "Effects of light polarization and crystal orientation on holographic recording efficiency in doped LiNbO<sub>3</sub> crystals" *Proc. SPIE*, vol. **7142**, (2008) 71420Z.
- 6. I.Mihailova, Vj.Gerbreders, E.Sledevskis, V.Kolbjonoks and E.Tamanis. Second harmonic generation in selenium-metal structures. *Proc. SPIE*, vol. **7142** (2008) 71420D.
- 7. S.Fomins, M.Reinfelde, A.Larichev, N.Iroshnikov, A.Gerbreders and M.Ozolinsh. Photoinduced AsSeS thin film phase plates as adaptive optics mirrors for eye aberration correction. *Proc. SPIE*, vol. **7142** (2008) 7142-43.

### Lectures on Conferences

# 24th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, February 20-22, 2008.

- 1. A.Gerbreders and J.Teteris, *Optical recording on chalcogenidew and organic polymer composites*. Abstract, p. 45.
- 2. E.Sledevskis, Vj.Gerbreders, V.Kolbjonoks, J.Teteris and A.Gulbis, *Photoinduced processes in selenium-metal structures*. Abstract, p. 48.
- 3. J.Teteris, An interaction between light and soft materials, Abstract, p. 44.
- 4. M.Reinfelde and J.Teteris, *Holographic self-enhancement in As-S-Se films*, Abstract, p. 46.
- 5. U.Gertners and J.Teteris, *Direct holographic recording of surface-relief gratings* on amorphous As<sub>2</sub>S<sub>3</sub> films. Abstract, p. 47.
- 6. A.Ozols and M.Reinfelde, *Wavefront inversion inLiNbO<sub>3</sub>:Cu crystals*. Abstract, p. 49.
- 7. J.Aleksejeva, J.Teteris and E.Laizane, *Surface relief formation in organic and inorganic polymers by UV holography*. Abstract, p. 50.
- 8. A.Danilovs and J.Teteris, *Creation of diffraction optical elements with focused beam.* Abstract, p. 57.
- 9. V.Duboviks and J.Teteris, *Surface-relief modulation of chalcogenide films by* 442 nm laser beam. Abstract, p. 58.

# 6th International Conference Advanced optical materials and devices", Riga, Latvia, August24-27, 2008.

- 1. J.Teteris. Interaction between Light and Soft Materials, Abstracts, p.34.
- 2. A.Ozols and M.Reinfelde. *Effects of light polarization and crystal orientation on holographic recording efficiency in doped LiNbO<sub>3</sub> crystals, Abstracts, p.33.*
- 3. A.Gerbreders and J.Teteris, V.Kolobjonoks, Holographic recording in polymer composites of organic photochromes and chalcogenides, Abstracts, p.35.
- 4. E.Sledevskis, Vj.Gerbreders, V.Kolbjonoks, J.Teteris and A.Gulbis, *Second harmonic generation in selenium thin films*. Abstracts, p.57
- 5. Vj.Gerbreders, A.Gerbreders, G.Kirilovs, J.Teteris, E.Sledevskis, A.Bulanovs, *Planar waveguides based on organic polymer and As*<sub>2</sub>*S*<sub>3</sub> *films*. Abstracts, p.65.
- 6. E.Laizane, I.Muzikante, J.Teteris, K.Kundzins and D.Gustina. *Optically induced surface relief grating of azobenzene containing polymer films*. Abstracts, p.79.
- 7. I.Mihailova, Vj.Gerbreders, E.Sledevskis, V.Kolbjonoks and E.Tamanis. *Second harmonic generation in selenium-metal structures*. Abstracts, p.55.

8. A.Bulanovs, Vj.Gerbreders and E.Sledevskis. *Investigation As*<sub>2</sub>S<sub>3</sub>-Al films for *dot-matrix holographic recording*. Abstracts, p.82.

# Third Int. Conf. on Optical, Optoelectronic and Photonic Materials and Applications – ICOOPMA2008, Edmonton, Canada, July 20-25, 2008.

J.Teteris. Interaction between light and soft materials. Abstracts, p. 180.

# International Baltic Sea Region Conference "Functional materials and nanotechnologies" FM&NT-2008, Riga, Latvia, April 1-4, 2008.

A.Trukhin, J.Teteris and A.Fedotov. *Photosensitivity of SiO*<sub>2</sub>-Al and SiO<sub>2</sub>-Na glasses and er ArF (193 nm) and  $F_2$  (157 nm) lasers. Abstracts p. 35.

# XVI<sup>th</sup> International Symposium on Non-Oxide and New Optical Glasses, Montpellier, France, April 20-25, 2008.

- 1. J.Teteris. *Direct holographic recording of surface-relief gratings on amorphous chalcogenide films*. Abstract, p.OC-48.
- 2. Vj.Gerbreders, E.Sledevskis, V.Kolbjonoks, J.Teteris and A.Gulbis. Second harmonic generation in selenium-metal structures. Abstract, P49.
- 3. A.Bulanovs, V.Gerbreders, E.Sledevskis and J.Teteris. *Dot-matrix holographic recording in As*<sub>2</sub>*S*<sub>3</sub>*-Al films*. Abstract, P53.
- 4. A.Gerbreders, J.Teteris and I.Mihailova. *Optical recording in organic polymer-chalcogenide composite thin films*. Abstract, P55.
- 5. E.Aleksejeva, E.Laizane, I.Muzikante and J.Teteris. *Surface-relief grating formation on organic and inorganic polymer films by UV holography.* Abstract, P56.

### EOS Annual Meeting 2008, Paris, France, 29 September – 02 October, 2008

J.Teteris, J.Aleksejeva, U.Gertners, A.Gerbreders and M.Reinfelde. *Direct photo-induced surface-relief formation on organic and inorganic amorphous polymer films*. Abstract, p.82.

# 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	PhD Students
1. Prof. I.Lācis	1. M.Sc. A.Švede
2. Prof. M.Ozolinsh	2. M.Sc. G.Ikaunieks
3. Dr. G. Krūmiņa	3. M.Sc. S. Fomins
4. M.Sc. R.Paeglis	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)
itury	Universita` di Roma "Tor Vergata" (Prof. I. Davoli)
Sweden	Chalmers TH, Sweden (Prof. L.Komitov)
Norway	Buskerud Høgskolan, Institutt for Optometri (Prof. J.R.Bruenich).
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 Laboratotry, 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.

# Main Results

### FERROELECTRIC LIQUID CRYSTAL GLASSES FOR AMBLIOPIA RESEARCH

#### Sergejs Fomins, Maris Ozolinsh, Gunta Krumina, Varis Karitans University of Latvia & Kengaraga Str. J.V. 1063 Riga Latvia

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 trough 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. Karitans<sup>1</sup>, M. Ozolinsh<sup>1</sup>, G. Kuprisha<sup>2</sup>

<sup>1</sup>Institute of Solid State Physics, University of Latvia, 8 Kengaraga Str., 1063 Riga <sup>2</sup>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: nonstability 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 CORTIAL MECHANISMS IN CONTRAST ADAPTATION

#### Didzis Lauva<sup>1</sup>, Maris Ozolinsh<sup>2</sup>

<sup>1</sup>Department of Optometry and Vision Science, University of Latvia <sup>2</sup>Institute of Solid State Physics, University of Latvia

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 asses 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

#### Gunta Krumina, Maris Ozolinsh, Gatis Ikaunieks

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

In routine eve examination the visual acuity usually is determined using standard charts with black letters on a white background, however contrast and colour are perception. The purpose of research was to study important characteristics of visual the perception of isoluminant coloured stimuli in the cases of true and simulated amlyopia. 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

#### Maris Ozolinsh<sup>1</sup>, Gunnar Andersson<sup>2</sup>, Gunta Krumina<sup>1</sup>, and Sergejs Fomins<sup>1</sup> <sup>1</sup>University of Latvia, 8 Kengaraga Str., LV-1063 Riga, Latvia <sup>2</sup>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

S. Fomins, M.Ozolinsh, G.Krumina, and V.Karitans. Ferroelectric liquid crystal glasses for amblyopia training. *Integrated Ferroelectrics*, V.103, pp.10-17 (2009).
 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).
 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).
 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).
 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).

#### **Reports in 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 Al<sub>2</sub>O<sub>3</sub>. Recently it was shown that some optical properties of nitride compounds are prospective for its application as new UV light and visible light emitters (Watanabe, Taniguchi), besides, features of AlN could rate it among materials available for UV light dosimetry (our results). Presently different forms of these materials are synthesized including a bulk material and its nanostructured forms and it is also known that their optical properties could be different. The interests of our research are largely focussed on revealing of the difference between the optical properties of the bulk material and its nanostructured forms. The spectral investigations performed in this laboratory are based on luminescence studies (photoluminescence (PL) and its excitation (PLE), optically stimulated luminescence (OSL) and thermoluminescence (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. Part of investigations was performed together with the collaboration partners from abroad.

#### **Scientific Staff**

PhD student 1. Dr. Hab.Phys, Assoc. Prof. B.Berzina 1 V Korsaks

**Students - Technicians** 1 D Jakimovica

2. Dr. L.Trinkler

#### **Scientific Visits Abroad**

B.Berzina, Frascati Research Center, Italy (10 days). L Trinklere, Frascati Research Center, Italy (8 days). V.Korsaks, Frascati Research Center, Italy (6 days). D.Jakimovica, Frascati Research Center, Italy (6 days).

### **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)

#### Main investigations and results

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

B. Berzina, L.Trinkler, V.Korsak, R.T.Williams<sup>1</sup>, B.Ucer<sup>1</sup>, D.Carroll<sup>2</sup>, S.Bellucci<sup>3</sup>

<sup>1</sup> Department of Physics, Wake Forest University, USA
 <sup>2</sup> Center of Nanotechnologies, Wake Forest University, USA
 <sup>3</sup>INFN-Laboratori Nazionali di Frascati, Italy

Our previous spectral investigations showed that the 395 nm photoluminescence (PL) is common for both the bulk h-BN (powder) and the multi-walled nanotubes (BNNT) synthesized from this powder. This luminescence could be related to the excitonic processes possibly influenced by some surface defects such as nitrogen vacancies. In the case of the bulk material the 395 nm PL band possesses well pronounced phonon-induced substructure with ~170 meV energy difference between two neighbour lines, whereas in the case of BNNT this substructure is hardly observable. Infrared (IR) light absorption measurements were performed in INFN National Laboratory Frascati, Italy. The 1370 cm<sup>-1</sup> absorption line was found for both the bulk h-BN and BNNT, coincident with the 170 meV phonon energy observed from PL spectra.

#### THERMOLUMINESCENCE OF Al<sub>2</sub>O<sub>3</sub> BULK AND NANOSIZE POWDERS

L.Trinkler, B.Berzina, D.Jakimovica

Thermoluminescence (TL) has been studied in the alumina (Al<sub>2</sub>0<sub>3</sub>) bulk and nanosize powders irradiated with UV light. The TL studies were carried out using the set-up for spectral measurements with an integrated sample heater, providing measurements of TL curves in the 20-300 °C temperature range and TL emission spectra under variable wavelength of the irradiation light. The studied alumina samples revealed the essential differences in the TL properties. The bulk Al<sub>2</sub>0<sub>3</sub> powder has 3 peaks (110, 170 and 280 °C) in the TL curve and 2 complex bands (around 450 and 700 nm) in the TL emission spectrum, whereas the nanosize powder is characterized with the very low TL intensity, one peak (80 °C) in the TL curve and one band (700-800 nm) in the TL emission spectrum.

The TL properties of alumina powders are explained with participation of intrinsic, surface and impurity defects in the luminescence processes. Some of these defects are identified basing on the analysis of photoluminescence spectra and literature data. Thus, TL spectra of bulk powders reveals the presence of F and F<sup>+</sup> intrinsic defects,  $Cr^{3+}$  and Fe<sup>3+</sup> impurity defects, whereas TL spectra of nanosize powders are determined mainly by the decisive role of surface defects. The studies of the luminescence processes in alumina powders are in progress.

#### **Scientific Publications**

1. R.T.Williams, K.B.Ucer, D.L.Carroll, B.Berzina, L.Trinkler, V.Korsaks, and R.Krutohvostov. *"Photoluminescence of self-trapped excitons in boron nitride nanotubes"*, J. of Nanoscience and Nanotechnology Vol 8 (2008) 1-5.

2. L.Trinkler, B.Berzina, D.Kasjan, L.-Ch. Chen, *"Luminescence processes induced by UV radiation in AlN nanotips and nanorods"*. Radiation measurements 43 (2008) 231-235.

3. Е.М.Шишонок, Л.Тринклер, С.В.Леончик, Б.Берзиня "*Люминесценция кубического нитрида бора, активированного тулием*". Журнал прикладной спектроскопии, 75, No 4 (2008) 547-555.

#### **Lectures on Conferences**

24<sup>th</sup> LU Scientific Conference of Institute of Solid State Physics, University of Latvia, February 20-22, 2007, Riga, Latvia

**1.** D.Kasjan, B.Berziņa, L.Trinklere, J.Grabis, I.Steins. "*Photoluminescence of Al<sub>2</sub>O<sub>3</sub> nanopowder*". Book of Abstracs, p 19.

International Baltic Sea Region Conference Functional Materials and Nanotechnologies (FM&NT), April 2-4, 2007, Riga, Latvia

**2.** V.Korsaks, L. Trinkler, B. Berzina, R.Williams, B.Ucer, and D.Carroll. *"Luminescence of multi-walled BN nanotubes and its raw material"*, Book of Abstracts, p.168.

**3.** Yu.Zhukovskii, S.Piskunov, B.Berzina, L.Trinkler, S.Belluci. "*Atomic and electronic structure of single-walled BN nanotubes containing nitrogen vacancies*", Book of Abstracts, p.25.

# 2008 International Conference on Excitonic Processes in Condenced Matter (EXCON'2008), June 22-27, 2008, Japan

**4.** B. Berzina, L. Trinkler, V. Korsak, R. T. Williams, K. B. Ucer, D. L. Carroll, and S. Bellucci. *"Excitonic and defect luminescence in h-BN powder and BN nanotubes"*. Kyoto University, Book of Abstarcts, p.89.

**5.** R. T. Williams, K. B. Ucer, D. L. Carroll, L.Trinkler, V.Korsaks, B. Berzina. "*Self-trapped excitons with vibronic structure on BN nanotubes*", Kyoto University, Book of Abstarcts, p. 88.

#### International Conference Nanoscience&Nanotechnology (n&n 2008) October 20-23, 2008, Frascati, Italy

**6.** B.Berzina, L.Trinkler, V.Korsaks, S.Bellucci, M.Piccinini, R.T.Williams, K.B.Ucer, and D.L.Carroll. *"Vibrational structure of photoluminescence and its approval by absorption in h-BN nanostructured materials"*. Laboratori Nazionali di Frascati, Book of Abstracts, 64.

# LABORATORY OF SURFACE PHYSICS

# Head of Laboratory Dr.phys. F.Muktepavela

#### **Research Area and Main Problems**

The research interests of the Laboratory of Surface Physics 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 2008

- 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

#### Technical Staff A.Petersons

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

#### PhD Student

Students

Mg.Phys.G.Bakradze

B.sc.R.Zabels
 B.sc R.Lisovskis

#### Scientific visits abroad

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

#### **Visitors from Abroad**

- 1. Dr.S.Stolyarova, Technion, Haifa, Israel (10 days).
- 2. Dr.V.Sursajeva, ISSP, Chernogolovka, Russia (2 weeks).

# Cooperation

#### Latvia

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

### **Main Results**

### PERCULIARITIES OF GRAIN BOUNDARY MICROMECHANICAL PROPERTIES IN POLYCRYSTALLINE ZINC

G. Bakradze, F. Muktepavela, V. Sursaeva<sup>1</sup>

<sup>1</sup> Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka

The influence of grain boundaries (GBs) properties on the development of grain boundary sliding (GBS) and vice versa - the influence of GBS on the mechanical properties of GBs - have been studied in pure Zn using precision microindentation technique, optical, electron and atomic force microscopy. Results have shown the different dependencies of microhardness from indentation depth for GBs and individual grains in bulk. When the plastic zone around the indent was comparable to the grain size, GBs acted as barriers for dislocation sliding bands and twins. At higher loads, a number of grains are involved in the process of deformation, but no increase of microhardness is observed due to the activation of GBS. At the same time, microhardness measurements performed directly on GBs and on triple junctions (TJs), have shown that microhardness values of GBs and TJs in polycrystalline Zn were higher than in the centre of grains. Thus, movement of the ensemble of defects to the GBs during microindentation is the activating factor for GBS in polycrystalline Zn. At the same time, during spreading of the deformation from GB to the centre of grain the activation of GBS was not observed.



Microhardness-distance profiles near grain boundaries in zinc polycrystal at three different loads (1.4mN, 4.4mN, 14.4mN) at room temperature



Single and polycrystalline Zn microhardness dependence on the indenter penetration depth at room temperature



The AFM image of plastic zone around imprint made using load P=0.2N at room temperature (initial stages of GBS).



Micrographs of indentation imprints made in polycrystalline Zn at RT P=50mN.

# ION-INDUCED MODIFICATION OF STRUCTURE AND MICROMECHANICAL PROPERTIES IN LIF CRYSTALS

### I.<u>Manika</u>, J. <u>Maniks.</u>, R.Lisovskis, K. Schwartz<sup>1</sup> <sup>1</sup> GSI, Darmstadt, Germany

Large penetration depth and ability to create radiation defects with nanoscale dimensions make swift heavy ions as an effective tool for the modification of physical and mechanical properties of solids. The track damage created in LiF crystals by swift U, Xe and Kr ions with a specific energy of 11.1 MeV per nucleon was studied using dislocation mobility measurements, track etching, SEM, AFM and optical microscopy. The results show high sensitivity of dislocation mobility to track core damage. For U tracks, continuity of etching and high obstacle strength for dislocations is observed while the tracks of Xe ions show discontinuities of etching and reduced obstacle strength. The efficiency of dislocation impeding by tracks decreases with decreasing the energy loss in the row of  $U \rightarrow Xe \rightarrow Kr$  projectiles. The ion induced reduction of dislocation mobility on irradiated surface is stronger compared to that in the bulk of irradiated layer. The results indicate redistribution of radiation defects by their migration to irradiated surface or interface between irradiated and unirradiated parts of the crystal.

#### Scientific publications

- 1. F.Muktepavela, G.Bakradze, V.Sursaeva. Micromechanical properties of grain boundaries and triple junctions in polycrystalline metals exhibiting grain boundary sliding at 293K.- *J. Mater. Sci*, 2008, vol.43, pp.3848-3854.
- 2. I. Manika, J. Maniks. Effect of substrate hardness and film structure on indentation depth criteria for film hardness testing. *-Journal of Physics D: Applied Physics*, 2008, vol.41, No.7, 074010 (1-6 p).
- 3. I. Manika, J.Maniks, K.Schwartz. Swift-ion-induced hardening and reduction of dislocation mobility in LiF crystals. *-Journal of Physics D: Applied Physics*, 2008, vol.41, No.7, 074008 (1-5 p).
- 4. M. Silinskas, A. Grigonis, V. Kulikauskas and I. Manika. Hydrogen influence on the structure and properties of amorphous hydrogenated carbon films deposited by direct ion beam. *-Thin Solid Films*, 2008, vol.516, No 8, pp.1683-1692.
- 5. I. Manika, J.Maniks, K. Schwartz. Investigation of heavy ion tracks in LiF crystals by dislocation mobility method. *Nuclear Inst. and Methods in Physics Research B*, 2008, vol 266/12-13, pp 2741-2744.
- M.Shorohov, F.Muktepavela, J.Maniks. Surface processing of TlBr crystals for Xand γ-ray detectors.- *Latvian Journal of Physics and Technical Sciences*, 2008, No.3, pp.13-19.
- F. Muktepavela, E.Platacis, R.Krishbergs, A.Shishko, A.Zik. Experimental studies of the strong magnetic field action on the corrosion of RAFM steels in Pb17Li melt flows.- *Proc.* 7<sup>th</sup> *International PAMIR conference of Fundamental and Applied MHD*, Presqu'Ile de Giens, France – 2008, Volume II, pp. 565-569.
- E.Platacis, R.Krishbergs, F. Muktepavela, A.Shishko. Analysis of the strong magnetic field influence on the corrosion of EUROFER steel in Pb17Li melt flows.-*Proc.* 7<sup>th</sup> International PAMIR conference of Fundamental and Appied MHD, Presqu'lle de Giens, France – 2008, Volume I, pp. 321-325.

# 7<sup>th</sup> International Symposium "Swift Heavy Ions in Matter (SHIM 08), Lyon, France, June 2-5, 2008.

1. I.Manika, J.Maniks, K.Schwartz. *Swift-ion-induced hardening and reduction of dislocation mobility in LiF crystals*. Abstracts, p.9 (oral presentation)

# International Baltic Sea Region Conference "Functional materials and nanotechnologies (FM&NT-2008)", April 1-4, 2008, Riga, Latvia.

- 2. G. Bakradze, F. Muktepavela, T. Petkova, P. Petkov, K.Kolev, V.Ilcheva. Influence of AgI on microhardness of (As<sub>2</sub> S<sub>3</sub>)<sub>100-x</sub> (AgI)<sub>x</sub> and (AsSe)<sub>100-x</sub>(AgI)<sub>x</sub> glasses. Abstracts, p.163 (poster presentation).
- 3. F.Muktepavela, G.Bakradze, L.Grigorjeva, R.Zabels, A.Gerbreders, E.Tamanis. Effect of the annealing on structure and properties of ZnO films obtained by mechanical oxidation. Abstracts ,p.172 (poster presentation).
- 4. A.Presz, W.Lojkowski, J.D.Fidelus, L.Griogorjeva, F.Muktepavela, J.Grabis, C.J.Monty Visualization of ZnO nanostrucures by scaning electron microscopy. Abstracts, p.173 (oral presentation)
- 5. I.Manika, J.Maniks, K.Schwartz. Diagnostics of ion-induced track damage in LiF single crystals by dislocation probe. Abstracts, p.57 (oral presentation).

# 6<sup>th</sup> Intern. Conf. "Advanced Optical Mater. and Devices (AOMD-08)", August 24-27, 2008, Riga, Latvia.

6. F. Muktepavela, L.Grigorjeva, R.Zabels, G. Bakradze, E. Tamanis. Nanohardness and structure of ZnO coatings.. Abstracts, p.59 (poster presentation).

# Intern. Conf. "Transparent Oxide Coatings (IS-TCO -2008)", October 22-26, 2008, Heraclion, Crete.

7. F. Muktepavela, G. Bakradze, L.Grigorjeva, R.Zabels, E. Tamanis Properties of ZnO coatings obtained by mechanoactivated oxidation. Abstracts p.130 (poster presentation).

### 4th Intern. Conf. on Mater. Science and Condens. Matter Physics, September 23-26, 2008, Chisinau, Moldova.

- 8. F. Muktepavela, L.Grigorjeva, R.Zabels, E. Tamanis. Micro-and nanohardness of ZnO obtained by mechanoactivated oxidation Abstracts, p.173 (poster presentation).
- 9. F.Muktepavela, G.Bakradze, V.Sursaeva. Micro- and nanohardness of grain boundaries in Zn. Abstracts, p.246 (oral presentation).
- 10. I.Manika, J.Maniks, R.Lisovskis. Dislocation impeding by ion tracks: surface and bulk effects. Abstracts, p.247 (oral presentation).

### 5<sup>th</sup> Intern. Conf. "Phase transformations and strength of crystals", November 17-21, 2008, Chernogolovka, Russia.

- 11. F. Muktepavela. Deformation behaviour of phase boundaries in fine grained Pb-Sn eutectics. Abstracts, p.83 (oral presentation).
- 12. B. Straumal, J.Kalniņš, A.Aslund, V.Kostjuchenko, F.Muktepavela, V.Pervezencov. Pb-Sn, Cu-Zn-Pb alloys for the restoration of historic organs. Abstract, p.181 (poster presentation).

# 7<sup>th</sup> PAMIR International Conference on Fundamental and Applied MHD, Presqu'île de Giens - France, September 8 – 12, 2008.

- 13. F. Muktepavela, E.Platacis, R.Krishbergs, A.Shishko, A.Zik.Experimental studies of the strong magnetic field action on the corrosion of RAFM steels in PB17Li melt flows (poster presentation).
- 14. E. Platacis, R. Krishbergs, F. Muktepavela., A Shishko. Analysis of the strong magnetic field influence on the corrosion of EUROFER steel in Pb17Li melt flows (oral presentation).

# **DEPARTMENT OF RADIATION PHYSICS**

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

#### **Research Area and Main Problems**

The Laboratory includes four research groups – the nuclear spectroscopy and theory, applied nuclear physics, oxide physics and fine particles cooperative effects study groups. The following main problems are developed in the laboratory:

- 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;
- study of the possibilities to use planned Salaspils cyclotron for activation analysis;
- study of magnetic ions exchange interaction in the antiferromagnetic oxides MeO-MgO solid solutions employing optical absorption, luminescence, EPR and Raman spectroscopy methods;
- study of exchange interaction between radiation defects and transition metals ions in the dielectric crystals doped with the transition metals ions;
- EPR retrospective dosimetry
- study of physical, structural and magnetic properties of solid state fine particles.

#### **International projects:**

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

#### Scientific Staff

- 1. Dr.hab. J.Berzins
- 2. Dr.hab. M.Balodis
- 3. Dr.hab. V.Bondarenko
- 4. Dr.hab. A.Afanasjevs
- 5. Dr. hab. U.Ulmanis †30.12.2008
- 6. Dr.hab. N.Mironova Ulmane
- 7. Dr. hab. J. Tambergs †25.11.2008
- 8. Dr. L.Simonova
- 9. Dr. T. Krasta
- 10. Dr. D.Riekstina

#### Technical Staff

1. S.Afanasjeva

- 11. Dr. V.Skvortsova
- 12. Dr. O.Veveris
- 13. Dr. A.Petrovs
- 14. Dr. J. Ruza
- 15. Dr. G. Smilskalne
- 16. Dr.Ing. A.Pavlenko
- 17. Mag. I.Motmillere
- 18. Mag. M. Polakovs
- PhD students
  - 1. Mg.J.Proskurins
- 1. D. Magone

Students

- 2. K. Bavrins
- 3. A. Jakimovičs
- 4. G. Māliņš

- 2. L. Neiburgs
- 3. A. Sotaks

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2. Mg. A.Andrejevs

#### Scientific visits abroad

Dr. hab. A.Afanasjev, Mississipi University, USA (7 months).

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

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

Dr. D. Dr. D. Riekstina, 21. Seminar Aktivierungsanalyse und Gammaspektroskopie (SAAGAS 21), Deutschland, (3 days).

Dr. hab. J. Dr. hab. J. Berzins, 5<sup>th</sup> Dresden Symposium "Hazards detection and management", Dresden, 3 -7 March 2008

Dr. D. Riekstina, 5<sup>th</sup> Dresden Symposium "Hazards detection and management", Dresden, 3 -7 March 2008.

Mag. J. Proskurins, 58<sup>th</sup> International Meeting on Nuclear Spectroscopy and Nuclear Structure "NUCLEUS-2008". Fundamental Problems of Nuclear Physics, Nuclear Methods in Nanotechnology, Medicine and Nuclear Power Engineering. Moscow, Russia, 23-27 June, 2008

Dr.hab. M.Balodis, 13<sup>th</sup> International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics (CGS13). Cologne, Germany, 25-29 August, 2008.

Mag. J.Proskurins, 13<sup>th</sup> International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics (CGS13). Cologne, Germany, 25-29 August, 2008.

Dr. D.Riekstina, LSC 2008, Davos, Schweiz, (6 days).

Dr.hab. phys. N.Mironova-Ulmane, Dresden, Germany

Dr.hab. phys. N.Mironova-Ulmane Institute of metal physics, Ekaterinburg, Russia (2 week)

Dr.V. Skvortsova. Gdansk, Poland, (1week).

Dr. V. Skvortsova, Lyon, France. (1week)

Dr. A.Pavlenko IAEA Wiena, Austria (10 mounth)

# Cooperation

### Latvia

1. Medical Academy of Latvia (Dr.hab., Prof. M.Eglite, 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 (Prof. J. Deghtjar).
- 8. National Diagnostic center.

# USA

- 1. Lawrence Livermore National Laboratory, California (Prof. R. W. Hoff).
- 2. Brookhaven National Laboratory, Upton (Prof. R.F. Casten).
- 3. Notre Dame University, Notre Dame, USA (Prof. S. Frauendorf).

### Germany

- 1. Technical University Munich (Prof. T. von Egidy, Dr. H.-F. Wirth)
- 2. Institüt für Physik, Johannes Gutenberg Universität Mainz, Mainz, Germany

### 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. Bőrner, 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, Ŕež (Dr. J.Honzatko).
- 2. Department of Nuclear Physics, Charles University (Prof. J. Kvasil).

# 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, Universitá Roma Tre, Rome (M. Piccinini)
- 3. INFM and Dipartimento di Fisica, Università di Trento, Povo (Trento)( G.Mariotto)
- 4. INFM 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).
- 2. Institute of Physics of the Ukrainian Academy of Science, Kiev (prof. S. Nepijko).
- 3. Pedagogical University, Kaluga, Russia (prof. K.Nikiforov),
- 4. Institute of Chemical Physics, Chernogolovka, Russia (prof.V.Petinov).

# Croatia

1. Ruder Boskovic Institute, Zagreb (Prof. S.Music).

### Poland

1. Institute of Pysics, PAS, Warshaw (Dr. A.Suchocki).

### 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)

# Austria

1. IAEA (Dr. A Shakhashiro)

# Denmark

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

#### **Main results**

### EXPERIMENTAL STUDY OF NUCLEAR PROPERTIES STRUCTURE OF THE ODD-ODD NUCLEUS <sup>188</sup>Re

#### M.Balodis, J.Bērziņš, Ļ.Simonova, V.Bondarenko, T.Krasta, J.Tambergs, A.Jakimovičs

Gamma-ray spectra of <sup>188</sup>Re are studied via thermal neutron capture in the <sup>187</sup>Re targets. Gamma-gamma coincidence spectra measured at Nuclear Research Institute, Prague, from 60 to 5800 keV, are evaluated. Partial evaluation is made for the single gamma-spectra from 100 to 800 keV, measured at the Institute Laue-Langevin, Grenoble. The <sup>188</sup>Re low-energy level scheme is developed and improved considerably. The scheme is interpreted, employing the rotor-plus-two-particle model. Two particle configurations are based on Nilsson proton orbits  $5/2^+[402]$ ,  $9/2^-[514]$  and neutron orbits  $1/2^-[510]$ ,  $3/2^-[512]$ . 7/2<sup>-[503]</sup>,  $9/2^-[505]$ . For six negative particle rotational bands with K=1,1, 2, 2, 3, and 4, the Coriolis mixing calculations are performed.

# EXPERIMENTAL AND THEORETICAL STUDY OF THE <sup>194</sup>Ir NUCLEUS

### M.Balodis, J.Bērziņš, N.Krāmere

The structure of <sup>194</sup>Ir is investigated via  $(n,\gamma)$ ,  $(n,e^{-})$ , (d,p), and  $(d_{pol},\alpha)$  spectroscopy. The use of different methods leads to an almost complete level scheme up to high excitation energies, including  $\gamma$ -decay and spin-parity assignments. A reanalysis of the formerly published  $(n,\gamma)$ , (n,e) data, including earlier unpublished spectrum above the 500 keV energy, was performed, taking into account the new (d,p) and  $(d_{pol},\alpha)$  transfer reactions data. The experimental level scheme is compared with model predictions, based on extended supersymmetry scheme. Herein, the classification of states was done with regard to quantum numbers, excitation energies, and  $(d_{pol},\alpha)$  transfer strengths. A one-to-one correspondence in excitation energies was obtained for the 23 lowest-lying theoretical states, with similar structures for the experimental and calculated level schemes. The two-nucleon transfer strengths show remarkable agreement. A classification of Nilsson states is discussed as well under the assumption of low-deformation prolate axial shape of the <sup>194</sup>Ir nucleus.

#### **Nuclear Theory**

#### STUDIES OF QUANTUM CHAOS AND PHASE TRANSITIONS IN THE FRAMEWORKS OF COMPLETE VERSION OF IBM-1 AND TRIAXIAL ROTATOR MODELS

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

Continuing the studies of quantum chaos and phase transition relationships in nuclear models, carried out according to the LSC research grant project No.05.1707, the nuclear theory group worked in two directions. The first one was the study of the classical energy functional of complete IBM-1 model version in terms of nuclear shape variables ( $\beta$ , $\gamma$ ), employing two essential control parameters ( $r_2$ ,  $r_1$ ) used in catastrophe theory formalism. The analysis of the dependence of nuclear energy surface equilibrium values from the deformation parameter  $\beta$  has been performed in the case when the triaxiality parameter  $\gamma=0^{\circ}$ . The results, obtained for critical points and phase transition lines between spherical ( $\beta=0$ ) and two deformed (prolate –  $\beta>0$  and oblate -  $\beta<0$ ) shapes

were compared with the results of our previous studies, in which the simplified extended Casten triangle version of the interacting boson model was used. A comparison of nuclear shape parameter  $\beta$  values, at which phase transitions occur, obtained both by our precise solution of the classical energy functional and by the expansion of the energy functional in Taylor series, in analogy with Landau theory of the second order phase transitions, has shown that, in order to obtain physical solutions, one should include in the Taylor series all power terms up to  $\beta^5$ . The second direction was the study of quantum chaos dynamical criteria (wave function entropy  $W(\Psi_i)$  and basis state fragmentation width  $\kappa(\Phi_k)$ ) in the frameworks of Bravin-Fedorov triaxial rotator model, which, in difference from the previously studied geometrical A.Davidov's rigid triaxial rotator model, depends on both nuclear quadrupole deformation parameters  $(\beta, \gamma)$ . The model Hamiltonian matrices have been diagonalized for all nuclear spin I values up to I=101, and corresponding chaos criteria of model energy states were evaluated. The obtained results, just like in the case of Davidov's model, have shown that one can determine correctly a theoretically predicted transition from the "soft" ( $\kappa(\Phi_k) \le 1$ ) to "hard" chaos ( $\kappa(\Phi_k) > 1$ ) only starting with nuclear spin values  $I \ge 50$ , when the number of mixed basis states n>26.

In addition, the studies of nuclear isospin symmetry effects were continued for  $N\approx Z$  p- and sd-shell nuclei, employing the Strictly Restricted Dynamics Model, and started for nuclei in the A~190 region in the frameworks of unified nuclear model.

#### Magnetic properties of solid state fine particles

#### **EXCHANGE BIAS EFFECTS IN FINE COBALT PARTICLES**

#### A.Petrovs, I.Kudrenickis, M.Maiorov

Magnetic characterization of Co nanoparticles, prepared by evaporation of massive cobalt in the flow of inert gases, have been studied. Particles were placed in nonmagnetic paraffin matrice. It was observed and interpreted the horizontal shift of the hysteresis loops, traced after magnetic field-cooling, as a result of magnetic exchange between surface spins (antiferromagnetic or spin-glass-like) and core (ferromagnetic) spins. The focusing attention is devoted to the investigations of exchange anisotropy of fine cobalt particles with oxidized surface . From the value of hysteresis loop shift the value of the exchange magnetic anisotropy constant and its dependence on the particle size (14-23 nm) has been determined. X-ray structure analysis has shown that the cobalt core of the particle is surrounded by a thin layer of the CoO which, in turn, is covered by a layer of the Co<sub>3</sub>O<sub>4</sub>. The numerical calculations of magnetic hysteresis loops have been carried out for the "unaxial+exchange" anisotropy. Corresponding values for changes of the relative remanent magnetization and for changes of coercitive force were evaluated. The calculated results show the arising the mechanism of "over pulling" of the magnetic loops and decreasing the values of the coercive force H<sub>c</sub>. The experimental data for the particles of all sizes, except the smallest one, are well fitting on the line with the value of the slope  $K_{exch}=0.29\pm0.02$  erg/cm<sup>2</sup>. The smallest particles with cobalt core radius 4 nm give the value  $0.21\pm 0.02$  erg/cm<sup>2</sup>, that might be connected with the size effect for this value defined, e.g., by decreasing the thickness of the CoO layer or decreasing the value of M<sub>s</sub> in dependence on the cobalt core diameter of the particle. The values of magnetic parameters of particle ensemble (H<sub>c</sub>, M<sub>r</sub>/M<sub>s</sub>, shift of the loop) are the result of complicated "game" of different kinds of anisotropies, their magnitudes and distribution of particles sizes in the ensembles. In the case of oxidized Co particles the effective uniaxial anisotropy arising from dipole-dipole interaction should be taken into account .
#### Laboratory of Applied Nuclear Physics

#### TRITIUM DETERMINATION WITH LSS FOR SOLVING SOME ENVIRONMENTAL PROBLEMS IN LATVIA

#### D.Riekstina, O.Veveris, G.Smilskalne

Tritium determination via a liquid scintillation method, employing the Packard TRI-CARB spectrometer with OptiPhase "HiSafe"3 optimized modes of using the scintillation liquid, was applied for the solution of 3 different problems:

**A.** Regular tritium control in ground water around the potentially dangerous objects as the decomissioning Salaspils nuclear reactor and the radioactive waste repository "Radon".

**B.** Investigations on the tritium diffusion (leachability) from concrete containing the tritium in water.

**C.** Control of drinking water in food industry and urban water-supply. With regards to the EU Directive 98/83 EC on the quality of drinking water, implemented in Latvia in 2003 (The Latvian Cabinet of Ministers Regulation Nr.235), the control of the tritium content in the sources of drinking water was started. More than 120 water sources from food industry and urban water-supply in Latvia were checked and it was established that the tritium concentration in neither of them exceeds 10 Bq/l limits.

#### RADIATION MONITORING AND CONTAMINATED TERRITORY CONTROL IN LATVIA

#### D.Riekstina, J.Berzins, O.Veveris, J.Malnacs

The control of the radioactive contaminated territory and monitoring of artificial radionuclides in the soil and groundwaters around the potentially most polluted regions of Latvia (the areas of the shut-down (1998) Salaspils research nuclear reactor) and the radioactive waste repository "Radons" has been carried out. The tritium monitoring of groundwaters in 19 wells was performed during 9 years period. Tritium concentration in certain wells varies within a wide range and seasonal changes are recognisable as well. The results of Cs-137 monitoring in soils demonstrated that the concentrations doesn't exceed the average value (260 Bq/kg) in Latvia soils. Difference in radionuclide concentration of various samples depends on the soil type.

The pollution by radium and its decay products in the rooms, sewage and special ventilation systems of the former medical facility as well as the migration of this pollution in the soils around this object was investigated. For a number of years in this facility the production of radon from radium salts for therapy purposes was carried out. According to the obtained data, the concentration of Ra-226 in many places in rooms exceeds natural background more than 100 times. Pollution of soil with Ra-226 was established in the depths up to 3 m.

Obtained data made it possible to prepare an action plan for the recovery of investigated area.

#### Laboratory of Transition Metals Compaunds Physics

#### **OPTICAL PROPERTIES OF HYDROGEN-CONTAINING MgO CRYSTAL**

V. Skvortsova, N. Mironova-Ulmane, L. Trinkler, L. Grigorjeva

The photoluminescence (PL), its excitation (PLE) and absorption spectra in ultraviolet, visible and infrared (UV-VIS-IR) regions were used to investigate the MgO single

crystals irradiated by fast neutrons. It is shown that the photoluminescence band of the MgO crystals at 730 nm belongs to the hydrogen-containing complex centers  $V_{OH}^{-}$ -Fe<sup>3+</sup>, which are transformed during the irradiation with fast neutrons. The behavior of the PL band 730 nm after fast neutron irradiation depends on the iron-chromium concentration. It is found that the fast neutron irradiation produces the interstitial proton H<sup>+</sup><sub>i</sub> and the Mg(OH)<sub>2</sub> microphase.

#### THE ELECTRON PARAMAGNETIC RESONANCE SPECTRA OF BLOOD

M.Polakovs, Nina Mironova- Ulmane, Andrejs Pavlenko and Eriks Reinholds<sup>\*</sup> \*P.Stradins Clinical University Hospital, Nuclear Medicine Department, Riga, Latvia

The aim of work is studying of radiation influence on blood of patients examined by radio-isotopes diagnosis (Tc99m) using electron paramagnetic resonance (EPR).

It is well known that EPR can be used to monitor paramagnetic metalloproteins contains  $Fe^{3+}$  (methemoglobin, transferrin) and  $Cu^{2+}$  (ceruloplasmin).

The EPR spectra were recorded using an EMX-6/1 spectrometer (BRUKER) working at X-band frequency with 100 kHz modulation. Magnetic field varied between 100 and 7000 Gauss. The g-factors of EPR signals were determined by reference to the external magnetic field. The EPR signal intensities of sample were measured against fixed standard signals using the standard crystal MgO- $Cr^{3+}$  placed in resonant cavity. The EPR spectra of blood have been studied at 77 K temperature.

Venous blood was donated by consenting patients before and after radio-isotopes diagnosis and collected under air in glass tubes containing a small amount of heparin used as an anticoagulant.

EPR spectra of patients blood was measured before and after radio-isotopes diagnosis. The EPR spectrum consists of the signals of some different paramagnetic centres. EPR spectra of some patients have the signal with g = 6 is caused by heme Fe<sup>3+</sup> ions in the high spin state assigned to methemoglobin [1]. It was observed that after radio-isotopes diagnosis the EPR signal intensity of methemoglobin increase. We can also detect EPR signals from the metal-protein transferrin (g= 4.3) that contains the non-heme rhombic iron Fe<sup>3+</sup> [1].

It is shown that EPR spectra of blood of patients after examination by radio-isotopes diagnosis has stronger signal of the ion  $Fe^{3+}$  of methemoglobin is in low-spin state with g = 2.005 and in the high spin state with g=6 than before radio-diagnosis.

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# 24-th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, 20-22 February, 2008.

1. J.Proskurins, K. Bavrins, A.Andrejevs, J. Tambergs, "Studies of phase transitions and quantum chaos in the framework of interacting boson and geometrical nuclear models", p.38.

2. J Ruža, "On present status of quantum measurements", p. 39.

3. M. Balodis, J. Bērziņš, Ļ. Simonova, V. Bonderenko, T. Krasta, I. Tomandl, M. Jentschel, P. Mutti, H. Boerner, "Nuclear structure study of <sup>188</sup>Re analysing  $(n,\gamma)$  reaction measurements", p.40.

4. A. Jakimovičs, T. Krasta, J. Tambergs, M. Balodis, "Structure of odd-odd nucleus <sup>188</sup>Re in the framework of the rotor plus two-quasiparticle model", p. 41.

5. O. Veveris, D. Riekstina, "Applying of liquid scintillation spectrometry in tritium analysis in environment", p. 42.

6. G. Malins, A. Andrejevs, J. Tambergs, "Study of inertioid model", p.53.

7. V. Skvorcova, "Luminescence of radiation and impurity defects in neutron irradiated magnesium oxide crystals", p.22.

# 5<sup>th</sup> Dresden Symposium "Hazards detection and management" Dresden, 3 -7 March 2008.

1. D.Riekstina, J. Berzins, O. Veveris, J. Malnacs, "Radiation monitoring and contaminated territory control in Latvia", p.38.

# International Baltic Sea Regional Conference "Functional materials and nanotechnologies", Riga, April 1-4, 2008

1. A.Petrov, V.Serga, M.Maiorov . "Size, structure and magnetic properties of extractive-pyrolytic, synthesized cobalt ferrite particles", p.117

#### EcoBalt'2008, Riga, May 15-16, 2008

1. J. Bērziņš, D. Riekstina, "Possible investigations in National multipurpose cyclotron center in Latvia, p.24.

#### LSC 2008 Advances in Liqud Scintillation Spectrometry, Davos, 25-30 May 2008

1. D.Riekstina, O. Veveris, G. Smilskalne, "Tritium determination with LSS for solving some environmental problems in Latvia", p.88.

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1. J.Bērziņš, M.Balodis, V.Bondarenko, Ļ.Simonova, T.Krasta, A.Jakimovičs, J.Tambergs, I.Tomandl, M.Jentschel, P.Mutti, H.Boerner, "Structure of <sup>188</sup>Re from the  $(n,\gamma)$  reaction", p.149-150.

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1. J.Ruža. "Conceptual aspects of von Neumann's quantum measurement scheme"

2. J.Ruža. "Entangled states in quantum mechanics".

#### 13<sup>th</sup> International Capture Gamma-Rays and Related Topics Symposium (CGS-13), Cologne (Germany), August 25-29, 2008

1. 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 <sup>188</sup>Re", p.149-150.

2. J. Proskurins, K.Bavrins, A.Andrejevs, T.Krasta, J.Tambergs. "Study of Quantum Chaos in the Framework of Triaxial Rotator Models", p.174-175.

#### DFG Physics School "Foundations of Quantum Physics", 21-26 September, Bad Honnef, Germany

J.Ruža. "Hidden variables in quantum mechanics". Scientific seminar of LU ISSP, Riga, 12 November, 2008 1.A.Andrejevs, J.Tambergs. "2008 Nobel price in physics".

#### Cyclotron Networking Meeting, Ispra, Italy, 3-5 December, 2008

1. J. Berzins "Multipurpose cyclotron center in Latvia"

# Scientific seminar of LU PMP Inst. of Atomic Physics and Spectroscopy "In memoriam Juris Tambergs", Riga, 4 December, 2008

1.A.Andrejevs, J.Tambergs. "2008 Nobel price in physics".

# 5<sup>th</sup> Dresden Symposium "Hazards Detection & Management", Dresden, Germany, 03-07 March, 2008

D. Riekstina, J. Berzins O. Veveris, J. Malnacs "Radiation monitoring and contaminated territory control in Latvia", p. 38.

#### International Conference "EcoBalt'2008, Riga, May 15-16, 2008

J. Berzins, D. Riekstina, "Possible investigations in national multipurpose cyclotron center of Latvia", p. 24

#### LSC 2008, Davos, Schweiz, May 25-30, 2008

D. Riekstina, O. Veveris, G. Smilskalne, "Tritium determination with LSS for solving some environmental problems in Latvia", LSC2008-88.

#### International Conference "Advances in Modern Natural Sciences", Kaulga, Russia 1.A.E.Petrov, I.V.Kudrenickis."Gadolinium Containing Ferrites and Superconductors after Thermal Neutron Irradiation (Comparing Consideration)" // ADVANCES IN MODERN NATURAL SCIENCES, International Conference Proceedings, Kaluga, Russia, 2008; p.144-152

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1. A.Petrov, I. Kudrenickis, M.Maiorov. "Exchange bias effects in fine cobalt particles", Conference Proceedings, Volume 1, p.50 – 56.

# International conference "Advanced Optical Materials and Devices, AOMD-6, August 2008, Riga, Latvia

1. M.Polakovs, N. Mironova-Ulmane, N.Kurjane, E.Reinholds, "Micro-Raman scattering of hemoglobin", p.38.

2. N. Mironova-Ulmane, A. Kuzmin, T. Dizhbite, I. Sildos, M. Pärs J. Grabis "Magnon and phonon excitations in nanosized NiO", p.53.

3. V. Skvortsova, N. Mironova-Ulmane, L. Trinkler, L. Grigorjeva. "Optical Properties of Hydrogen-Containing MgO Crystal", p. 56.

# "16<sup>th</sup> International Conference on Solid Compounds of Transition Elements Dresden, Germany. 2008.g. 26-31 July

N. Mironova-Ulmane, A. Kuzmin, M. Grube. "Raman and infrared spectromicroscopy of manganese oxides".

# International Baltic Sea Region conference "Functional materials and nanotechnologies" Riga, April 1-4, 2008.

N.Mironova-Ulmane, A.Kuzmin, M.Grube. "Microspectroscopy of manganise oxides", p.51.

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N. Mironova-Ulmane, A.Kuzmin, T.Dizhbite, I.Sildos, M.Pärs, I.Steins, J.Grabis "Raman scattering in nanosized Ni<sub>c</sub>Mg<sub>1-c</sub>O solid solution".

#### 14th Nordic – Baltic Conference on Biomedical Engineering – NBC-2008.

M.Polakovs, N.Mironova-Ulmane, A.Pavlenko, E.Reinholds. "The electron paramagnetic resonanse spectra of blood".

#### "The 15 th Conference on Luminescence and Optical Spectroscopy of Condensed Matter (ICL '08), Lyon (France), 7 -11. July

V. Skvortsova, L. Trinkler, "Luminescence of impurity and radiation defects in magnesium oxide crystals irradiated by fast neutrons", p.We-P057.

#### International Workshop on Advanced Spectroscopy and Optical Materials. Gdansk (Poland), 13-17 July 2008

Skvortsova V., Mironova- Ulmane N., Trinkler L. "Influence of transition elements impurities and radiation defects on luminescence and absorption spectra of MgO crystals", p.2-P-1.



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#### 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)	

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

### 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, A. Jurgis).

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- 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).

#### France:

- 1. Laboratoire de Chimie Inorganique et Matériaux Moléculaires, Université Pierre et Marie Curie, Paris, (Dr.habil. M.Bouvet).
- 2. Laboratoire POMA, Université d'Angers, Angers (Prof. J.M.Nunzi).

#### 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)

### Main results

#### OPTICAL INDUCED PROPERTIES OF POLYMER FILMS CONTAINING AZOBENZENE DERIVATIVES

#### HOLOGRAPHY RECORDING IN AZOBENZENE CONTAINING POLYMER FILMS

#### E.Laizāne, K.Kundziņš, I.Muzikante, J.Teteris, D.Gustiņa, E.Markava In co-operation with Latvian Institute of Organic Synthesis

Since the first proposition of the D.Gabor, holography has been widely use for various optical information processes. In recent years polymers and low molecular organic compounds are studied due to their potential application as photoactive media for information storage and processing. One of the hot topics is surface relief grating (SRG) in polymers doped with azobenzine molecules. The main advantage of azobenzene molecules are changes of there geometry and optical properties by irradiation with fixed wavelength light. In experiments influence of structure of 2 original low molecular azobenzene derivatives (A-45, A-48 see figures above) on SRG of polymer matrix is studied. We observed up to 200 nm and 70 nm high surface reliefs for polymer doped with A-45 molecules and A-48 molecules respectively.



A-45 6-[4-(4-Dicyclohexylsulfamoyl-phenylazo)phenoxy]-hexanoic acid

A-48 6-{4-[4-(Hexyl-phenyl-sulfamoyl)phenylazo]-phenoxy}-hexanoic acid

The formation of photoinduced SRG of azobenzene containing polymer films is caused by photoisomerisation process.

This work is supported by the National Research Program of Latvia in Materials Science.

#### **OPTICAL AND ELECTRICAL PROPERTIES OF N,N-DIMETHYLAMINO-BENZYLIDENE 1,3-INDANDIONE (DMABI) AND IT DERIVATIVES**



DMABI

#### IMPACT OF AGGREGATES ON EXCITATION DYNAMICS IN TRANSPARENT POLYMER FILMS DOPED BY DIPOLAR MOLECULES

S.Jursenas, N.Kurilcik, R.Karpicz, V.Gulbinas, L.Valkunas, M.Rutkis, I.Muzikante In co-operation with Institute of Physics, Vilnius, Lithuania Institute of Materials Science and Applied Research, Vilnius University, Vilnius, Lithuania

The impact of aggregate states on the optical properties of PMMA films doped (up to 25wt.%) with dipolar DMABI molecules was studied. Formation of DMABI nanocrystallites up to micrometers in sizes was shown to have a minor impact on absorbance properties of the films. Meanwhile excitation recombination pathways were significantly altered by occurrence of the aggregates by increasing their size. Competition in the emission from the DMABI monomer and from the self-trapped exciton in the crystallite has been observed by varying the dopant concentration. Resonant energy transfer enhancing with the dopant concentration leads to the change in the emission colour of the DMABI/PMMA films from green (for the low dopant concentration below 1 wt.%) to red in highly doped films (N10 wt.%). Due to the lower energy absorption band and to the pronounced exciton-phonon coupling, the aggregate states act as excitation energy trapping centers with the high fluorescence output. Selectively excited fluorescence sensing can be applied as an indicator of the aggregate state formation in the blends doped by dipolar molecules. In particular, transparent polymer films doped with dipolar DMABI can be applied as time-temperature indicators. However, for high intensity excitation the DMABI nanocrystals operate as nonradiative traps due to efficient exciton-exciton annihilation. To explain the

experimental data the enhancement of exciton–exciton annihilation with the increase in the size of submicron crystallites is suggested.

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

#### INFLUENCE OF CORONA POLING PROCEDURES ON LINEAR AND NON-LINEAR OPTICAL PROPERTIES OF POLYMER MATERIALS CONTAINING INDANDIONE DERIVATIVATIVES AS A CROMOPHORES

#### A.Vembris, M.Rutkis, E.Laizane

Second harmonic generation (SHG) efficiency of the poled guest - host polymer system is proportional to the concentration and orientation degree of non-linear optical (NLO) active molecules (chromophores). Corona poling realized at elevated temperatures could cause concentration decrease of NLO- active molecules due to centrosymmetric crystallization. Our studies showed that number density of crystallites is depending on orientation procedure. To obtain the best orientation procedure for guest - host systems containing four different chromophores based on DMABI we have compared optical images and SHG efficiency of corona poled films. According to our observations external poling electric field applied from the very beginning of the sample heating process can reduce crystallite grow. The optical quality is improved and SHG efficiency in some cases is up to 1.6 (depending on molecule structure) times larger after our suggested orientation sequence compared to classic corona poling procedures. The NLO efficiency of the investigated guest - host films are affected by crystallite grow in the sample. The reduction of crystallisation process is possible in several ways. First is well known chemical modification of molecule structure (in our case it is attachment of a tret- butyl moiety). Second is to decrease the time when sample is exposed to elevated temperature. Third is our suggested orientation procedure where corona discharge is switched on all the time. The number density of the crystallites could be kept approximately the same as in unheated (fresh) sample by applying of the corona discharge during initial heating step to poling temperature. SHG efficiency in comparison to classic corona poling procedures in case of this poling sequence is increased more then 1.5 times. The maximum enhancement by the first type of orientation

sequence was observed in the range of concentrations optimal with respect to SHG efficiency.

#### NEW FIGURE OF MERIT FOR TAILORING OPTIMAL STRUCTURE OF THE SECOND ORDER NLO CHROMOPHORE FOR GUEST – HOST POLYMERS

M. Rutkis, A. Jurgis, V. Kampars, A. Vembris, A. Tokmakovs, V. Kokars In co-operation with Institute of Physical Energetics, Institute of Applied Chemistry, Riga Technical University

Reliability to forecast SHG efficiency using two sets of non linear optical (NLO) chromophore figures of merit (*FOM*) was tested. One of them predicts that SHG efficiency  $d_{33}$  of the poled guest - host polymer is proportional to ground state dipole ~  $\mu_g$ , another to ~  $1/\mu_g$ . Correlation of maximal achieved second order NLO efficiency of the **PMMA** based systems containing eight dimethylaminobenzylidene -1, 3 - indandione (**DMABI**) related chromophores with proposed *FOM* have been analyzed.

The best correlations were obtained with second set of *FOM*, especially if high dipole moment ( $\mu_g$ >7D) chromophores are included in analysis.



is linear fit for eight, dashed for six chromophores.

This work is supported by the National Research Program of Latvia in Materials Science.

#### SUPRAMOLECULAR ASSEMBLY OF INDANDIONE BASED BINARY CHROMOPHORE ORGANIC GLASSES FOR NLO APPLICATIONS

M. Rutkis, V. Kampars, V. Kokars, A. Vembris, A. Tokmakovs, A. Jurgis In co-operation with Institute of Applied Chemistry, Riga Technical University Institute of Physical Energetic

There is an enduring interest to use organic molecular systems as an active material in the nonlinear optical (NLO) devices. One of the possibilities to create such material is electrical field poled organic glasses containing noncentrosymmetrically arranged chromophores. High NLO efficiency and stability are essential criteria's for device use. Key issues to achieve these goals are high molecular NLO efficiency of chromophore, as well, as high load of them. Unfortunately, highly effective chromophores have large dipole moments and tend to aggregate in atiparallel configuration, diminishing NLO efficiency. To ensure their spatial separation one could use a host capable to bind chromophore at specific sites by supramolecular forces. In this case host themselves is not NLO active and acts just as matrix maintaining separation of chromophores. Further increase in efficiency can be achieved within new class of organic NLO materials binary chromophore organic glasses (BCOG), where both host and guest contains NLO active molecules. Challenge, what one has to overcome, is molecular assembly of both chromophores in such spatial way that their nonlinearity is additive and not subtractive. In our presentation we would like demonstrate such supramolecular assembly of chromophores. Up to 50% enhancement of NLO efficiency was obtained in our novel BCOG build from dimethylaminobenzylidene 1, 3 - indandione containing hosts and zwitterionic indandione-1,3 pyridinium betaine as a guest.



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

#### POLYMERS FILMS WITH INDANDIONE DERIVATIVES AS ALTERNATIVES TO AZOBENZENE POLYMERS FOR OPTICAL PATTERNING

B.Stiller, M.Saphiannikova, K.Morawetz, J.Ilnytskyi, D.Neher, I.Muzikante, P.Pastors, V.Kampars In co-operation with University of Potsdam, Institute of Physics, Potsdam, Germany Leibniz Institute of Polymer Research, Dresden, Germany Institute for Condensed Matter Physics, Lviv, Ukraine Institute of Applied Chemistry, Riga Technical University

Surface relief gratings (SRGs) on organic thin films are studied extensively for both scientific interest and in relevance to the applications. Among the chromophores being used the azobenzenes showed the best performance, but the use of alternative photosensitive groups provides better general understanding of the phenomena. A thermodynamic theory and molecular dynamics simulations of photoinduced effects are discussed. In this study we use indandione derivatives, known as promising materials for photonics applications, as an alternative to the azobenzenes. We consider their photoreactions when incorporated into a polymer film. We have demonstrated that the optically induced mass transport is not limited to azobenzene containing materials. Also indandione (DMABI and it derivatives) containing guest-host polymer films show mass transport effects and can be used to generate gratings optically. SNOM experiments and the spectral diffraction dependence of gratings made from indandione containing guesthost polymer films show that the topography grating is superimposed by a refractive index grating. Spectral diffraction dependence and optically ordering of indandiones opens up new possibilities for applications in data storage and safety devices. Surface relief gratings can be generated using low power lasers to exclude thermal modification of the samples. Indandione (DMABI) moieties were aligned by polarised light and the molecular order were detected by UV VIS spectroscopy using polarised light. As theoretically predicted by thermodynamic theory of light induced material transport and by the molecular dynamics study, the optical induced mass transport is based on the change in photo orientation of chromophores in thin organic films.



This work was supported by the Deutsche Forschungsgemeinschaft (DFG), the Ministry of Culture and Science (BMBF) of Germany and by National Research Program of Latvia in Materials Science.

#### ANALYSIS OF PHOTOELECTRICAL PROPERTIES OF POLYMER FILMS CONSISTING OF INDANDIONE DERIVATIVES BY KELVIN PROBE

#### J.Sīpols, V.Kampars, P.Pastors, I.Muzikante, E.Fonavs In co-operation with Institute of Applied Chemistry, Riga Technical University

The optically induced switching of electrical properties is important for investigation of opto-electronic effects in polymer systems. One of the possibilities to have polymer films with definite properties is incorporation of photosensitive organic molecules in host-guest systems.

In this work novel indandione type organic molecules, which consist of acceptor and donor groups bridged by delocalized  $\pi$ -electron system, are investigated. Both calculation and experimental data show a reversible highly dipolar photoinduced intramolecular electron transfer (PIET) of DMABI molecule. When molecule is irradiated at PIET spectral region a large change of dipole moment from ground state to excited state takes place. These large changes allow to investigate photoelectrical properties of molecule. Especially it is possible to detect changes of surface potential of host-guest thin films consisting of DMABI molecules or it derivatives by Kelvin probe method. In this work influence of concentration of molecules on changes of photoinduced surface potential (amplitude and response time to irradiation) between 1 and 25 wt% will be discussed.



#### ELECTRO-PHYSICAL PROPERTIES OF VACUUM DEPOSITED THIN ORGANIC FILMS OF DMABI AND IT DERIVATIVES WITH HETEROJUNCTION

#### J.Latvels, K.Pudzs, I.Muzikate, E.Fonavs, P.Pastors, V.Kampars In co-operation with Institute of Applied Chemistry, Riga Technical University

Nowadays, thin films of organic materials having semiconducting properties are being extensively studied due to the very promising applications in organic electronics. For the realization of logic circuits both p- and n-channel materials are necessary. Consequently investigations of electrical properties of organic devices with heterojunction are of great importance. The rectification effect of metal-organic semiconductor (Me/OS) junction attributed to Schottky barrier formation in the interface and is described by many authors.

The rectification effect due to heterojunction between two organic semiconductors may be realized due to the occurrence of an energy barrier between both molecular materials with shifted HOMO and LUMO energy levels going from one material to another one. In our work double layer structure of DMABI and it derivatives are investigated. According to quantum chemical calculations two compounds with more shifted HOMO and LUMO levels were chosen. Experimental data concern to studies of the DC currentvoltage (I-U) characteristics and activation energies Ea(U) of a molecular material based heterojunction. The experiments with monolayer of DMABI or it derivatives sandwichtype samples show symmetrical I-U characteristics, whereas double layer samples show asymmetrical character. The rectifying I-U behavior of Schottky barrier devices is usually assumed to follow the standard thermionic emission theory for conduction across the junction metal/organic layer. In applying this theory to the present system, the current is assumed to be controlled by the transfer of carriers across the interface of the metal/organic layer, and the interface between two DMABI derivatives. In the bilaver sample, we are introducing a new electrical feature - a self-bias (known as built-in potential) motivated by the contact between two DMABI derivatives, which accumulates in each respective side holes and electrons. This entails the formation of a space-charge layer between the semiconducting materials.



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- 2. M.Rutkis, A.Jurgis, V.Kampars, A.Vembris, A.Tokmakovs, V.Kokars, Optimizing the second order NLO performance of the host guest polymer systems by tailoring the chromophore structure, *Molecular Crystals and Liquid Crystals*, Vol. 485, pp.903–914, 2008
- 3. I.Aulika, J.Pokorny, V.Zauls, K.Kundzins, M.Rutkis, J.Petzelt, Structural and optical characterization of Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub> PLD deposited films, *Optical Materials*, Vol.30, pp 1017–1022, 2008.
- 4. S.Jursenas, N.Kurilcik, R.Karpicz, V.Gulbinas, L.Valkunas, M.Rutkis, I.Muzikante, Impact of aggregates on excitation dynamics in transparent polymer films doped by dipolar molecules, *Thin Solid Films*, Vol. 516, Iss.24, pp. 8909-8916, 2008
- B.Stiller, M.Saphiannikova, K.Morawetz, J.Ilnytskyi, D.Neher, I.Muzikante, P.Pastors, V.Kampars, Optical patterning of azobenzene and indandione containing films, *Thin Solid Films*, Vol. 516, Iss.24, pp. 8893-8898, 2008
- A.Vembris, M.Rutkis, V.Zauls, E.Laizane, Stability of the Functional NLO Polymers - Optical Induced De- poling of the DMABI Molecules in sPMMA Matrix, *Thin Solid Films* Vol. 516, Iss.24, pp. 8937-8943, 2008
- 7. A.Vembris, M.Rutkis, E. Laizane, Influence of corona poling procedures on linear and non-linear optical properties of polymer materials containing indandione derivatives as a cromophores, *SPIE Proceedings, Organic optoelectronics and photonics III*, Eds. P.L.Heremans, M.Muccini, A.Meulenkamp, Vol, 6999, 699924, 2008.
- 8. O.Vilītis, P.Šipkovs, D.Merkulovs, Refrakcijas indeksa noteikšana šķidrumiem cilindriskā kivetē, *Latvian J.Physics Techn. Sciences*, Vol.45, No.3, pp.50-62, 2008

#### **Conference presentations**

# International Symposium Towards Organic Photovoltaics, Linz, Austria, February 5-9, 2008

 I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, M.Plotniece, M.Roze, J.Kalnachs, A.Murashov, P.Shipkovs, V.Parra, G.Rozite, Photosensitivity of bi-layer GaOHPC: C<sub>61</sub>(CO<sub>2</sub>Et)<sub>2</sub> and P3HT:PCBM bulk heterojunction cell, Book of Abstracts, p.118

# International Conference, Course, Exhibition Photonics Europe (Organic Optoelectronics and Photonics II), Strasbourg, France, 7-10 April, 2008

1. A.Vembris, M.A.Rutkis, E.Laizane, Influence of corona poling procedures on linear and non-linear optical properties of polymer materials containing indandione derivativatives as a cromophores, CD

#### International Baltic Sea Region Conference on Functional materials and Nanotechnologies FM&NT 2008, April 1-4, 2008, Riga, Latvia

- 1. M.Rutkis, A. Jurgis, A.Vembris, Roadmap for the NLO polymer material design. Enhancement of the polar order stability: one more reason to change the best chromophore paradigm, Book of Abstracts, p. 70
- A.Ozols, D.Saharov, V.Kokars, V.Kampars, G.Mezhinskis, A.Maleckis, A.Pludons, M.Rutkis, Spectroscopic studies of the red light surface relief grating recording in stilbene azobenzene derivatives, Book of Abstracts, p. 71
- I.Muzikante, J.Latvels, E.Fonavs, M.Bouvet, Electrical properties of double layer organic thin films based on heterojunction – for design of molecular diode, Book of Abstracts, p. 72
- I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, J.Kalnachs, A.Murashov, M.Plotniece, M.Roze, P.Shipkovs, G.Rozite, V.Kampars, V.Parra, Wide spectral range photosensitive bi-layer organic bulk heterojunction system, Book of Abstracts, p. 133
- A.Tokmakovs, M.Rutkis, V.Kokars, V.Kampars, Design and characterization of the novel indandione derivatives based binary chromophore organic glass material for NLO applications, Book of Abstracts, p. 135
- 6. E.Jecs, M.Rutkis, J.Kreicberga, A.Jurgis, V.Kampars, NLO properties of polymer systems containing 4'-{N,N-bis[2-ethanol]amino}-4-nitroazobenzene derivatives as a chromophores, Book of Abstracts, p. 136
- 7. I.Bidermane, E.Laizane, E.Fonavs, I.Muzikante, D.Gustina, E.Markava, Reversible photo surface potential of azobenzene containing polymer films role of photoisomerization and molecular structure, Book of Abstracts, p. 137
- A.Vembris, M.Rutkis, E.Laizane, Recording of information in doped polymer system by modifying second harmonic generation efficiency, Book of Abstracts, p. 138
- 9. J.Sipols, I.Muzikante, E.Fonavs, V.Kampars, P.Pastors, Photoelectrical properties of polymer films consisting of indandione derivatives, Book of Abstracts, p. 140

#### The European Materials Research Society 2008 Spring Meeting, Symposium Q: Functional supramolecular architectures for organic electronics and nanotechnology, May 26 - 30, 2008, Strasbourg, France

 M.Rutkis, V.Kampars, V.Kokars, A.Vembris, A.Tokmakovs, A.Jurgis, Supramolecular assembly of indandione based binary chromophore organic glasses for NLO applications, <u>www.emrs-strasbourg.com/index</u>, E-MRS 2008 Spring Meeting, Book of Abstracts

# The 6<sup>th</sup> International Conference Advanced Optical Materials and Devices AOMD 6, August 24-27, 2008, Riga, Latvia

- 1. M.Rutkis, A.Jurgis, A.Vembris, Second order NLO polymer material design lessons learned from computer modelling of the external field poling and polar order relaxation dynamics, Abstracts, p. 28
- 2. I.Muzikante, E.Fonavs, J.Sipols, I.Bidermane, Photo surface potential of host-guest systems containing polar molecules, Abstracts, p. 27
- I.Kaulachs, I.Muzikante, L.Gerca, G.Shlihta, J.Kalnachs, A.Murashov, M.Plotniece, P.Shipkovs, G.Rozite, V.Parra, PV effect of wide spectral range bi-layer organic bulk heterojunction system containing hydroxygallium phthalocyanine, Abstracts, p. 12
- 4. E.Laizane, D.Gustina, E.Markava, I.Muzikante, Synthesis and optical properties of some azobenzene alcoxy carboxylic derivatives, Abstracts, p. 78
- 5. E.Laizane, I.Muzikante, J.Teteris, K.Kundzins, D.Gustina, Optically induced surface relief grating of azobenzene containing polymer films, Abstracts, p. 79
- 6. A.Vembris, M.Rutkis, E.Laizane, Impact of different corona poling procedures on non-linear optical properties of doped polymer materials, Abstracts, p. 77

# 10<sup>th</sup> School-Conference Advanced Materials and Technologies, August 27-31, 2008, Palanga, Lithuania

- 1. I.Muzikante, Photoelectrical properties of organic monolayers, multilayer and mixed systems. Charge carrier photogeneration and transport processes, Book of abstract, p. 14 and CD
- 2. M.Rutkis, Second order NLO polymer materials: design strategy, characterization, applications and achievements, Book of abstract, p. 15 and CD
- 3. A.Vembris, M.Rutkis, E.Laizane, Investigation of nonlinear optical efficiency of the polymer materials doped with indandion derivatives, Book of abstract, pp. 144
- 4. E.Laizane, I.Muzikante, J.Teteris, K.Kundzins, D.Gustina, Optical pattering of azobenzene containing polymer films, Book of abstract, p. 145

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

#### **Scientifical Staff**

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

#### **Technical Staff**

- 1. I.Guza
- 2. L.Gvardina
- 3. J.Melderis
- 4. J.Veinbergs
- 5. A.Grablevskis

### 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. *Apollo AS* Ltd
- 9. AlarmLat Ltd
- 10. .Mikoniks Ltd

11. Energoremonts *Rīga* Ltd

Denmark DanBalt Electronics

#### Russia

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

2. Competence Centre ELIKO

The prospects of the instruments look at appendix 1

Estonia 1. Tallinn

University of

Technology

#### **Our Clients**

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

etc.

#### **Lectures on Conferences**

# 24<sup>th</sup> Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2008

- 1. P.Annus, M.Min, A.Kristiņš. *Simple waveforms for signal processing* Abstracts, p.71
- 2. I.Gvardina, J.Kleperis, A.Kristiņš. *Monitoring of the environment temperature and relative humidity using the DS1923*. Abstracts, p.74
- 3. S.Zeļenkovs, A.Kristiņš, J.Melderis. *Designing of the AVR 8-bit microcontroller based air compressor station control unit.* Abstracts, p.59
- 4. D.Gusevs, J.Veinbergs, I.Gvardina, J.Melderis *The soft start devices with three-phase management on the PIC 18F4431 controller base*. Abstracts, p.60.
- 5. A.Grabļevskis, E.Garkājs *Frequency converter on the dsPIC30F4011 microcontroller base.* Abstracts, p.75.
- 6. A.Grabļevskis, E.Garkājs, A.Kristiņš. *The Analog Devices and Microchip DSPmicrocontroller functionality comparative analysis for the engine built-in control systems*.Abstracts, p.61.
- 7. D.Gusevs, V. Kutevs. Usage of fleet managment systems on example of NaviFleet system. Abstracts, p.76.

#### The outlook "High Tech in Latvia 2008" LTP and RTU

- 1. A.Kristiņš. Monitoring of the environment temperature and relative humidity, p.33.
- 2. A.Kristiņš. Soft start devices with three-phase control, p.49.



## Monitoring of the environment temperature and relative humidity

The climate monitoring system has been developed for grain warehousing and drying. It performs a temperature registration in a range from -20°C up to +85°C with the step of 0.5°C and a registration of relative humidity in a range 0 % up to 100 % with the step of 0.64%. This system was designed on the base of five the DS1923 Hydrochron Temperature/Humidity Logger iButtons. Such logger has no any own means of indication and control. Therefore all functions on its service and information exchange with it are carried out at contact between its case and supporting device using 1-Wire protocol. This system allows as tracing the current situation on a computer in a real time, as collecting the saved up data a posteriori. It provides controlling of the logger's parameters, storing and graphic representation of the data fixed by the loggers.





Scope of applying of such system is, first of all, monitoring sensitive to temperature and/or the humidity foods, pharmaceutical and medical reasons and propagations at a at their transportation storage

medical reagents and preparations, etc. at their transportation, storage and processing.

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#### **Our address**



### 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.

Our address:



### **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<sup>TM</sup> 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:	$\leq 40 \text{ mA}$	
System in alarming mode (defined by alarming device):	<4 A	
Access time:	20 seconds	
Detectors with disconnecting ability:	$\leq$ 4 pcs.	
Detectors without disconnecting ability:	$\leq$ 3 pcs.	
Possible combinations of keys:	$2,8 \cdot 10^{14}$	
Maximal number of user keys:	56 (250) pcs.	
Dimensions:	115x55x30 mm	

Our address:



## 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<sup>TM</sup> 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):	$\leq 8 \text{ mA}$
Armed only engine deactivation:	$\leq$ 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	6000

Automatic switching on of the immobilizing mode after ignition switching off - in 20 secs.

Our address:



### 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"

Our address:



### **Electronic Documentation**

There is a portable system based on Dallas Semiconductor firm Touch Memory<sup>TM</sup> chips for data saving and moving without paper. The silicon chip packs in TM memory more as 8000 signs ( $\sim 4-5$  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 ( $\emptyset$  17,4 x 5,89 mm) and is tolerant to mechanical shock, static electricity, and electromagnetic fields and to other harmful environmental factors.

TM has an ambient temperature range -40°C to +85°C.

Touch Memories can accommodate over one million data changes.

Our address:



## **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.

Our address:



### 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<sup>TM</sup> 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**

+(10 - 15) V
$\leq 8 \text{ mA}$
< 0,5A (typically)
5 seconds
Immediately
5 seconds
$2,8 \cdot 10^{14}$
$\leq$ 56 pcs.
83x55x35 mm

Our address:



## 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<sup>TM</sup> 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 • 10 <sup>14</sup>
Number of user keys (standard):	56 pcs.
Number of events registered:	500
Time of data retention in Master-key:	over 10 years

Our address:



### 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 ( $210 \times 297 \text{ mm}$ ) 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  $(0 \div 0.15 \text{ s})$ .

The device can be used for testing of 10 types of breakers: BBIII-110; BB5-110; BBY-110; BBH-110/6; BB-3305; 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".

Our address:



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

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

In the developed remote control systems "Rabbit" controllers are used.

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

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

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

Practical applications:

1. The system of access, control and management is worked out for LatRosTrans company. The system consists of 24 controllers (number of technological blocks on Russia-Ventspils oil pipeline), dispatcher program (in Daugavpils) and some client applications.

2. Entrance in/out system for "Latvijas Gāze" company is worked out, which consists of three in/out gates with automatic barriers, server administrator and guard programs and some other client applications.

3. The system including checkpoint, the authorized access in cabinets and the security signal system for two buildings of the Latvian Shipping Company with a unified database.

Our address:



### 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<sup>TM</sup> 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.

Our address:



### **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  $\emptyset$ 17.35 x 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.

Our address:



## 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.



Our address:



## **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.



Our address:

## Appendix 2

Instrument title	Dektak 150 Surface Profile Measuring System		
Photo			
Technical details	Measurement Technique Measurement Capability	Stylus profilometry Two-dimensional surface profile measurements	
	Sample Viewing	640 x 480-pixel (1/3informat) camera, USB;	
	manual zoom	variable 0.67 to 4.29mm	
	(644X to 100X with 17in.	monitor)	
	Stylus Sensor	Low-Inertia Sensor (LIS 3)	
	Stylus Force	0.03 to 15mg (N-Lite sensor)	
	Stylus options Stylus radius	12.5um	
		2.5µm	
	Sample Stage	Manual X/Y/O, 100 x 100mm X-Y translation,	
		anual levelling	
		optional X-Y auto stage, 150mm (6in.) travel,	
		1µm repeatability, 0.5µm resolution	
	Computer System	PC with Pentium® D Dual Core processor	
	Software	Dektak software running under Windows XP,	
		Step Detection software (std.)	
		Stress Measurement software	
	Performance		
	Scan Length Range	55mm (2.16in.)	
	Data Points Per Scan	60,000 maximum	
	Max. Wafer Size	150mm (6in.)	
	Step Height Repeatability	6Å, 1 sigma on 0.1µm step	
	Vertical Range	1mm (0.039in.) 1Å may (at 6.55µm range)	
A 11 /1 .	Transparent films/photoresis	t thickness, thin- and thick-film measurements.	
Application example	roughness studies, surface q	uality and defect review and etc.	
Responsible	Mārtiņš Rutkis,	L.	
(name, second name, e-	E-mail: martins.rutkis@cfi.lu.	IV,	
nall, phone, room number)	Room number 226.		

Instrument title	NANO Indenter G200 for nanomechanical testing:		
	depth sensing measurement of nano- and		
	microhardness, Young modulus, scratch tests		
Photo	Nano Indenter* G200		
	Coil/magnet assembly		
	Leaf spring Capacitance gauge Indenter Sample		
Technical details Maximum load 500 mN			
	Load resolution 50 nN		
	Displacement resolution <0.01nm		
	<ul> <li>Usable sample area 40x40 mm</li> </ul>		
	Motorized sample manipulation table, positioning $\pm 1 \mu m$		
	<ul> <li>Pre-mounted diamond indentation tip (Berkovich)</li> <li>Ontical imaging system</li> </ul>		
	video screen, objectives 10x&40x		
	Operating and data analysis software		
Application example	<ul> <li>Measurements of nanohardness,</li> <li>Measurements of Young modulus</li> </ul>		
	<ul> <li>Measurements of Young modulus,</li> <li>Scratch tests</li> </ul>		
	of surfaces, thin and ultra thin films		
Responsible: (name, second name, e- mail, phone, room number)	Jānis Maniks, E-mail: <i>manik@latent.lv,</i> Phone (371) 6 7261132, Room number 319.		

Instrument title	X-ray Diffractometer X'Pert Pro MPD
Photo Technical details	High resolution vertical gonigmenter equipped with long fine focus ceramic tube.
	type PW3373/00, Cu anode, wavelength 0.154 nm, max. 2.2 kW, 60 kV.
	Detector: PIXcel, wide dynamic range solid-state detector.
	Non-ambient chamber TTK-450+LNC, temperature range from -190 to +450'C.
	Open Eulerian stage for texture and stress analysis, can be mounted samples with maximum diameter of 100 mm and maximum height of 25 mm
	(Psi -595deg, Phi 0360deg, accuracy 0.1 deg)
	Software: X'Pert Data collector, Reflectivity, Texture etc.
Application example	high resolution powder diffraction, phase identification and quantitative phase analysis.
	analysis of thin films and coatings,
	crystallite size and strain determination, kinetic and non-ambient experiments.
Responsible	Anatolijs Mišņovs,
(name, second name, e- mail, phone, room	E-mail: amish@lanet.lv, Phone (371) 6 7260896
number)	Room number 411, 433,
	Kārlis Kundziņš,
	E-mail: <i>kkarils@gmail.com,</i> Phone (371) 6 7187875
	Room number 405.
Instrument title	Vacuum deposition system of metal and organic
------------------------	--
	material thin films EDWARDS AUTO 306
Photo	
Technical details	<ul> <li>Vacuum chamber: A stainless steel front-loading high vacuum chamber, 400mm diameter by 500mm high with viewport in chamber door.</li> <li>2 evaporation sources: Single resistance evaporation source with clamps capable of holding filament or boat evaporation sources.</li> <li>2 sources for evaporation of organic materials: Provides precisely-controlled thermal evaporation of organic molecular material Easily changeable crucible with 2cc capacity Working temperature range of 50 to 600C Direct-contact thermocouple for precise temperature measurement Temperature control accuracy ±0.1C.</li> <li>Sample work-holder: Static Fluid cooled and heated workholder with 100 mm usable diameter, -20 °C to + 90°C operation range. External desktop closed-loop heater-cooler (-20 to +90 °C), with fluid reservoir and electronic temperature control.</li> <li>Film thickness measuring system: Quartz crystal thin film deposition system with digital display of deposition rate and deposition thickness (10nm - 3µm), information storage for 11 sputtering materials. Facility to control up to 2 source shutters automatically and close shutters when pre-programmed termination thickness values are achieved.</li> </ul>
Application example	System is provided for preparing thin films of organic material with metal
-	electrodes for investigation of electrical and photoelectrical properties for molecular electronics and photonics
Responsible	Inta Muzikante
(name, second name, e-	F-mail: inta.muzikante@cfi.lu.lv.
mail, phone, room	Phone (371) 6 7260787.
number)	Room number 309.

Instrument title:	Nanostructure Imprint System for Fabrication of Surface relief Nanostructures		
Photo:			
Technical details:	Low-noise, single	Power (W)	>8
	laser Verdi V-8	Wavelength (nm)	532
		Linewidth (MHz)	<5
		Beam Diameter (mm)	2.25 ±10%
		Beam Divergence (mrad) Pointing Stability (urad/°C)	<0.5 2
		Power Stability (%)	±1
		Noise (% rms)	<0.03
		Polarization	vertical, >100:1
	Motorized XYZ Translation Stage	X and Y travel range	50 mm (2x ATS50-50)
	A 1 550+Ensemble	Z travel range	25 mm (ATS50-25)
		Travel resolution	< 0.5 μm
		Computer control	Motion controller included (3x Ensemble MP + software)
		Input power	50 Hz, 220-230 VAC
Application example:	Recording and nvestigation of materials.	on of holographic grating's p	roperties for different classes
Responsible: (name, second name, e- mail, room number)	Jānis Teteris, E-mail: <i>teteris</i> @ <i>latnet.lv</i> , Room number 308.		

Instrument title:	Picosecono	d Fluorescence Spectrometer
Photo:		
Technical details:	Excitation Source	Picosecond solid state laser including second and third harmonic generator and OPG
	Spectral region Scanning accuracy Pulse duration Repetition rate Output pulse energy Linewidth Detection System Temporal resolution Spectral resolution Spectral region Sample Chamber Temperature region Vacuum Shroud Vacuum System for the Sample Chamber Ultimate total pressure Computer System	210-2300 nm 0.1 nm ~15 ps 10 Hz ≥ 0.3 mJ for spectral region 450 nm – 1000 nm; ≥ 1 mJ for spectral region 250 nm – 500 nm; ≥0.05 mJ for spectral region 220 nm – 410 nm ≥0.15 mJ for spectral region 250 nm – 300 nm < 6 cm <sup>-1</sup> Spectrograph and streak camera 15 ps 0.1 nm 200 nm – 850 nm Closed cycle He cryostat 4 K – 350 K 5 ports for optical experiments Oil-free pumping system based on turbomolecular pump <5 x 10 <sup>-7</sup> mbar PC with 4 Pentium (dual core) RAM 1GB, HD 80 GB, 22 in. flat panel display LabView driver, HPD-Ta Image acquisition and processing software
Application example:	Time-resolved spectral mea	surements: spectral region 250 nm – 950 nm,
Pasnonsible	temperature region 4 K – 35	0 К.
(name, second name, e- mail, phone, room number)	E-mail: (anatoly@cfi.lu.lv), Phone (371) 6 7187471, Room number 512.	

Instrument title	Microwave High Temperature Furnace MKH-4,8	
Photo	$\sim$	
Technical details	Heating Chamber 135 x 135 x135 mm <sup>o</sup> , useful volume $\sim 2 \text{ Litres}$ . The chamber is gas and vacuum tight	
	<b>Microwave supply:</b> 6 independent magnetrons, 800 W each: total MW power 4.8	
	kW, adjustable from 15 - 100 %	
	power density up to104 W/Litre frequency 2450 MHz +/- 50 MHz.	
	to 1750°C (short terms operation). Temperature measuring by pyrometer, range	
	Heating of non-conductive material is possible due to use SiC susceptors.	
	Protective gases supply. Heating in protective gas is possible. Two gas	
	connections with shut-off valves and needle closing valves are installed. The flow	
	meter with needle valve for the protective gas is in the gases supply lines. In the	
	<b>Process Guiding Software.</b> Software ECS-2000 and controller SE 402 are used.	
Application sample	Furnace is applicable for sintering of ceramics, superconductor	
	processing, sample annealing as well as driving out organic materials and pre-	
Responsible	Larisa Grigorjeva,	
(name, second name, e-	E-mail: lgrig@latnet.lv,	
mail, phone, room number)	Phone: (371) 6 7260880,	
	Room number 413.	

Instrument tittle	PCT Pro-2000 hydrogen sorption - desorption
	equipment with RGAPro-100 masspectrometer
Photo	
Technical details:	<ul> <li>Possibility to measure:</li> <li>PCT Isotherms</li> <li>Sorption Kinetics</li> <li>Absorption/Desorption Cycling PCT and Kinetics</li> <li>Temperature Programmed Desorption</li> <li>Masspectrometer attachment for the detection of desorbed gases, (100 AU and up to 200 bar direct input pressure)</li> <li>Next specific features: <ol> <li>Sample size: 4-6 ml, 5 calibrated dosing volumes desirable rated for full pressure range 0.001 to 200 bar)</li> <li>Integrated automatic PID control of working gas.</li> <li>Heated Gas Manifold (+29 °C).</li> <li>Automatic Pressure Range Switching (high (200 bar limit) and low (5 bar limit) pressure transducers).</li> </ol> </li> </ul>
Application example:	5) Software Control (including Kinetics, PCT, Cycling Kinetics and Cycling PCT). Classical material for hydrogen storage is LaNi <sub>5</sub> ; with PCTPro-2000 it is easy to measure PCT (pressure – composition – temperature) isotherms for hydrogen
	absorption – typically in range of 2-6 bars at temperatures +30 - +60 °C.
Responsible (name, second name, e- mail, phone, room number)	Janis Kleperis, E-mail: <i>kleperis</i> @ <i>latnet.lv</i> , Phone: (371) 6 7262145, Room: 214

Instrument title	X-ray fluorescence (XRF) spectrometer for elemental
	analysis with micro-focused X-ray excitation and
	energy-dispersive detector.
Photo	
Technical details	Sample excitation by X-rays (Rh tube) focused by polycapillary fiber lens, minimum spot size 50 microns (fwhm). Energy-dispersive liquid N2-cooled Si detector with Be window, suitable for detecting of XRF of chemical elements ranging from Na to U.Large sample chamber with computer-controlled translation (x-y-z) stage. Analysis can be performed in air or vacuum (in case of light elements). Linear (1-D) and 2-D distributions (maps) of chemical elements in the sample can be measured. Manufacturer: EDAX/Ametek, Model: Eagle III microprobe. Built-in additional options: set of filters in the primary (excitation) X-ray beam, and variable focusing spot size
Application example	General application for express-analysis of elemental composition of different materials. Compared to electron microscope-based XRF microanalyzers, no special sample preparation is required and the analysis can be typically completed within few minutes. The main limitation is the inability to detect elements lighter than sodium (Na). Both basic components and trace impurities can be analyzed. During the initial tests we have successfully detected trace amounts of chlorine in synthetic SiO <sub>2</sub> glass (sensitivity better than 100 ppm).
Responsible (name, second name, e- mail, phone, room number)	Einards Skuja E-mail: <i>skuja@lanet.lv</i> , Phone: (371) 6 7260756, Room: 313.

Instrument title	Vacuum device for UV-radiation
Title	Resonant Frequency doubler for CW single-frequency lasers, model FD-SF-
	07
Photo	
Technical details	Smart Auto-Relock function for CW single-frequency lasers (Ti:Sapphire, Dye, Ar, DPSS etc.)that opens possibilities for laser wavelength conversion in the visible and near IR ranges into the blue and UV domains .Optimized resonator of FD-SF-07 in combination with high-quality mirrors ensures relatively high level of output second-harmonic power. Pumped with 1 W fundamental radiation power the double outputs: more than 250 mW with in the 350-475 nm range (for 700 - 950-nm input),> 200 mW within the 275 – 350 nm range(for 550 – 700 -nm input), and >150 mW with in the 244 – 275 nm range.
Title	Turbo-molecular vacuum pump SST 1001
Photo	
Technical details	Final pressure - 1x10 <sup>-10</sup> mbar
	Velocity of rotation - 38000 1/min
Application example	Recording and investigation of holographic grating's properties for UV
Responsible	Jānis Teteris,
mail, phone, room	E-mail. <i>Telens elamet.iv</i> ,
number)	

Instrument tittle	HR4000 User-configured Spectrometer
Photo	
Technical details:	Dimensions: 148.6 mm x 104.8 mm x 45.1 mm Weight: 570 grams Detector: Toshiba TCD1304AP linear CCD array Detector range: 200-1100 nm Pixels: 3648 pixels Pixel size: 8 μm x 200 μm Pixel well depth: ~100,000 electrons Sensitivity: 130 photons/count at 400 nm; 60 photons/count at 600 nm Computer interface: USB 2.0 Next parts: Light source: DH-2000 Deuterium Light Source Difraction grating: 300 and 600 lines/mm Software: SpectraSuite
Application example:	Thin film materials for proton conducting membranes – light scattering and light absorption edge determination; concentrations of metal (Fe, Ni) ions in electrolyte
<b>—</b>	solution – obtained from visible light absorption spectra
Responsible:	Janis Kleperis E-mail: <i>kleperis@latnet.lv</i> Phone: (371) 6 7262145 Room number 212

Instrument tittle	Fume Cupboard with angled front
Photo	
Technical details:	Dimensions: 1500x630x2050/2550 Weight: 570 grams Construction: stainless steel, The sink (300x150 mm) from stainless steel; Electricity (220V, 2200 W), lighting Gas ubing (inlet for pressured air/Nitrogen Upper body: 13 mm acide proof and heavy burning SGL plastic
	Producer: SIA "BIO NAMS" Slāvu Street 2a, Daugavpils, LV-5404, Latvia E-mail: bionams@inbox.lv; Web: www.bionams.lv
Application example:	Preparation of Thin film materials for proton conducting membranes, preparation of metal hydride materials in an environment washed with nitrogen
Responsible:	Janis Kleperis E-mail: <i>kleperis</i> @ <i>latnet.lv</i> Phone: (371) 6 7262145 Room number 214