

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



# **ANNUAL REPORT**

**2006**

Riga 2007

**Annual Report 2006, Institute of Solid State Physics, University of Latvia.**

Editor: A.Krumins. Composed matter: A.Muratova. Set up at the Institute of Solid State Physics, University of Latvia, *Kengaraga Str.8, Riga LV – 1063, Latvia.*

*Riga, Institute of Solid State Physics, University of Latvia, 2007, p. 143*

Director: **Dr. hab. A.Sternberg**  
**Institute of Solid State Physics, University of Latvia**  
*8 Kengaraga Str., LV-1063 Riga*  
*Latvia*  
**Tel.:** +371 7187816  
**Fax:** +371 7132778  
*<http://www.cfi.lu.lv>*

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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 largest physics research institute in Latvia.

Four laboratories from the Institute of Physics of the Latvian Academy of Sciences, working in the field of solid state physics 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 Latvian 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**. Three research staff members of the Institute have been elected as professors of the University of Latvia. Post graduate and graduate curricula are 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 was established at ISSP.

Research and training in optometry and vision science is taking place in the Laboratory of Optical Materials 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 student and staff.

### **The research of the ISSP includes:**

- studies of electronic and ionic processes in wide-gap materials with different degree 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 **Council** of 21 members elected by the employees of the Institute (Table 2). Presently Dr. phys. L.Trinklere is the elected chairman of the ISSP Council. The Council appoints director and its deputy.

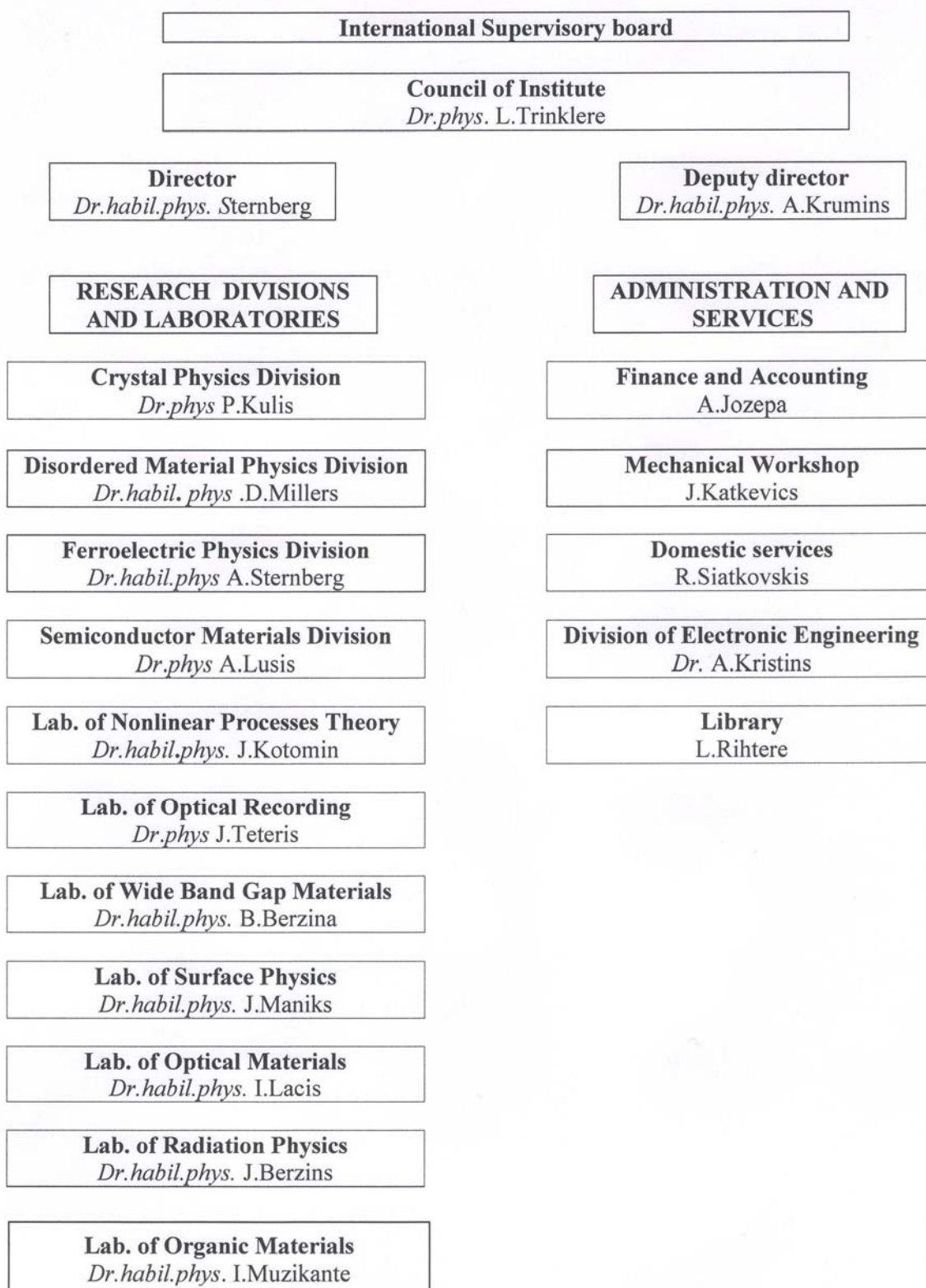
**The International Supervisory** board of ISSP was established in 1999 and it consists of 7 members (Table 3).

The Scientific Board of the ISSP is eligible to award **PhD degrees** in physics in the specialities mentioned above and in medical physics.

The interdisciplinary nature of research at the ISSP is reflected by its **highly qualified staff**. At present there are 180 employees working at the Institute, 28 of 87 members of the research staff hold Dr.habil.degrees, 45 hold Dr. or PhD. At the end of 2006 there were 15 PhD students and 46 undergraduate and graduate students in physics and optometry programmes working at the ISSP. Educational activities of the Institute were continued and extended in 2006.

*Table 1*

**ORGANISATION STRUCTURE OF THE ISSP IN 2006**



*Table 2*

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

1. Laima Trinklere, Dr.phys., chairman of the Council
2. Liga Grinberga, PhD. student
3. Janis Kleperis, Dr.phys.
4. Eriks Klotins, Dr.phys.
5. Andris Krumins, Prof., Dr.habil.phys.
6. Peteris Kulis, Dr.phys.
7. Jurijs Kuzmins, Prof., Dr.phys.
8. Janis Maniks, Dr.habil.phys.
9. Donats Millers, Dr.habil.phys.
10. Inta Muzikante, Dr.habil.phys.
11. Daina Riekstina, Dr.phys.
12. Uldis Rogulis, Dr.habil.phys.
13. Janis Ruhmanis
14. Andrejs Silins, Prof., Dr.habil.phys.
15. Linards Skuja, Dr.habil.phys.
16. Maris Springis, Dr.habil.phys.
17. Andris Sternbergs, Dr.habil.phys.
18. Ivars Tale, Prof., Dr.habil.phys.
19. Janis Teteris, Dr.phys.
20. Anatolijs Truhins, Dr.habil.phys.
21. Vismants Zauls, Dr.phys.

*Table 3*

### **International Advisory Board of the Institute**

1. Prof. Dr. Gunnar Borstel, University of Osnabruck, Germany
2. Prof. Niels E.Christensen (chairman), University of Aarhus, Denmark
3. Prof. Claes – Goran Granqvist, Uppsala University, Sweden
4. Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia
5. Prof. Sergei Tuituinnikov, Joint Institute for Nuclear Research, Dubna, Russia
6. Prof. Juris Upatnieks, Applied Optics, USA
7. Prof. Harald W.Weber, Atomic Institute of Austrian Universities, Vienna, Austria

The annual report summarizes research activities of the ISSP in 2006. The staff of the Institute has succeeded in 31 **national science grants** and in the **two national cooperation projects** (Functional Materials and Technologies for Microelectronics and Photonics and Nanomaterials and Nanotechnologies), with the total financing 245.5 thous. Ls.

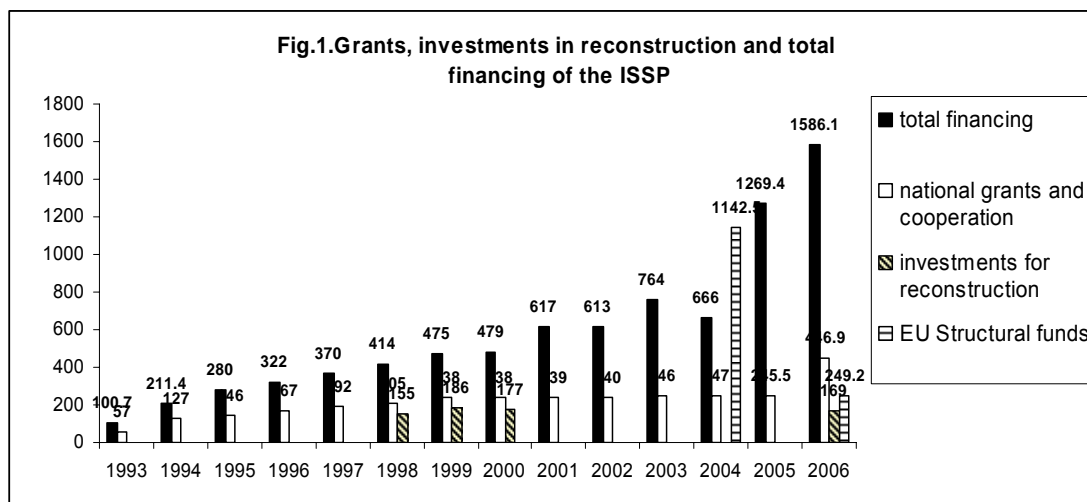
In 2005 the new Law of Science was passed by Parliament of Latvia. According to this law the state budgetary financing in Latvia for science have to increase yearly per 0.15% from GDP up to reaching a 1% value in the future. The budgetary increase was focused on scientific infrastructure financing and launching of National research programmes. One of the scientific priorities in Latvia is materials science. ISSP became coordinating institution for the Programme attracting 228,3 thous. Ls budget in 2006. The infrastructure financing for ISSP for in 2006 was 281,9 thous. Ls. and it was partly used also for the salaries of the scientific and maintenance staff of the institute. (Table 4)

**Table 4**

INCOME OF ISSP, THOUSAND Ls, FROM 1993 - 2006

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Rent of space	Structural funds from EU
1993	100.7	56.8	-	40.8	-	3.1	
1994	211.4	127.8	-	64.2	9.6	9.8	
1995	281	145.7	45	38.2	40	12.1	
1996	322.5	167.1	11.7	62.4	68	13.3	
1997	370	192.1	39	93	26	15.2	
1998	414 + 156	205.2	26	114	42	26.5	
1999	475.6+186	238.1	48.8	156.5	16.5	15.6	
2000	478.8 + 77	238.3	36.9	146.3	43	14.3	
2001	617.3	238.8	64.5	116.5	183	14.5	
2002	612.8	239.9	90.0	133.0	131	18.9	
2003	764.6	245.7	172.3	152.5	179	15.1	
2004	<b>1 809</b>	<b>246.7</b>	<b>123.5</b>	<b>166.5</b>	<b>121.8</b>	<b>8.0</b>	<b>1142,5</b>
2005	<b>1 269,4</b>	<b>245,5</b>	<b>358,8 + 120)*</b>	<b>172,8</b>	<b>387,6</b>	<b>4,7</b>	
2006	<b>1586,1</b>	<b>466,9</b>	<b>403,4 + 169)*</b>	<b>152,4</b>	<b>135,6</b>	<b>9,6</b>	<b>249,2</b>

\*) – investment for building reconstruction



### Main achievements in 2006

1. Institute succeeded in receiving 5 projects from EU Structural funds for applied science with total financing at 2006 249,2 thous. Ls (B.Berzina, I.Tale, J.Zvirgzds, J.Teteris, J.Kleperis)
2. Dr.habil.phys. I.Muzikante was elected a correspondent member of Latvian Academy of Science.
3. Mg.phys. A.Sharakovskis received a 2006 award for young scientists in physics.
4. D.Grjaznov was acquired degree of doctor of physics at Germany.
5. 4 master students started PhD studies in physics at Institute.
6. Under the supervision of our scientists 3 M.Sc. thesis and 8 B.Sc. thesis in physics were defended.
7. Four International conferences and seminars were organised in 2006:
  - Conference of Baltic Sea region “Functional materials and nanotechnologies” 27.-29.03.2006.
  - EFDA Remote Participation Workshop 20.-21.06.2006.
  - 10. European Conference of Organised Films, 21.-24.08.2006.
  - ERA-NET seminar “Modern Trends in Materials Science and Technology”, 11.-12.10.2006.
8. The conferences take place in the reconstructed Conference hall of the Institute, which was finished at 2006.
9. The number of scientific publications by the co-workers of the Institute was 131.
10. About 40 young researchers, mainly students from Physics Department University of Latvia, have been associated with the scientific projects of the Institute.

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 6<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



**Master of Science (M.Sc.) and Bachelors of Science (B.Sc.)  
Thesis prepared at the Institute in 2006**

**M.Sc. thesis**

<b>No</b>	<b>Author</b>	<b>Title</b>	<b>Supervisor</b>
1.	D.Bocharov	Quantum chemical interpretation of x-ray absorption spectra in perovskite type compounds	Dr.phys.A.Kuzmin
2.	L.Brikmane	Photo- and thermostimulated process in complex systems	Dr.habil.phys. M.Springis
3.	A.Slishans	Investigation of oxifluride composites	Dr.habil.phys. U.Rogulis

**B.Sc. thesis**

<b>No</b>	<b>Author</b>	<b>Title</b>	<b>Supervisor</b>
1.	D.Dinsbergs	The Bell's inequalities in the framework of classical and quantum mechanics	Dr.habil.phys. J.Tambergis
2.	A.Ivanovs	Ferroelectric thin film characterization using scanning electron microscope	Mag.phys. R.Krutohovostovs
3.	E.Laizane	Optical induced phenomena in solid state and solution of azobenzene molecules	Dr.habil.phys. I.Muzikante
4.	G.Marcins	Acquisition of thin layers of gallium nitride	Dr.habil.phys. prof.I.Tale
5.	G.Osheniaks	Spectral characteristics of AlN nanopowder	Dr.habil.phys. B.Berzina
6.	E.Tjutjunnika	Spectral characterization of AlN nanotips and nanorods	Dr.habil.phys. B.Berzina
7.	I.Valdabe-Kaleja	Effect of grain boundary sliding on the polycrystalline Zn mechanical properties	Dr.phys. F.Muktepavela
8.	A.Vembris	Optically induced orientation and disorientation of chromophore molecules in host – guest system (PMMA-DMABI)	Dr.phys. M.Rutkis

# CRYSTALS PHYSICS

Head of Division Dr. 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. Investigations on a new class of materials - oxifluoride composites. One of the goals is to obtain fluoride micro- and nanocrystals with controlled size and properties in the oxide glass matrix. First samples of oxifluorides on the basis of lithium borate glasses with lanthanum fluoride component have been obtained; investigations of their properties are in progress. The second goal is development of light emitters, detectors and visualization systems on oxyfluoride nanocomposite basis with enhanced quantum efficiency. In special conditions, oxyfluoride compounds containing lanthanide ion-doped fluoride crystallites may exhibit emission of photons of greater energy than those absorbed during the excitation (“up-conversion” of energy). These properties are essential to achieve the mentioned goal. For this purpose, the oxyfluoride composite glass samples based on  $\text{Li}_2\text{CO}_3$ ,  $\text{B}_2\text{O}_5$ ,  $\text{LaF}_3$ ,  $\text{LiF}$  and  $\text{RbF}$ , activated with Ce, Eu and Er, were synthesized and studied. The microscopy and X-ray diffraction measurements were performed to identify the crystallites liable to occur during the thermal processing of glass compounds and really the  $\text{LiF}$  crystallites were found in most cases. The possibility was checked to create also the crystallites of  $\text{RbF}$  in glass matrix. The “up-conversion” luminescence was observed in lithium and boron containing oxyfluoride glasses activated with Er ions.
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 photonic 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 the multiple ionised metal ions and the charge exchange emission during ionization of evaporated metal ions.

## **Scientific Staff**

1. Dr. P. Kulis
2. Dr. hab. U. Rogulis
3. Dr. hab. M. Springis
4. Prof., Dr. hab. I. Tale
5. Dr. J. Trokss
6. Dr. A. Veispals
7. Mg. J. Jansons

## **Technical Staff**

J. Straumens

## **PhD Students**

1. J. Butikova
2. L. Dmitrichenko
3. E. Elsts
4. A. Fedotovs
5. A. Sharakovsky

## **Students**

1. Dz. Berzins
2. M. Chubarovs
3. U. Grube
4. G. Marcinshs
5. A. Petruhins
6. A. Voitkans

## **Scientific visits abroad**

1. Dr. hab. phys. U. Rogulis, University of Paderborn, Germany (4 months);
2. Dr. hab. phys. I. Tale, University Milano-Bicocca, Milano, Italia (9 days);
3. Dr. hab. phys. I. Tale, Instituto Superior Tecnico (IST), Lisbon Portugal (2 weeks);
4. Dr. hab. phys. I. Tale, University of Rostock, Germany (2 weeks);
5. Mg. A. Sharakovsky, University Milano-Bicocca, Milano, Italia (9 days);
6. Mg. L. Dmitrichenko, University Milano-Bicocca, Milano, Italia (9 days);
7. Mg. A. Fedotovs, University Milano-Bicocca, Milano, Italia (9 days);
8. Mg. A. Fedotovs, , Lviv University, Ukraine (9 days);
9. Mg. J. Butikova, Max Plank Institute of Plasma Physics, Garching, Germany (4 weeks);
10. Mg. A. Sharakovsky, Instituto Superior Tecnico (IST), Lisbon Portugal (5weeks);
11. G. Marcinshs, Aixtron, Achen, Germany (2 week)
12. Mg. L. Dmitrichenko, , Aixtron, Achen, Germany (2 week)

## **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" Aachen, Germany
4. Max Plank Institute of Plasma Physics, Garching, Germany

### Portugal

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

## Main Results

### RADIATION – INDUCED PHOTOLUMINESCENCE OF Fe ACTIVATED LiBaF<sub>3</sub> CRYSTALS

**A. Sharakovsky, M. Springis, P. Kulis**

Activated alkali halides, alkali-earth halides, and alkali-alkali-earth halides including perovskite type fluorides are known as radiation-induced photostimulated and thermostimulated luminescent materials for x-ray storage systems, including dosimeters. In the present paper we report results on the optical spectroscopy of the radiation-induced defects in Fe doped LiBaF<sub>3</sub> crystals. After x-ray irradiation photoluminescence maximum at about 2.25 eV was observed. The intensity of the photoluminescence band increases with the exposure dose. Luminescence polarization and spectra have been measured at different temperatures and it is likely that the several axial centres involving Fe are responsible for the x-ray induced photoluminescence. Concentration of the axial centres related to the PL band at 2.25 eV grows when the x-ray dose is increased.

Parameters important for the potential PL dosimeter based on LiBaF<sub>3</sub>:Fe are considered.

In order to consider the possibility of using LiBaF<sub>3</sub>:Fe crystals in radiation dosimetry the concentration of Fe ions has to be optimised and diffusion-controlled processes have to be studied more in details.

### EPR OF F TYPE CENTRES IN LiBaF<sub>3</sub>

**A.Fedotovs, E.Elsts, U.Rogulis, I.Tale, M.Nikl<sup>1</sup>, N.Ichinose<sup>2</sup>, K.Shimamura<sup>2</sup>**

<sup>1</sup>*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*

<sup>2</sup>*Laboratory of Material Sciences and Technology, Waseda University, Tokyo, Japan*

In this research we studied EPR spectra of pure LiBaF<sub>3</sub> sample of high quality. For EPR measurements LiBaF<sub>3</sub> sample was X-irradiated at room temperature, but spectra could be observed at low temperatures - at 77K. We could well resolve all hyperfine structure lines of F-type centre. Qualitative analysis with g-tensor parameters derived from magneto-optical measurements show that the F-type centre observed earlier by MCD-EPR techniques is the same F-type centre we observe in the EPR.

## X-IRRADIATION INDUCED PHOTO- AND THERMOSTIMULATED LUMINESCENCE OF CsCdF<sub>3</sub>:Mn CRYSTALS

**M. Springis, A. Sharakovsky, I. Tale, U. Rogulis**

Perovskite type fluoride crystals doped with rare-earth ions and other activators are promising materials for laser hosts and detectors of ionising radiation. The radiation-induced effects have been studied in a number of fluorides and the main defects (F- and V<sub>K</sub>-type) have been identified. Considerably less information on radiation effects is available for CsCdF<sub>3</sub>. Here we present a study of photo- and thermostimulated luminescence (PSL and TSL respectively) of previously X-irradiated CsCdF<sub>3</sub> crystal doped with Mn. After X-irradiation of CsCdF<sub>3</sub> crystal at 8 K luminescence bands about 300 nm and 550 nm appear, when the crystal is optically stimulated at the same temperature. Several stimulation bands can be revealed for luminescence at 300 nm and 550 nm. According to Molwy-Ivey relation for halide crystals the stimulation band at 340 nm seems to be related to F-type centre absorption band. Subsequent heating of the crystal after X-irradiation at 8 K shows two groups of TSL peaks in temperature regions 8 K – 90 K and 200 K – 300 K. The spectral composition of the peaks involves both the emission band at 300 nm and 550 nm, moreover in spectra at low temperatures 300 nm emission band prevails, while in spectra of the most intense TSL peaks at 245 K and 295 K the emission band at 550 nm is dominant. Performed experiments allow us to suggest that the PSL band at 300 nm should be a result of electron recombination with self-trapped holes (STH), but the luminescence at 550 nm is related to Mn ions. Mechanisms of radiative recombinations as well as thermal stability of both STH and Mn ions are investigated.

## OPTICALLY DETECTED MAGNETIC RESONANCE INVESTIGATION OF A LUMINESCENT OXYGEN-VACANCY COMPLEX IN LiBaF<sub>3</sub>,

**B. Henke<sup>1</sup>, U. Rogulis, S. Schweizer<sup>1</sup>**

*<sup>1</sup>Department of Physics, University of Paderborn, Germany*

The structure of an oxygen-related luminescence centre in manganese-doped LiBaF<sub>3</sub> was investigated by photoluminescence (PL) and PL-detected electron paramagnetic resonance (PL-EPR). At 20 K this centre shows two luminescence bands peaking at about 430 and 475 nm, when excited at 220 nm. These bands can be attributed to an excited triplet state (S=1) of an oxygen-vacancy complex with the z-axis of the fine structure tensor parallel to the <110> direction. This complex is believed to be next to a Mn<sup>2+</sup> impurity on a Ba<sup>2+</sup> site and can be described by an oxygen on a fluorine lattice site with a nearest fluorine vacancy along the <110> direction.

## OPTICAL PROPERTIES OF Ce-DOPED OXIFLUORIDE COMPOSITES

**U. Rogulis, A. Veispals, L. Dimitrocnko, M. Springis, P. Kulis, A. Fedotovs**

Oxy-fluoride composites have been obtained based on lithium borate glass with lanthanum fluoride. Glasses without lanthanum fluoride are transparent up to 275 nm. In samples doped with Ce-activator, an additional absorption at about 300 nm and intense photoluminescence could be observed. After x-irradiation, EPR spectrum appears with a slightly resolved structure and a thermo-luminescence could be observed. At the present stage it is still unclear under what conditions fluoride crystallites are created in a glass matrix, however specific thermal treatment makes them observable.

## **ELECTRON PARAMAGNETIC RESONANCE STUDIES OF RADIATION DEFECTS IN LiYF<sub>4</sub> CRYSTALS**

**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 obtained results have shown 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. Based on the estimated  $g$ -values, the authors have suggested 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 angular dependence, which have been explained by the  $g$ -anisotropy and hyperfine interaction of the unpaired electron spin with two neighbouring fluorine nuclei.

## **RECOMBINATION PROCESSES IN LiBaF<sub>3</sub> CRYSTALS**

**P. Kulis, M. Springis, I. Tale, A. Sharakovsky, L. Dimitrichenko**

The creation of radiation defects in LiBaF<sub>3</sub> crystals at 10 K and the processes of their thermostimulated recombination are investigated. The methods of optical absorption, thermal bleaching of colour centers, thermostimulated and optically stimulated luminescence are used. The radiation defects anneal in a multi-stage process accompanied with thermo-luminescence at 20, 46, 105, 130, 170, 210 and 270 K. Differences in the optical absorption spectra measured before and after the TSL peaks are obtained and recombination parameters are determined. The TSL peak at 20 K arises from the delocalization of H-centers. The presence of two TSL peaks related to V<sub>K</sub>-centers at 105 and 130 K indicates that 60° and 90° migration hops occur. The absorption band of H-centers is at 3.8 eV, but V<sub>K</sub>-centers are characterized with two absorption bands at 3.2 and 4.3 eV.

## **EPR HYPERFINE STRUCTURE OF THE Mo-RELATED DEFECT IN CdWO<sub>4</sub>**

**E.Elsts, U.Rogulis**

The hyperfine structure (hf) of the electron paramagnetic resonance (EPR) spectrum of Mo-related impurity defects in CdWO<sub>4</sub> crystal observed previously is reconsidered with account for interactions with two different groups of neighbouring Cd nuclei. The best fit of calculated EPR spectrum to the experimental is obtained with account for 2 groups of 3 and 2 equivalent Cd nuclei, respectively.

## **MAGNETO-OPTICAL RESONANCE INVESTIGATIONS ON Eu- AND Nd-/Dy- CODOPED CaAl<sub>2</sub>O<sub>4</sub> AND SrAl<sub>2</sub>O<sub>4</sub> SINGLE CRYSTALS**

**S. Schweizer<sup>1</sup>, B. Henke<sup>1</sup>, U. Rogulis, W. M. Yen<sup>2</sup>**

<sup>1</sup> *Faculty of Sciences, Department of Physics, University of Paderborn,  
Paderborn, Germany*

<sup>2</sup> *Department of Physics and Astronomy, University of Georgia, Athens, GA, USA*

We present first magneto-optical measurements on the single crystalline persistent phosphors  $\text{MAl}_2\text{O}_4$  ( $\text{M} = \text{Ca}$  and  $\text{Sr}$ ) crystals doped with  $\text{Eu}$  and  $\text{Nd}$  or  $\text{Dy}$ , respectively. Their photoluminescence and microwave-induced changes in the recombination luminescence were investigated. The analysis of the magneto-optically detected electron paramagnetic resonance spectra, recorded after ultraviolet excitation at 4.2 K, shows that donor and acceptor centers are involved in the recombination process. The  $g$  value of the donor is 1.99 in  $\text{CaAl}_2\text{O}_4$  and 1.97 in  $\text{SrAl}_2\text{O}_4$ ; in both systems the  $g$  value of the acceptor is 2.01.

## **CARRIER LOCALIZATION EFFECT IN POLARIZED INGAN/GAN MULTIPLE QUANTUM WELLS**

**M. Springis, I. Tale, C. C. Yang<sup>1</sup>, S. Jursenas<sup>2</sup>**

<sup>1</sup>*Graduate Institute of Electro-Optical Engineering, Department of Electrical Engineering, National Taiwan University*

<sup>2</sup>*Institute of Materials Science and Applied Research, Vilnius University*

Improving performance of InGaN-based light-emitting devices requires quantitative characterization of localized states and built-in electric fields in InGaN quantum wells. We report on distinguishing between the localization and built-in field effects in InGaN quantum wells based on photoreflection (PR), photoluminescence (PL), PL excitation (PLE), selective excitation of PL (SEPL), PL excitation power (PLEP), and time-resolved PL (TRPL) spectroscopy. Two sets of samples containing 5 InGaN quantum wells separated by 9 nm-wide GaN barriers were fabricated by using MOCVD technique. In the first set, the quantum well width was gradually changed from 2 to 4 nm at a fixed InGaN content (15%), while in the second set, the In content was varied at a fixed well width (2.5 nm).

PR spectra revealed reliable values of built-in field (typically about 0.5 MV/cm for 15% In content). Meanwhile a remarkable Stokes shift between the PR feature and the PL peak position was observed. The Stokes shift increased with both the well width and In-content. We attributed this Stokes shift to solely the localization effect. Temperature behavior of the Stokes shift and PL linewidth was shown to be consistent with phonon-assisted carrier tunneling (hopping) through the random distribution of states confined in the band potential minima within large In-rich regions. The scale of the band potential profile fluctuations within the In-rich regions and the dispersion in the average band gap energy of the regions were quantitatively estimated from the PL temperature behavior using Monte Carlo simulation of in-plane carrier hopping. These estimations were compared with the observations of the band tail in the PLE measurements.

The characteristic blue shift of the PL peak with increasing the excitation power was examined using different energies of the incident photons for PL excitation (SEPL). At comparable carrier densities, an increase in incident photon energy resulted in a significant enhancement of the blue shift. This effect was more prominent in MQWs with wider wells and larger In-content. Such a dynamics of the excitation-power-induced blue shift was attributed to filling of the band-tail states. In our MQWs, the blue shift was shown to be dominated by band-tail filling rather than by screening of built-in field. Transient behavior of band-tail filling under conditions of screened built-in field was revealed by TRPL measurements in highly excited MQWs.

# INVESTIGATION OF METAL IONS IN FUSION PLASMAS USING EMISSION SPECTROSCOPY

**I. Tale, A. Sharakovsky, M.Springis**

The Latvian and Portugal Associations are performing development of advanced plasma – facing system using the liquid metal limiter. 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.

The fusion plasmas are related to the dense hot plasmas. The required average ion temperature according to the ITER project (International Thermonuclear Experimental Reactor) is 8.0 keV ( $9.3 \times 10^7$  K), the average electron temperature – 8.9 keV ( $1.04 \times 10^8$  K). Plasma temperature operated in the research tokamak ISSTOK, involved in testing of liquid metal limiter concept is considerably less, being of order of  $10^5$  K.

The ionisation degree of metal atoms considerably depends on the plasma ion temperature. Density of metal vapours in plasma can be estimated using the following two spectroscopic methods:

- The fluorescence of the multiple ionised metal ions in steady state concentration;
- The charge exchange emission during ionisation of evaporated metal ions.

In the first step of development of testing system of metal vapours the equipment and instrumentation for charge exchange spectroscopy of Ga and In has been elaborated taking into account the following features of plasma emission. The Ga emission lines occur on the background high temperature plasma black body emission and stray light. Radial distribution of Ga in plasma in the facing plane of Ga flux is desirable. For spectroscopy of fusion plasma theoretical and experimental investigation of fluorescence of multiple ionised Ga and In ions in laser created plasma will be performed.

## LASER ABLATION SPECTROSCOPY FOR IMPURITY DEPTH PROFILING AND CONCENTRATION IMAGING IN PLASMA FACING MATERIALS

**I. Tale, J. Butikova, P. Kulis,, A. Sarakovsky.**

Particle fluxes from the plasma (ions, electrons, atoms) results in complex processes of the plasma-wall interaction. They are crucial for possibility of application of the material in the fusion devices. Understanding these processes is necessary for improving of the wall materials as well as leads to optimize plasma discharge operation conditions. Investigation of the material modification under plasma exposure, development of new plasma facing materials and development of methods of their characterization are actual tasks into the development of plasma facing components. It is stated that plasma – wall material interaction results in several processes such as: erosion of material, migration of materials in fusion devices involving tungsten migration, deposition of carbon layers, tritium co-deposition, and diffusion of hydrogen isotopes in plasma facing materials.

Several methods for investigation of the surface and impurity content in near-surface layers are applied. They involves X-ray photoelectron spectroscopy, the deuterium depth profiling by analysis of energy spectrum of alpha particles resulting the nuclear reaction  $D(^3\text{He},p)^4\text{He}$  in the near-surface layers of solids. Using different  $^3\text{H}$  energy depth profiles from 1  $\mu\text{m}$  up to  $>10 \mu\text{m}$  can be obtained. For obtaining of composition of hydrocarbon layers and their optical properties ion beam techniques is applied

The alternative method for obtaining of impurity content in solid materials is laser ablation spectroscopy. Two techniques are available for impurity analysis: fluorescence spectroscopy and mass spectroscopy.



The advantage of fluorescence spectroscopy is high sensitivity, disadvantage for spectroscopy of plasma facing materials – extremely close spectral line position of the hydrogen isotopes ( for 434,04 nm line of H and D the difference is  $\Delta\lambda=0.12$  nm).

Mass spectroscopy allows separate H, D and T however the sensitivity is considerably lower.

The laser ablation fluorescence spectroscopy, proposed to set up for impurity analysis permits to provide both the impurity depth profiling and the content layer after layer imaging in the course of the laser beam scanning.

Proposed investigations is focused on deposition characteristics of surface layers, migration effects of W and carbon, accumulation of hydrogen isotopes in plasma facing and divertor materials. They can be obtained by analysis of the camping- integrated results of tungsten- coated graphite tiles installed in the main chamber and divertor regions.

### Scientific publication

Published in 2006

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2. U. Rogulis, A. Veispāls, L. Dimitročenko, M. Springis, P. Kūlis, A. Fedotovs, *Optical properties of Ce-doped oxy-fluoride composites*, - Latvian Journal of Physics and Technical Sciences, 2006, vol. 2, p. 111-115.
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4. A. Fedotovs, U. Rogulis, L. Dimitročenko, *Electron paramagnetic resonance studies of radiation defects in LiYF<sub>4</sub> crystal*, - Latvian Journal of Physics and Technical Sciences, 2006, vol. 6, p. 60-65.
5. B. Henke, U. Rogulis, and S. Schweizer, *Luminescent oxygen-vacancy complex in Mn-doped LiBaF<sub>3</sub> investigated by optically detected magnetic resonance*, Proceedings of the 8<sup>th</sup> International Conference on Inorganic Scintillators and their Use in Scientific and Industrial Applications, SCINT 2005, Institute for Scintillation Materials, Ukraine, Kharkov, 2006, p. 70-73.
6. A. Fedotovs, E. Elsts, U. Rogulis, I. Tale, M. Nikl, N. Incinose, K. Shimamura, *EPR of F-Type Centres in LiBaF<sub>3</sub>*, - Proceedings of the 8<sup>th</sup> International Conference on Inorganic Scintillators and their Use in Scientific and Industrial Applications, SCINT 2005, Institute for Scintillation Materials, Ukraine, Kharkov, 2006, p. 156-158.
7. P. Kulis, M. Springis, I. Tale, A. Sharakovsky, L. Dimitrichenko, *Recombination Processes in LiBaF<sub>3</sub> Crystals*, - Proceedings of the 8<sup>th</sup> International Conference on Inorganic Scintillators and their Use in Scientific and Industrial Applications, SCINT 2005, Institute for Scintillation Materials, Ukraine, Kharkov, 2006, p. 159-161.
8. A. Fedotovs, L. Dimitrocenko, U. Rogulis, *EPR of Radiation Defects in LiYF<sub>4</sub> Crystals*, - - Proceedings of the 8<sup>th</sup> International Conference on Inorganic Scintillators and their Use in Scientific and Industrial Applications, SCINT 2005, Institute for Scintillation Materials, Ukraine, Kharkov, 2006, p. 162-164.

9. A. Sharakovskiy, M. Springis, I. Tale, *Luminescence of CsCdF<sub>3</sub>:Mn Crystals*, - Proceedings of the 8<sup>th</sup> International Conference on Inorganic Scintillators and their Use in Scientific and Industrial Applications, SCINT 2005, Institute for Scintillation Materials, Ukraine, Kharkov, 2006, p.188-190.
10. B. Henke, U. Rogulis, S. Schweizer, *Optically detected magnetic resonance investigation of a luminescent oxygen-vacancy complex in LiBaF<sub>3</sub>*, - Journal of Physics: Condensed Matter, 2006, vol. 18, p. 1577-1583.
11. S. Schweizer, B. Henke, U. Rogulis, W.M. Yen, *Magneto-optical resonance investigations on Eu- and Nd-/Dy-codoped CaAl<sub>2</sub>O<sub>4</sub> and SrAl<sub>2</sub>O<sub>4</sub> single crystals*, - Science and Technology of Dielectrics in Emerging Fields -and- Persistent Phosphors (PV 2005-13), pp. 191-198. Published by: The Electrochemical Society, 2006. Editors: Worhoff, Misra, Mascher, Sundaram, Yen, and Capobianco ISBN: 1-56677-511-6.

## Lectures on Conferences

### **22nd Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, March 29-30, 2006.**

1. A. Fedotovs, U. Rogulis, L. Dimitrochenko, *EPR of radiation defects in LiYF<sub>4</sub> crystal*, - Abstracts of the 22 Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, March 29-30, 2006, p. 7 (oral presentation).
2. E. Elsts, A. Fedotovs, U. Rogulis, A. Guļāns, I. Tāle, M. Nikl, N. Ichinose, K. Shimamura, *EPR of F-Type Centres in pure LiBaF<sub>3</sub> crystal*, - Ibid. p. 8 (oral presentation).
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4. J. Jansons, *Professor of physics Fricis Gulbis (1891-1956)*, - Ibid. p. 25 (oral presentation).
5. J. Buitikova, *Rutherford backscattering measurements or LIBS standards*, - Ibid. p. 41 (oral presentation).

### **2<sup>nd</sup> Latvian conference “Functional materials and nanotechnologies” Riga, March 27-28, 2006.**

1. A. Gulans, I. Tale, *Ab initio calculation of GaN nanowires*, - 2<sup>nd</sup> Latvian conference “Functional materials and nanotechnologies” Riga, March 27-28, 2006, Book of abstracts, p. 19 (poster presentation).
2. E. Klotins, M. Springis, *Critical dynamics in nanoscale*, - Ibid. p. 31 (oral presentation).
3. P. Kulis, G. Marcins, M. Springis, I. Tale, A. Veispals, A. Voitkans, *Implementation of the MOCVD technique for growth of III group nitride nanostructures*, - Ibid. 37 (oral presentation).
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5. U. Rogulis, A. Veispāls, L. Dimitročenko, M. Springis, P. Kūlis, A. Fedotovs, *Optical properties of Ce-doped oxy-fluoride composites*, - Ibid. p. 61 (poster presentation).

### **10<sup>th</sup> Europhysical Conference on Defects in Insulating Materials, EURODIM-10, Milano, University of Milano-Bicocca, Italia, July 10-14, 2006.**

1. P. Kulis, A. Sarakovskis, M. Springis, I. Tale, *Trap spectroscopy of N- and B-doped 6h-SiC*, - 10<sup>th</sup> Europhysical Conference on Defects in Insulating Materials,

- EURODIM-10, Conference program and book of abstracts, Milano, University of Milano-Bicocca, Italia, July 10-14, 2006, p. 58 (oral presentation).
2. S. Schweizer, B. Henke, U. Rogulis, W.Yen, *Recombination processes in rare-earth doped  $M\text{Al}_2\text{O}_4$  ( $M=\text{Ca}, \text{Sr}$ ) persistent phosphors investigated by optically-detected magnetic resonance*, - Ibid. p. 40 (oral presentation).
  3. B. Henke, S. Schweizer, U. Rogulis, *Optical and electron paramagnetic resonance studies on radiation defects in Mn-activated  $\text{RbCdF}_3$* , - Ibid. p. 56 (oral presentation).
  4. L. Dimitrocenko, U. Rogulis, A. Veispals, M. Springis, P. Kulis, A. Fedotovs, *Luminescence of Ce-doped borate-oxyfluoride glass ceramics*, - Ibid. p. 136 (poster presentation).
  5. A. Sharkovsky, K. Smits, M.Springis, *Luminescence of radiation defects in  $\text{LiBaF}_3:\text{Fe}$* , - Ibid. p.223 (poster presentation).
  4. A. Gulans, I. Tale, Ab initio calculation of wurtzite-type GaN nanowires, - Ibid. p. 245 (poster presentation).
  5. A. Fedotovs, E. Elsts, U.Rogulis, A. Gulans, I. Tale, M.Nikl, N. Ichinose, K. Shimamura, *EPR hyperfine structure of F-type centres in pure  $\text{LiBaF}_3$  crystal*, - Ibid. p.340 (poster presentation).

**6<sup>th</sup> European Conference on Luminescent Detectors and Transformers of Ionizing Radiation LUMDETR'2006, Lviv, Ukraine, June 19-23, 2006.**

1. A. Fedotovs, U. Rogulis, L. Dimitročenko, *Electron paramagnetic resonance studies of radiation defects in  $\text{LiYF}_4$  crystal*, - Abstract of the International conference LUMDETR'2006, Lviv, Ukraine, June 19-23, 2006, p.190 (poster presentation).

**Popular scientific articles**

1. J. Jansons, *Latvijas Universitātes Fizikas institūts vācu nacistu okupācijas laikā - "Zinātņu vēsture un muzejniecība"*: LU Raksti, 693. sēj./ Zinātniskais redaktors prof. M. Baltiņš. – Rīgā: Latvijas Universitāte, 99 – 107, 2006.
2. J. Jansons, *Professor of physics Fricis Gulbis (1991-1956)*, - Abstracts of XXII Baltic Conference on the History of Science, Vilnius, October 5-6, 2006, p. 34 – 35.
3. J. Jansons, *Fizikas profesors Fricis Gulbis (1891–1956)*, - LU Apgāds, 2006, 128 lpp.

# DISORDERED MATERIAL PHYSICS

Head of Division Dr.hab.phys.D.Millers

**Solid state radiation physics laboratory**  
Head of Laboratory,  
Dr.hab.phys.L.Grigorjeva

**Defect studies group**  
Head of Group  
Dr.hab.phys. L.Skuja

**Solid state optics laboratory**  
Head of Laboratory,  
Dr.hab.phys.A.Trukhin

## Research area and Main Problems

The main materials studied are: LiNbO<sub>3</sub>, YVO<sub>4</sub>, TlBr, YAP/YAG, CaWO<sub>4</sub>, ZnO, ZrO<sub>2</sub>, glassy SiO<sub>2</sub>, Ge-doped silica). Studies of single crystals, nanocrystals, ceramics, glasses and fibers were carried out.

Time-resolved optical spectroscopy has been used for fast relaxation processes responsible for excited states formation, excited states radiative and nonradiative decay, charge and energy transfer. The Fourier-transform infrared (FTIR) spectroscopy was used for detection of molecular species, paramagnetic centers were studied by electron paramagnetic resonance (EPR).

### Laboratory of solid state radiation physics

1. Dr. hab.phys. S.Chernov
2. Dr. hab.phys. L.Grigorjeva
3. Dr. hab.phys. D.Millers
4. Dr.phys.V.Pankratov

### Technical Staff

1. Eng. A.Sitdikov
2. Eng. E.Arhipova

### Doktorants

1. K.Smits
2. M.Shorohov

### Students

A.Kalinko

### Defect studies group

1. Dr.hab.phys. A. Siliņš
2. Dr.hab.phys L. Skuja
3. Dipl. phys. A. Lukjanska

### Laboratory of solid state optics

1. Dr.hab.phys.A.Trukhins
2. Dr..phys.K.Trukhins



## Scientific Visits Abroad

1. Dr.hab.phys. L.Grigorjeva, Poland, (6 days).
2. Dr.hab.phys.D.Millers, Poland, (6 days).
3. Dr.phys.V.Pankratov, Poland, (6 days).
4. K.Smits, Poland, (6 days)
5. Dr.V.Pankratov, Italy, (7days)
6. K.Smits, Italy, (7days)
7. Dr.hab.phys. L.Grigorjeva, Italy, (7days).
8. Dr.hab.phys.D.Millers, France (7 days).
9. Dr.hab.phys. L.Grigorjeva, France, (4days).
10. Dr.hab.phys. L.Grigorjeva, Italy, (7days).
11. K.Smits, France, (14days)
12. D.Millers, Lithuania (4 days).
13. V.Pankratov Lithuania (2 days).
14. L.Grigorjeva, Lithuania (2 days).
15. D.Millers, Romania (5 days).
16. L.Grigorjeva, Romania (5 days).
17. L.Skuja, Italy 7 days,
18. L.Skuja, A. Siliņš, Germany (5 days)
19. L.Skuja, Japan (30 days)

## Visits from Abroad

Dr. C. Monty, CNRS/PROMES, France

Prof. R. Piticescu, National Research and Development Institute for Non-ferrous & Rare Metals, Romania

Dr.J. Fidelus, High Pressure Research Center, Polish Academy of Sciences, Poland

Dr. K.A.Gross, the University of Melbourne

## Cooperation

### Latvia

University of Latvia, Institute of Biology (Dr. O.Mutere).

SIA "Baltic Scientific Instruments" (Dr.V.Gostillo).

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

SIA "OPTICS", (V.Jakovlev).

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

### USA

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

Department of Physics and Engineering, Sweet Briar College (Prof. Hank Yochum).

### Estonia

Institute of Physics, Tartu (Dr.V.Nagirnyj, M.Kirm, V.Babin)

### Russia

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

Burjatija State University (A.V.Nomoev)

### Poland

High Pressure Research Center, Polish Academy of Sciences UNIPRESS  
(Prof.W.Łojkowski, Dr.J.Fidelus)

Institute of Physics, University of Rzeszow (Dr.P.Potera)

Institute of Low Temperatures and Structure Researches, PAS, Wrocław  
(Prof. W. Streck)

**Romania**

Institute for Non-Ferrous and Rare Metals (Dr. R.M. Piticescu, Prof. R. Piticescu)

**France**

CNRS/Proc. Mat. Eng. Solaire, Font-Romeu (Dr. Claude Monty)

**Japan**

Tokyo Institute of Technology (Prof. H. Hosono)

ERATO-SORST Frontier Collaborative Research Center, Japan Science and  
Technology Agency (Dr. M. Hirano, K. Kajihara)

**Italy**

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

**The main results**

**LUMINESCENCE OF ZnO NANOSTRUCTURED POWDERS**

**L. Grigorjeva, D. Millers, A. Kalinko, W. Łojkowski<sup>1</sup>, T. T. Strachowski<sup>1</sup>,  
R. Piticescu<sup>2</sup>, C. Monty<sup>3</sup>, J. Grabis<sup>4</sup>**

<sup>1</sup> *High Pressure Research Center, Polish Academy of Sciences*

<sup>2</sup> *Institute for Non-Ferrous and Rare Metals, Bucharest, Romania*

<sup>3</sup> *CNRS/Proc. Mat. Eng. Solaire, Font-Romeu, France*

<sup>4</sup> *Institute of Inorganic Chemistry, Riga Technical University, Riga, Latvia*

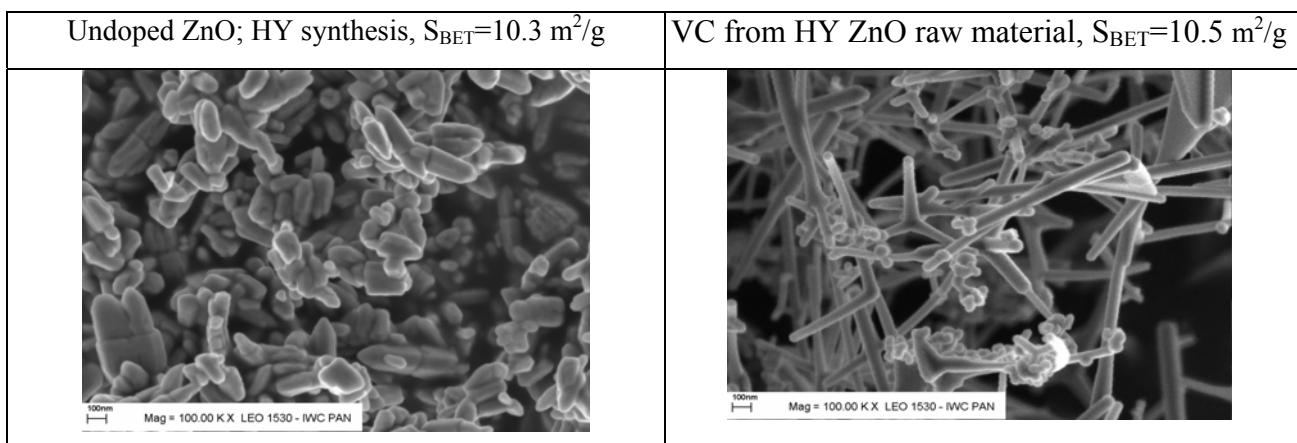
The luminescence properties of ZnO nanocrystals synthesized by microwave driven hydrothermal process (HY), plasma synthesis and evaporation-condensation (VC) in solar reactor were under investigation.

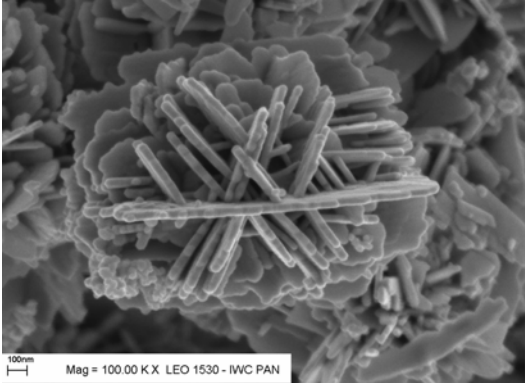
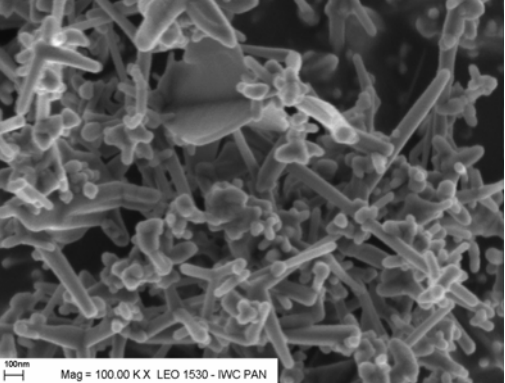
The FTIR absorption, x-ray diffraction and SEM images were used for nanopowders characterization.

The analysis of luminescence spectra and decay kinetics in defect band (1.8-2.5 eV) shows that the different luminescence centers are in HY powders and powders obtained after VC; the decay is not simple exponential. We find that for ZnO powders prepared by HY method the luminescence decay kinetics plot in **logI-logt** coordinates is a straight line at  $t \gg \Delta t$ , where  $\Delta t$  is excitation pulse duration.

The VC powders show whiskers-type structures. The luminescence intensity in excitonic band considerably increases after VC process and superlinear intensity dependence on excitation density is observed.

**The SEM images of typical nanopowders:**



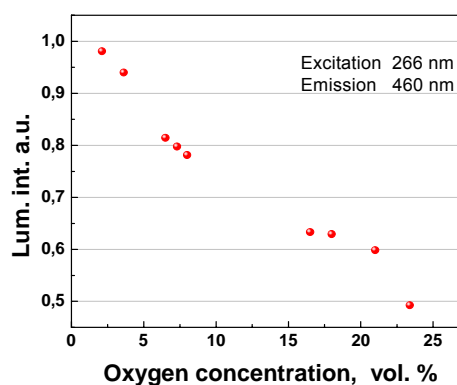
ZnO:Al (0.05 w%); HY synthesis; $S_{\text{BET}}=14.36, \text{ m}^2/\text{g}$	VC from HY ZnO:Al (0.05W%) raw material, $S_{\text{BET}}=20.1 \text{ m}^2/\text{g}$
	

## THE LUMINESCENCE PROPERTIES OF PURE, YTTRIUM AND EUROPIUM DOPED $\text{ZrO}_2$ NANOCRYSTALS

**D. Millers, L. Grigorjeva, K. Smits W. Lojkowski<sup>1</sup>, A. Opalinska<sup>1</sup>, J. Fidelus<sup>1</sup>**  
<sup>1</sup> High Pressure Research Center, Polish Academy of Sciences, Poland, Warsaw

The time-resolved luminescence of **pure** tetragonal nanocrystals shows two luminescence bands with different decay times. Both luminescence bands excitation is possible within band to band excitation and it is suggested that intrinsic defects are responsible for the observed luminescence. Additional strong luminescence band peaking at 3.5 eV was found in **yttrium stabilized tetragonal**  $\text{ZrO}_2$  nanocrystals. It is shown that the heating in vacuum results in strongly reduced intensity of luminescence excited by pulsed electron beam. It is proposed that the luminescence intensity reduction is due to the oxygen loss during the annealing of nanocrystals in vacuum. It was found that the effect can be used in luminescence-based oxygen sensors.

$\text{ZrO}_2$  nanocrystals luminescence intensity dependence on oxygen concentration

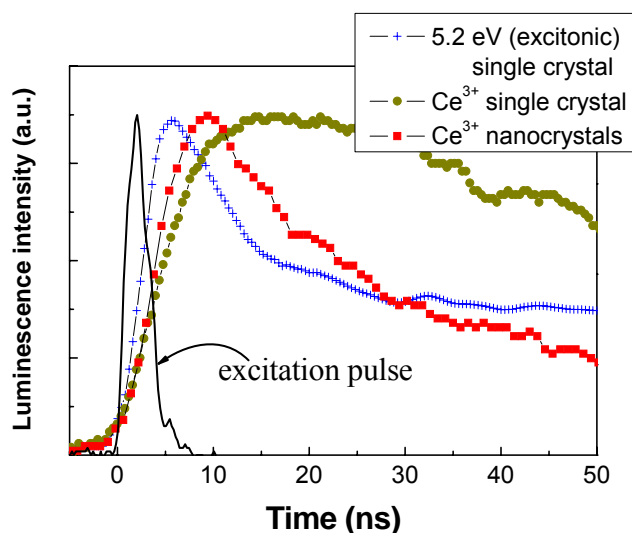


## LUMINESCENCE OF RARE-EARTH DOPED YAG AND YAP NANOPOWDERS

**V. Pankratov, D. Millers, L. Grigorjeva, T. Chudoba<sup>1</sup>,**  
<sup>1</sup> High Pressure Research Center, Polish Academy of Sciences, Warsaw, Poland

The YAG nanopowders doped by rare-earth ions could be a perspective raw material for transparent scintillating ceramic. Nominally pure, Ce, Nd and Eu doped YAG nanopowders with grain size  $\sim 20$  nm were obtained by Pechini and co-precipitation methods. The time-resolved luminescence spectroscopy was applied for defect studies and energy transfer processes in pure and doped nanopowders as well as in pure and

doped YAG single crystals. It is shown that an energy transfer rate from the host lattice to the  $\text{Ce}^{3+}$  ions is higher in YAG nanocrystals as compared to YAG single crystal. Intrinsic luminescence bands well known for single crystals were detected also in undoped nanopowders. The new intrinsic luminescence band was not observed in nanopowders. In Ce doped YAG nanopowders the intrinsic luminescence disappears. The effects of dopand concentration and nanopowders grain size to luminescence decay time were studied.



Initial part of time evolution for  $\text{Ce}^{3+}$  related luminescence in YAG nanopowder and single crystal under e-beam excitation at 80 K.

## TRANSIENT AND NEAR-EDGE ABSORPTION IN $\text{YVO}_4$ CRYSTALS

H.M. Yochum<sup>1</sup>, L. Grigorjeva, D. Millers, V. Pankratov, P. Potera<sup>2</sup>

<sup>1</sup>Department of Physics and Engineering, Sweet Briar College, Sweet Briar, VA, USA

<sup>2</sup>Mat-Phys Department, Institute of Physics, University of Rzeszow, Poland

Yttrium orthovanadate  $\text{YVO}_4$  (YVO) crystals doped with rare-earth ions such as  $\text{Nd}^{3+}$ ,  $\text{Tm}^{3+}$ ,  $\text{Ho}^{3+}$  and  $\text{Er}^{3+}$  are a well-known laser host materials.  $\text{YVO}:\text{Nd}$  is one of the most promising materials for diode-pumped lasers with a low threshold and high laser output. The process of near-edge absorption annealing in air was studied up to 1500C in  $\text{YVO}_4$ . In this annealing process, two stages with activation energies of 0.16 eV and 0.38 eV, were obtained. In addition to the annealing study, the transient absorption induced by pulsed electron beam excitation (270 keV, 8 ns) was studied on a set of  $\text{YVO}_4$  samples with different near-edge absorption levels in the spectral region 3.2-3.5 eV. The spectral range from  $\sim 1.25$  eV up to 3.0 eV is covered by a strong transient absorption. Transient absorption spectra show at least three broad overlapping bands ( $\sim 1.3$  eV,  $\sim 2.0$  eV and  $\sim 3.0$  eV). The 3 eV peak position is close to the near-edge absorption band and correlation between transient absorption bands and absorption due to stable colour centers was studied. It is suggested that absorption bands at  $\sim 1.3$  eV and  $\sim 2.0$  eV are due to electron and hole polarons, correspondingly.



## A NEW TYPE OF HYDROGEN-RELATED E'-CENTER IN WET SILICA GLASS

**L.Skuja<sup>1,2</sup>, K. Kajihara<sup>2</sup>, M.Hirano<sup>2</sup>, A. Saitoh<sup>3</sup>, H.Hosono<sup>2,3</sup>**

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

<sup>2</sup>*Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Japan;*

<sup>3</sup>*Tokyo Institute of Technology, Japan*

Since their discovery by electron paramagnetic resonance (EPR), E'-centers have proved to be nearly ubiquitous in all types of irradiated silica glass and have evolved to the most studied class of defects in silica and alpha quartz. The generic E' center in silica comprises a paramagnetic Si dangling bond, its properties being modified by variations in surroundings. Many different forms of E'-centers have been identified. We report an EPR-based evidence for a new, distinct type of E' center, which is observed in any wet silica glass, irradiated at 80K by F<sub>2</sub> laser photons (7.9eV). This type of centers is stable at 300K and is distinguished by a 0.08mT splitting of its low-field peak in derivative spectrum. Comparison between X-band and Q-band EPR spectra proves that this splitting is due to shf coupling. Deuteration experiments show that this coupling is associated with proton. The proximity of proton is confirmed by electron spin echo envelope modulation (ESEEM) technique. Computer simulation of the EPR spectrum yields principal g values  $g_1=2.00176$ ,  $g_2=2.00065$ ,  $g_3=2.00037$  and the principal values of proton hfs matrix (in mT):  $a_1=0.105$ ,  $a_2=0.021$ ,  $a_3=0$ . We attribute this signal to generic E' center having one of the surrounding three bridging oxygens substituted by a hydroxyl (OH) group. The center can be denoted as E'(OH) center. The magnitude of the observed shf splitting is consistent with the theoretical estimates.

## FLUORINE LASER-INDUCED SILICON HYDRIDE Si-H GROUPS IN SILICA

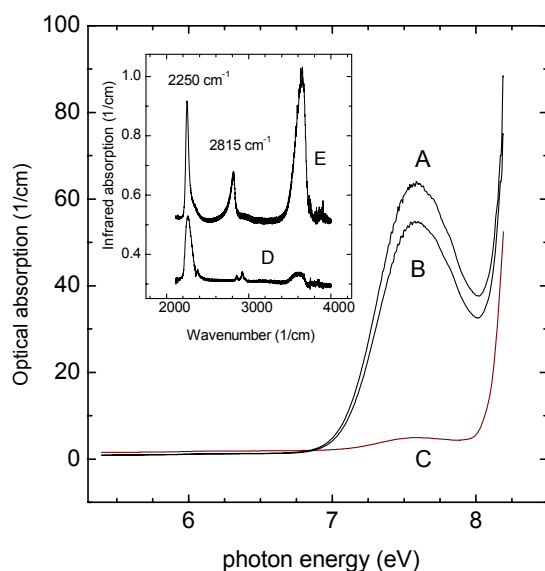
**Linards Skuja,<sup>\*,\*\*</sup> Koichi Kajihara<sup>\*\*</sup>, Masahiro Hirano<sup>\*\*</sup>, and Hideo Hosono<sup>\*\*,\*\*\*</sup>**

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

<sup>\*\*</sup>*Transparent Electro-Active Materials Project, ERATO-SORST, Japan Science and Technology Agency in Materials and Structures Laboratory & Frontier Collaborative Research Center,*

<sup>\*\*\*</sup>*Tokyo Institute of Technology*

Three distinct types of silicon hydride (Si-H) groups are identified by infrared (IR) spectroscopy in silica glass irradiated by 7.9 eV photons from fluorine laser. Irradiation of H<sub>2</sub>-loaded glasses creates an IR band around 2250 cm<sup>-1</sup> due to "isolated" SiH groups comprising Si atom coordinated by H and 3 bridging oxygens. Irradiation of wet silica at T=80K creates room-temperature stable SiH groups absorbing at 2237 cm<sup>-1</sup> and an unstable component, absorbing at 2221 cm<sup>-1</sup>. The 2237 cm<sup>-1</sup> band is assigned to hydride group neighbored by a silanol (SiOH) group, bound to the same silicon atom ("Si-H(OH)"). The cross section for photolysis of isolated SiH groups by 7.9 eV photons is below  $<4 \times 10^{-21}$  cm<sup>2</sup>, indicating that their optical absorption probably does not decrease the vacuum ultraviolet transparency of silica.



Vacuum ultraviolet absorption spectra of dry oxygen deficient silica before treatment (A), after H<sub>2</sub>-loading at T=423 K (B) and after 830 J/cm<sup>2</sup> irradiation at 295K by F<sub>2</sub> laser photons (7.9 eV) (C). Inset shows the corresponding irradiation-induced changes of IR absorption in this sample (D) and in H<sub>2</sub>-loaded chlorine-containing dry silica (E).

## Scientific Publications

Published in 2006

1. L.Grigojjeva, D.Millers, W.Łojkowski, T.Strachowski. Luminescence and FTIR spectroscopy of ZnO nanocrystals. Materials Science Forum, Trans Tech Publications, **vol.514-516**, 2006 p.1230-1234..
2. Vladimir Pankratov, Donats Millers, Larisa Grigorjeva, Witold Lojkowski, Robert Fedyk, Tadeusz Chudoba, Wieslaw Strek, Darek Hreniak, Piotr Mazur. Intrinsic Luminescence of Pure and Doped YAG Nanopowders. Proc.of the 8<sup>th</sup> International Conference on Inorganic Scintillators and their Use in Scientific and Industrial Applications, Ukraine, Kharkov, 2006, p.224-227.
3. S. Chernov, L. Grigorjeva, D. Millers, V. Pankratov. Luminescence Center Formation under Pulsed Electron Beam Excitation in CaWO<sub>4</sub> Crystal. Ibid, p.25-27.
4. M.Shorohov, L.Grigojjeva, D.Millers. Optical properties and spectroscopic performance of TlBr detector crystals. Nucl.Instruments and Methods in Physics Research A. **563** 2006, p.78-81.
5. K. Kajihara, M.Hirano, L.Skuja, H.Hosono, Role of Interstitial Voids in Oxides on Formation and Stabilization of Reactive Radicals: Interstitial HO<sub>2</sub> Radicals in F<sub>2</sub> - Laser-Irradiated Amorphous SiO<sub>2</sub>. J. Amer.Chem.Soc., v.128, p.5371-5374 (2006).
6. K. Kajihara, M.Hirano, L.Skuja, H.Hosono, Interstitial OH radicals in F<sub>2</sub>-laser-irradiated bulk amorphous SiO<sub>2</sub>. J.Phys.Chem.B v.110, p.10224-10227 (2006).
7. L.Skuja, K. Kajihara, M. Hirano, A. Saitoh, H. Hosono, An increased F<sub>2</sub> laser damage in "wet" silica glass due to atomic hydrogen: a new hydrogen-related E'<sup>2</sup>-center. J. Non-Crystalline Solids, v.352, p.2297-2302 (2006).
8. K. Kajihara, L.Skuja, M.Hirano, H.Hosono, In situ observation of the formation, diffusion, and reactions of hydrogenous species in F<sub>2</sub> -laser-irradiated SiO<sub>2</sub> glass using a pump-and-probe technique. Phys. Rev. v. B74, p.094202(1-11) (2006).

## Lectures in Conferences

**2<sup>nd</sup> Latvian Conference "Functional materials and nanotechnologies", 27-28 March, 2006, Riga, Latvia.**

1. D.Millers, K.Smits L.Grigojjeva, V.Pankratovs. Investigation of oxide nanopowders: outlook for sensors, scintillators and lasers. Proceedings, p.47.

2. A.Kalinko, L.Grigorjeva, D.Millers, K.Smits. Photoluminescence of nanostructured ZnO obtained by different technologies., Proc. p.23.
3. B.Polyakov, J.Prikulis, L.Grigorjeva, D.Millers, V.Zauls, J.D.Holmes, D.Erts. High density arrays of germanium nanowire photoresistors. p.58.
4. L. Skuja, K. Kajihara, M. Hirano, and H. Hosono, Vacuum-ultraviolet absorption of Si-H groups in glassy SiO<sub>2</sub> Proc. p.69.

**The 8<sup>th</sup> International Conference-School “Advanced Materials and Technologies”, Palanga, Lithuania, 27-31 August, 2006**

1. D.Millers, L.Grigorjeva, K.Smits. Luminescence – a Tool for Nanocrystal study.
2. V.Pankrativ. The study of Scintillators, phosphors and laser materials by means of time-resolved spectroscopy.

**Network for nanostructured materials, NANOVED 2006 – NENAMAT, May 14-17, 2006, Stara Lesna, Slovakia**

1. K.Smits, L.Grigorjeva, D.Millers, W.Lojkowski, A.Opalinska, J.Fidelus. Yttrium stabilized tetragonal ZrO<sub>2</sub> luminescence. Book of abstracts, p.124.
2. A.Kalinko, L.Grigorjeva, D.Millers, J.Grabis, W.Lojkowski, C.J.Monty. Time-resolved luminescence in mokro and nanostructured ZnO powders. Ibid, 88

**6<sup>th</sup> European Conference on Luminescent Detectors and Transformers of Ionizing Radiation, LUMDETR 2006, June 19-23, 2006, Lviv, Ukraine**

V.Pankratov, L.Grigorjeva, D.Millers, T.Chudoba. Luminescence of Rare-Earth doped YAG Nanopowders. Book of Abstracts, p.49.

**6th Symposium SiO<sub>2</sub>, advanced dielectrics and related devices, June 25-28, 2006, Palermo, Italy.**

1. L. Skuja, K. Kajihara, M.Hirano, H.Hosono. Silicon hydride Si-H groups in silica.Abstacts p.82.
2. K. Kajihara, M.Hirano, L. Skuja, H. Hosono Reactions of chlorine-related species in silica., p.23

**8th International Otto-Schott Colloquium, July 23-27, 2006, Jena, Germany.**

1. L. Skuja, K. Kajihara, M.Hirano, H.Hosono. Ultraviolet absorption of hydrogen-related species in glassy silica.
2. A.Silins Light Energy Accumulation and Emission Processes in Optical Glasses.

**European Material Research Society Fall Meeting (E-MRS 2006), 4-8 September, 2006, Warsaw, Poland.**

1. D.Millers, K.Smits, L.Grigorjeva, J.Fidelus. Luminescence of Europium doped ZrO<sub>2</sub> nanopowder. Book of abstracts, p.89.
2. L.Grigorjeva, D.Millers, Claude J.Monty, J.Kouam, K.Djessas. The luminescence properties of ZnO:Al nanopowders obtained by sol-gel; and vaporization-condensation methods.. Ibid, p.82.
3. J.Fidelus, W.Lojkowski, D.Millers, L.Grigorjeva, P.P Piticescu. Zirconia-based nanomaterials for oxygen sensors-generation, characterization and optical properties. Ibid, p.88.
4. V.Pankratov, L.Grigorjeva, D.Millers, T.Chudoba, R.Fedyk, W.Lojkowski. Time-resolved Luminescence Characteristics of doped YAG and YAP Nanopowders. Ibid, p.91.
5. L.Grigorjeva, D.Millers, RR.R.Piticescu, T.Strachowski, K.Smits, W.Lojkowski, Claude J.Monty. Cathodoluminescence of Al doped ZnO nanopowders. Ibid, p.92.

**10<sup>th</sup> Europhysical Conference on Defects in Insulating Materials, July 10-14, Milano, Italy.**

1. V.Pankratov, L.Grigorjeva, D.Millers, H.M.Yochum. Intrinsic luminescence and energy transfer process in pure and doped YVO<sub>4</sub> crystals. Book of abstracts, p
2. D.Millers, H.M.Yochum, V.Pankratov, P.Potera, L.Grigorjeva. Transient and near-edge absorption in YVO crystals. Ibid, p. 353.
3. L.Grigorjeva, D.Millers, A.LKalinko, W.Lojkowski, C.J.Monty, J.Grabis. Defect and donor-acceptor luminescence in nanostructured zinc oxide. Ibid, p.139.
4. K.Smits, L.Grigorjeva, D.Millers, J.D.Fidelus, W.Lojkowski. Luminescence of oxygen related defects in zirconia nanocrystals. Ibid, p.149.

**XI International Conference on the Physics of Non-Crystalline Solids (PNCS XI), Oct.29- Nov.2, 2006, Rhodes, Greece.**

1. L. Skuja, K. Kajihara, M.Hirano, A. Saitoh, H.Hosono. A New Type Of Hydrogen-Related E'-Center In Wet Silica Glass. Abstract NoO-EC2, p.86.
2. K. Kajihara, T.Miura, H.Kamioka, M.Uramoto, Y.Morimoto, M.Hirano, L. Skuja, H. Hosono Diffusion And Reactions Of Oxygen Species In Amorphous SiO<sub>2</sub>. Abstract No I-EC-2, p.84.

**Latvian Physics Teachers Conference, Liepāja, Latvia, 10-11 Nov., 2006**

K.Smits. Nanophysics

**Organizing the International Workshop FUN-NANOS (ECO-NET 2006) in Riga, 25February – 1 March.**

**Workshop ECO-NET project “Functional Nanomaterials”, 15-22 October, Romania.**

1. **D.Millers.** ZrO<sub>2</sub>:Eu Nanocrystals Luminescence
2. **L.Grigorjeva** Progress in ZnO Luminescence Studies

# **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 (Bragg grating and related optoelectronic devices).

### **Scientific staff**

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

### **Scientific Visits Abroad**

1. Professor, Dr. hab. Phys. A. Trukhin, Symposium SiO<sub>2</sub> advanced Dielectrics and Related Devices, Palermo, Sicily, Italy, June 2006. the International Conference on the Physics of Non-Crystalline Solids, Rhodes, Greece, 28 October - 3 November 2006
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. N.A. Bendeliani)

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**

Wake Forest University, Winston Salem, North Carolina (Professor, Ph.D. R.T. Williams)

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, (Prof. A. Revcolevchi, Dr. B. Poumellec)

Laboratoire de Physique des Lasers, Université des Sciences et Technologies de Lille, France (Prof. B. Capoen)

## **Italy**

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

## **Estonia**

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

## **The main results**

### **RADIATION PROCESSES IN OXYGEN-DEFICIENT SILICA GLASSES. IF ODC(I) IS A PRECURSOR OF E'-CENTER?**

**Anatoly N. Trukhin**

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

Accumulation of radiation-induced defects under non-destructive x-ray and destructive cathodoexcitation was studied in pure silica KS-4V glasses possessing absorption band at 7.6 eV. The correspondence between existence of this band and creation of the E'-center by radiation was checked. Detection of induced defects was realised by measurements of the luminescence during irradiation, post irradiation afterglow or phosphorescence, induced optical absorption and thermally stimulated luminescence. In all samples these observed phenomena show on charge trapping and recombination on oxygen deficient luminescence center. Others centers luminescence were not significant. In some samples the intensity of 7.6 eV absorption band was deliberately increased by treatment in hydrogen at 1200 C during 100 hours. The intensity of luminescence in hydrogen treated sample was smaller because of known quenching effect of hydrogen on the luminescence of oxygen deficient centers. The optical absorption method does not reveal induced absorption band of E' center in the hydrogen-free samples with different level of oxygen deficiency. Therefore, we did not detect transformation of the defect responsible for the 7.6 eV absorption band or the ODC(I) defect into E' center. In the hydrogen treated sample the absorption of the E' center was detected. The E' centers creation in the hydrogen treated sample was connected with precursors created by treatment ( $\equiv\text{Si-O-H}$  and  $\equiv\text{Si-H}$ ) in the network of glass. The destructive e-beam irradiation reveals rise up with dose of ODC luminescence intensity in the sample with small 7.6 eV band. That means that corresponding luminescence centers are created. Optical absorption measurements in that case detect the E' centers and a broad band at 7.6 eV. A compaction of irradiated volume was detected. Therefore, we came to known conclusion that E' center could be obtained when heavy damage of the glass network takes place or from precursors.

**Acknowledgements** This work was partly supported by the grants 05.1710 of the Latvian Council of Science and was partly supported by Latvian National research programme in Materials sciences.

# ABSORPTION AND LUMINESCENCE IN AMORPHOUS SILICA SYNTHESIZED BY LOW-PRESSURE PLASMACHEMICAL TECHNOLOGY

A.n. Trukhin<sup>1</sup>, K.M. Golant<sup>2</sup>,

<sup>1</sup>*University of Latvia, Solid State Physics Institute, LV-1063, Riga, Latvia*

<sup>2</sup>*Fiber Optics Research Center RAS, 119333, Moscow, Russia*

Amorphous silica was produced by a low-pressure plasmachemical deposition method at temperatures lower than  $T_g$  on a silica substrate tube with the use of hydrogen-free gaseous raw materials. Undoped (nominally pure) and fluorine-doped samples have been fabricated. Parts of substrates tubes with deposited layers have been collapsed by heating with an external burner to form rods, synthesized glass being situated in the cores. Comparison study of as-deposited and remelted silica samples were performed with the aim to recognize whether glass forming processing affected fundamental optical absorption and defects formation.

Raman scattering of laser light, optical absorption in the vacuum ultraviolet region as well as luminescence at different temperatures and different excitations were measured and compared for amorphous and fused silica.

The optical gap both in amorphous and fused silica is situated at 8.2 eV in the fluorine-free samples. The absorption spectrum in this region is exponential and corresponds to the intrinsic absorption threshold coinciding with known threshold of silica glass. The difference between as deposited amorphous and fused silica is in slope and temperature behavior (Urbach rule). For non-melted silica the exponent is slightly sloping than in fused silica and the slope is not changing with the change of the temperature (Urbach rule characteristic for disordered system presents a parallel shift of the spectra with temperature). Contrary for fused silica the slope is changing with the change of the temperature, presenting Urbach rule known for silica previously and exhibiting "crystal-like" behavior. In amorphous fluorine-containing silica the optical gap is situated at 8.1 eV. In the fused fluorine-containing silica the optical gap is situated at 8.25 eV expressing shift to higher energy relatively to position of the intrinsic absorption threshold known for silica doped with fluorine.

Raman spectra for amorphous silica samples both fluorine-containing and fluorine-free are coinciding within experimental errors. This spectrum is very similar to ordinary fused silica glass used for tube substrate. Only intensities in amorphous silica are a bit smaller than in substrate sample.

In the optical transparency range the absorption spectrum of studied silica possesses a band at 7.6 eV. It is on the level of 50-70  $\text{cm}^{-1}$  in the initial amorphous silica and it become smaller in the fused samples and reaches the level of 1-2  $\text{cm}^{-1}$ . It is concluded that ODC(I) defects are created in amorphous silica during plasmachemical deposition process. High level of ODC(I) in amorphous silica is related with deposition process with initial stage is deposition of Si-O molecules. Diminishing of the absorption intensity with fusion is related to decreases of the concentration of corresponding defect. The x-ray excitation of the samples reveals luminescence of the self-trapped exciton in silica glass both for amorphous and fused sample at low temperature (70-80 K).

Analogous situation is with fluorine-containing samples. That shows on existence of continuous network of tetrahedron. Luminescence of oxygen deficient centers modified with presence of chlorine and/or fluorine was detected as well at room temperatures and it existence correlates with existence of optical absorption band at 7.6 eV in as received samples known as ODC(I).

**Acknowledgements** This work was partly supported by the grants 05.1710 of the Latvian Council of Science and was partly supported by Latvian National research programme in Materials sciences.

## RECOMBINATION LUMINESCENCE OF OXYGEN-DEFICIENT CENTERS IN SILICA

A.N. Trukhin<sup>1</sup>, K.M. Golant<sup>2</sup>, Y. Maksimov<sup>3</sup>, M.Kink<sup>3</sup>, R.Kink<sup>3</sup>

<sup>1</sup>*University of Latvia, Solid State Physics Institute, LV-1063, Riga, Latvia*

<sup>2</sup>*Fiber Optics Research Center at the GPI of the Russian Academy of Science, 119991, Moscow, Russia*

<sup>3</sup>*Institute of Physics, University of Tartu, Estonia*

The luminescence of pure dry silica glasses prepared by PCVD and KS-4V methods was studied under ArF laser (193 nm) pulses in the range of temperatures 10-300 K. The PCVD samples were of two kinds: one was 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, at least, stimulates formation of ODCs at 193 nm. The decay kinetics possesses fast and slow components. The slow component of the ODC blue band is faster and that of the UV band is slower than for the case of lone twofold coordinated silicon. This corresponds to the recombination process of luminescence excitation. The model of processes is presented as charge separation under excitation and creation of a nearest self-trapped hole and electron trapped on the twofold-coordinated silicon modified by surrounding.

**Acknowledgements** This work was partly supported by the grants 05.1710 of the Latvian Council of Science and was partly supported by Latvian National research programme in Materials sciences.

### Presentation at conferences

1. A. Trukhin, M. Kink, Y. Maksimov, J.Jansons, R. Kink, Luminescence of GeO<sub>2</sub> rutile-like crystals, comparison with GeO<sub>2</sub> a-quartz-like crystals and GeO<sub>2</sub> glass, 22. CFI LU Zinātniskās konferences referātu tēzes, Rīga, Latvija, 7.-9. Februāris 2006, 5.lpp.
2. A.N. Trukhin, K.M. Golant, Absorption and luminescence in amorphous silica synthesized by low-pressure plasmachemical technology, book of abstracts of 6<sup>th</sup> Symposium SiO<sub>2</sub> advanced Dielectrics and Related Devices, Palermo, Sicily, Italy, June 2006, p.84-85.
3. A.N. Trukhin, K.M. Golant, Y. Maksimov, M.Kink, R.Kink, RECOMBINATION LUMINESCENCE OF OXYGEN-DEFICIENT CENTRES IN SILICA, Book of abstract of the International Conference on the Physics of Non-Crystalline Solids, Rhodes, Greece, 28 October - 3 November 2006, p.276

### Scientific papers published in 2006

1. A.N. Trukhin, Radiation processes in oxygen-deficient silica glasses: is ODC(I) a precursor of E'-center? *Journal of Non-Crystalline Solids*, 352 (2006) 3002-3008
2. Trukhin A.N., Kisand V., Kink R., Kink I., Energy transport in  $\alpha$ -quartz at 10 K. *Физика*, 49, N4 (2006) 155-160.
3. Raphael Blum, Anatolijs Truhins, Bertrand Poumellec and Suling Zhao The use of X-ray-induced and thermostimulated visible and UV luminescence for understanding X-ray poling of silica glasses • *Journal of Luminescence*, 122-123 (2007) 137-141



# PHYSICS OF FERROELECTRICS

**Head of Division Dr. hab. phys. A. Sternberg**

## Research Area

The research issues of the Division of Ferroelectric Physics includes various aspects of theoretical modelling, sample production related material synthesis, processing and characterization of ferroelectrics. Synthesis of ceramics is based on chemical coprecipitation and two stage hot pressing technologies. Production of thin films is made by pulsed laser ablation or sol-gel deposition techniques. Characterization methods include X-ray diffraction, atomic force microscopy and piezo response force microscopy, electron scanning microscopy with EDX option, dielectric spectroscopy and hysteresis measurements, optical studies. Phase transitions and ordering effects in “ordinary” ferroelectrics and ferroelectric relaxors are studied along with new compositions, including doped multicomponent systems and thin film ferroelectric and antiferroelectric heterostructures. A possible applications of ferroelectric materials in electronics, photonics and microelectromechanical systems are considered.

## Main research topics in 2006

### **Lattice Representation of Joint Hamiltonian and Stochastic Dynamics for Field Induced Polarization Switching**

#### **Synthesis of Ferroelectric Ceramics**

- Investigation of Ceramic Compositions Based on Lead Containing Niobates;
- Obtaining of Lead Free Ferroelectric Materials on the Bases of Alkaline Niobates;
- Production of Transparent Electrooptic PLZT Ceramics for Vision Science Applications, Synthesized by Hydroxopolymer, Molten Salts and Sol-Gel Methods.
- Investigation of Surface Microstructure of Ceramics and Thin Films

#### **Dielectric Properties of Perovskite Ferroelectric Relaxor Ceramics and Thin Films**

- Dielectric Impedance Fourier Spectroscopy and Characterization of Functional Materials.

#### **Structural and Optical Properties of Ferroelectric Thin Films**

- Structural and Optical Studies of  $\text{NaNbO}_3$  Thin Films Grown by PLD on  $\text{SrRuO}_3$  Bottom Electrode;
- Structural and Optical Characterization of  $\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$  PLD Deposited Films.

#### **Nanoscale Piezoresponse and Electrostatic Force AFM Imaging**

- Diffraction Grating Lines on Si/PMMA by Electron Lithography

#### **Ferroelectric and Antiferroelectric Thin Films for Future Thermonuclear Reactor Diagnostics Applications**

- Physical Properties of Ferroelectric and Antiferroelectric Thin Films After Electron Irradiation;
- Characterization of active components for use in bolometric radiation diagnostics systems.

#### **Optical Materials for Vision Science**

- Dynamics Of Eye Aberration Detected By High-Speed Hartmann-Shack Aberrometer;

- Application of PLZT and PDLC Passive and Active Optical Elements in Infrared Laser Systems for Bio-Optical Experiments and Medicine.

#### **Scientific staff**

1. Dr. phys. Eriks Birks
2. Dr. phys. emeritus Karlis Bormanis
3. Dr. sc. ing. emeritus Maruta Dambekalne
4. Dr. habil. phys. Vilnis Dimza
5. Dr. phys. Eriks Klotins
6. Dr. habil. phys. Andris Krumins
7. Dr. phys. Maris Kundzins
8. Dr. phys. Anatolijs Mishnovs
9. Dr. habil. phys. Maris Ozolins
10. Dr. habil. phys. Andris Sternberg
11. Dr. phys. Vismants Zauls
12. Dr. habil. phys. Juris Zvirgzds
13. Mg. chem. Maija Antonova
14. Mg. phys. Laila Chakare-Samardzija
15. Mg. chem. Marite Kalnberga
16. Mg. chem. Anna Kalvane
17. Mg. phys. Romans Krutohovostovs
18. Mg. phys. Karlis Kundzins

#### **Technical staff**

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

#### **Doctorants**

1. Mg. phys. Ilze Aulika

#### **Students**

1. Reinis Arajs
2. Andrejs Belijs
3. Marija Dunce
4. Sergejs Fomins
5. Eriks Klotins (junior)
6. Ainars Kuznecovs

#### **Visitors from Abroad**

1. Stud. **Robertas Grigalaitis**, University of Vilnius, (1 month)
2. Dr. phys. **Barbara Garbarz – Glos**, Institute of Physics, Krakow Pedagogical University, Poland (2 weeks);
3. Mg. **Wlodimierz Smiga**, Institute of Physics, Krakow Pedagogical University, Poland (2 weeks);

#### **Scientific Visits Abroad**

##### **Mg. Maija Antonova**

1. The Fourth Internacional Conference on Microwave Materials and their Applications 2006, Oulu, Finland (1 week).

##### **Mg. phys. Ilze Aulika**

1. University of Vienna, Institute of Experimental Physics, Vienna, Austria (1 month);
2. Meeting of MIND project participants, London, England (3 days);
3. Meeting of MIND project participants, Paris, France (3 days);
4. "ICOM2006" conference, Herzeg-Novi, Montenegro (1 week);
5. "E-MRS 2006" conference, Warsaw, Poland (1 week);
6. Seminar of Woollam „Spectroscopic Ellipsometry“, Darmstat, Germany (1 week).

##### **Dr. phys. Karlis Bormanis**

1. The Fourth Internacional Conference on Microwave Materials and their Applications, Oulu, Finland (1 week);
2. Internacional Conference Advanced Optical Materials and Devices (AOMD-5), Vilnius, Lithuania (1 week);
3. Hahn-Meitner-Institute Berlin, Germany (2 weeks);
4. AMPERE Workshop Advanced Materials as Studied by Spectroscopic and Diffraction Techniques, Vilnius, Lithuania (1 week).

Dr. sc. ing. **Maruta Dambekalne**

1. International Conference "Electroceramics", Toledo, Spain (1 week).

Mg. chem. **Anna Kalvane**

1. The Fourth International Conference on Microwave Materials and their Applications, Oulu, Finland, (1 week).

Dr. phys. **Eriks Klotins**

1. Third Annual Meeting COST ACTION P-10 Physics of Risk & Workshop on Complex System Science, Vilnius, Lithuania (3 days);
2. Workshop: PATTERNS, Portoroz, Slovenia (4 days).

Mg. phys. **Karlis Kundzinsh**

1. European Synchrotron Research Facility, ESRF Grenoble, France(1 week).

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

1. ICO Topical Meeting on Optoinformatics/Information Photonics - 2006, ITMO, St.Peterburg, Russia (1 week);
2. Annual Meeting of Applied Vision Association – 2006 "Vision in Perception and Cognition", Bradford University (1 week);
3. Annual Meeting of European Optical Society, Paris, France (1 week).

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

1. 100<sup>th</sup> Anniversary of Electro Ceramic Process Symposium, Tokyo, Japan (1 week);
2. The 8th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity RCBJSF-8, Tsukuba, Japan (1 week);
3. 32<sup>nd</sup> International Conference Micro- and Nano-Engineering 2006, Barcelona, Spain (1 week).

Dr. phys. **Vismants Zauls**

1. European Synchrotron Research Facility, ESRF Grenoble, France (1 week).
2. Piezoceramics for end-users II. POLECER International Conference, Hafjell, Lillehammer, Norway, (1 week).
3. Max-Plank Institute of Plasma Physics, Garching, Germany (3 days).

## Cooperation

### Latvia

1. Daugavpils University (Dr. habil. phys. G. Liberts).
2. Riga Technical University, Faculty of Material Science and Applied Chemistry (Prof. M. Knite, Prof. A. Ozols, Dr. R. Cimdins).
3. University of Latvia, Institute of Chemical Physics (Dr. D. Erts).
4. Riga Technical University, Institute of Inorganic Chemistry (Prof. J. Grabis)

### Austria

1. Atomic Institute of Austrian Universities, Technical University Vienna (Prof. H.W. Weber).
2. Institute for Experimental Physics, University Vienna (Prof. A. Fuith).

### Belorussia

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

**Czech Republic**

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

**Denmark**

1. Ferroperm, Ltd., Kvistgard (W. Wolny).

**Estonia**

1. Institute of Physics, University of Tartu (Dr. R. Jaaniso, Dr. V. Sammelselg).

**Finland**

1. University of Oulu (Dr. J. Levoska).
2. Colour Research Laboratory, University of Joensuu (Prof. J. Parkkinen).

**France**

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

**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. Grigas, Prof. J. Banys).

**Norway**

1. Kongsberg Optometric Institute, Buskerud Highschool (Prof. J.R. Bruenich, Dr. K.I. Daae).

**Poland**

1. Institute of Physics, Krakow Pedagogical University, Krakow (Prof. Cz. Kus, Dr. B. Garbarz – Glos, Dr. W. Smiga, Dr.hab. J. Suchanicz).
2. Institute of Physics, University of Silesia, Sosnowiec (Prof. Z. Surowiak, Mg. M. Plonska).

**Portugal**

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

**Russia**

1. Ural State University, Ekaterinburg (Prof. V. Shur).
2. Volgograd State Architectural and Engineering 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).

**Slovenia**

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

## Spain

1. Laboratory of Optics, University of Murcia (Prof. H.M. Bueno, Prof. P. Artal)
2. CIEMAT, Madrid (Dr. E. Hodgson).

## MAIN RESULTS

### LATTICE REPRESENTATION OF JOINT HAMILTONIAN AND STOCHASTIC DYNAMICS FOR FIELD INDUCED POLARIZATION SWITCHING

**Eriks Klotins**

Essential properties of advanced functional materials are determined by intrinsic mesoscopic scale structures, the ferroelectric domains, undergoing birth, growth and field controlled switching which dominate in numerous applications. The kernel of this phenomenon is ergodicity breaking formally explained by conventional thermodynamic theory. Unresolved questions that naturally emerge are what determine the temporal behavior of material and whether it's intrinsic structure can be favored by some physical principles. The answer requires solution of statistical problem of joint regular (Hamiltonian) and stochastic dynamics.

Developments reported here are focused on the kinetics of domains on the grounds of the model Hamiltonian and the impact of bosonic environment formulated in lattice representation, namely, each site of a cubic lattice is assigned to overdamped anharmonic oscillator obeying Landau-type dynamics affected by noise and by the interaction with first neighbor. In spite of simplicity and canonical axiomatic level, the lattice representation displays essential features of polarization response as well as the impact of electric and elastic boundary conditions associated with model Hamiltonians of arbitrary complexity. The mathematical technique includes Fokker-Planck and imaginary time Schrödinger equations as well as selfconsistent solution of this problem found by symplectic integration.

New results concern (i) field induced polarization switching and (ii) nucleation and sideways growth of domains in uniaxial lattice models.

### OBTAINING OF LEAD FREE FERROELECTRIC MATERIALS ON THE BASES OF ALKALINE NIOBATES

**M. Dambekalne, A. Kalvane, M. Antonova, M. Livins, K. Bormanis, A. Mishnov, and M. Kalnberga**

The  $ABO_3$ -type compounds with perovskite structure are one of the most interesting groups of materials. Among them the niobates are of great interest from the point of view of fundamental research as well as regarding their possible applications. Alkaline niobates such as  $NaNbO_3$  and  $LiNbO_3$  are considered to be a promising class of lead free piezoelectric materials representing an environment- friendly alternative for a wide range of practical applications. The sodium niobate is the best known of all niobates which is an antiferroelectric with very attractive dielectric and semi-conducting properties. The system  $NaNbO_3$ - $LiNbO_3$  becomes especially interesting when Li-content in solid solution increases. These materials would be good candidates for the fabrication of piezoelectric and pyroelectric elements working in high temperature. A great attention is focused on crystalline- and ceramic  $NaNbO_3$  as well as  $NaNbO_3$ -based solid solutions, which are the most useful materials for many applications. Particularly crystalline and

polycrystalline  $\text{Na}_{1-x}\text{Li}_x\text{NbO}_3$  have been extensively investigated. X-ray diffraction, structure, electrical properties, thermal expansion and high-temperature calorimetry of  $\text{Na}_{1-x}\text{Li}_x\text{NbO}_3$  with low Li-ion concentrations ( $x \leq 0.12$ ) have been investigated.

## STRUCTURAL AND OPTICAL STUDIES OF $\text{NaNbO}_3$ THIN FILMS GROWN BY PLD ON $\text{SrRuO}_3$ BOTTOM ELECTRODE

I. Aulika, J. Petzelt<sup>1</sup>, A. Deyneka<sup>1</sup>, J. Pokorny<sup>1</sup>, V. Zauls, and K. Kundzins

<sup>1</sup>Institute of Physics, Academy of Sciences of the Czech Republic

$\text{NaNbO}_3$  (NN) thin films with a flat surface morphology (Fig. 1) and good crystallinity were deposited by PLD on substrates of Pt/SRO and Si/SRO. The structural and optical properties of the films were analyzed using X-ray diffraction analysis, Raman spectroscopy, AFM, and spectroscopic ellipsometry.

Almost all phonon modes were detected simultaneously in Raman spectrum (Fig. 2) due to the random distribution of

the crystallographic axes in the granular samples for NN films. The mode Raman shifts  $\omega$  at  $\sim 240$  and  $620 \text{ cm}^{-1}$  of NN deposited on Pt/SRO lay at lower values of  $\omega$  in comparison with those of NN on Si/SRO. Detected reduced value of the dielectric permittivity and enlarged value of the loss factor for Pt/SRO/NN film,

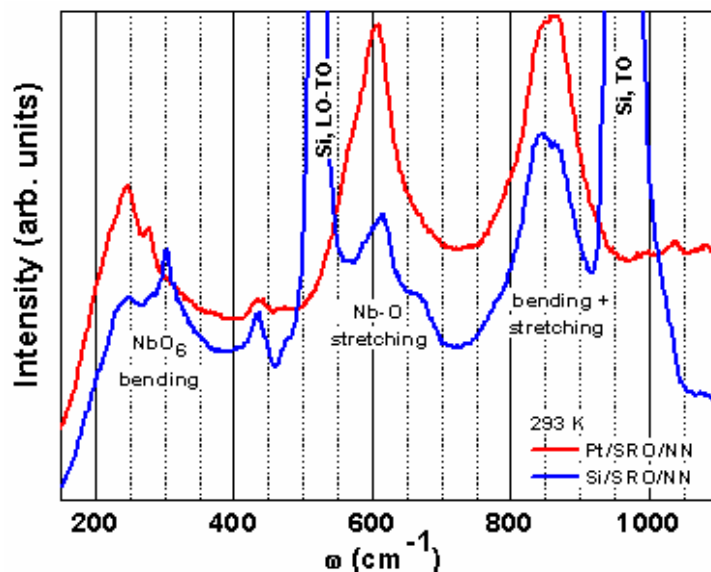


Fig. 2. Room temperature Raman spectra of NN deposited on Pt/SRO and Si/SRO substrates.

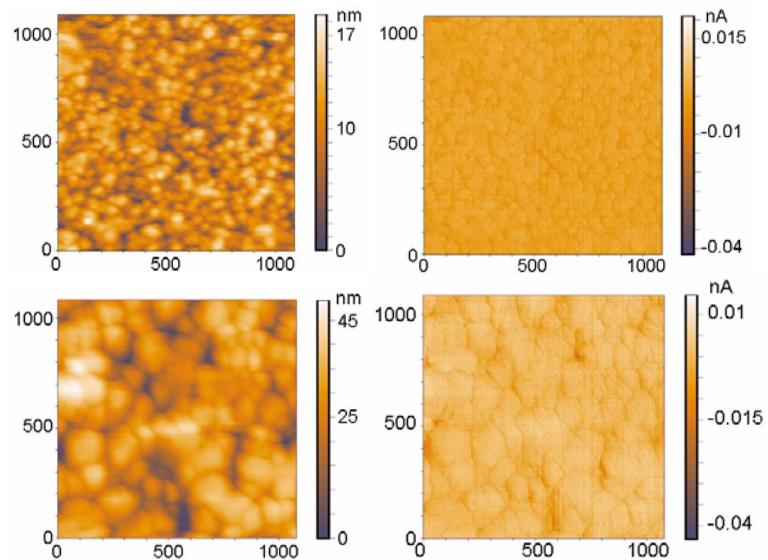


Fig. 1. Surface topography (left) and lateral force images (right) with scanned area  $(1 \times 1) \mu\text{m}^2$  for NN on a) Pt/SRO, and b) Si/SRO. The RMS roughness for the given images is 3 and 8 nm.

phonon modes frequencies for NN thin films in comparison with ceramics as well as lower optical properties of the second phase might be due to the size-induced phase transformation and/or grain boundary effects. Applying a multilayer model, where film was considered to consist from host material and voids (grain boundary effect), to the experimental data, the good numerical fit to experimental data was

found. Refractive index of Pt/SRO/NN samples is in a good agreement with those detected for single crystals.

This work was supported by subtask of collaboration Program of fundamental and applied research No. **05.0026.1.**, Latvian Council of Science.

## **STRUCTURAL AND OPTICAL CHARACTERIZATION OF Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub> PLD DEPOSITED FILMS**

**I. Aulika, J. Petzelt<sup>1</sup>, J. Pokorny<sup>1</sup>, V. Zauls, K. Kundzins, and M. Rutkis**  
*<sup>1</sup>Institute of Physics, Academy of Sciences of the Czech Republic*

The Raman scattering and optical properties of amorphous and polycrystalline Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub> (BST) thin films coated on Pt, Si, and Si/SRO substrates by PLD technique have been investigated by the Raman spectrometer and spectroscopic reflectometry. Almost all phonon modes were revealed for polycrystalline BST thin films coated on Pt and Si, but just two modes for amorphous BST on Si/SRO. The symmetry-forbidden first order Raman scattering was observed for all films above the phase transition temperature. The A<sub>1</sub>(TO) and B<sub>1</sub>+E mode in the films has significantly larger frequency compared to the bulk. This can be explained by the presence of the polar grain boundaries and/or polar nanoregions and/or misfit dislocations, which generates accommodation of the strains at the film/substrate interface.

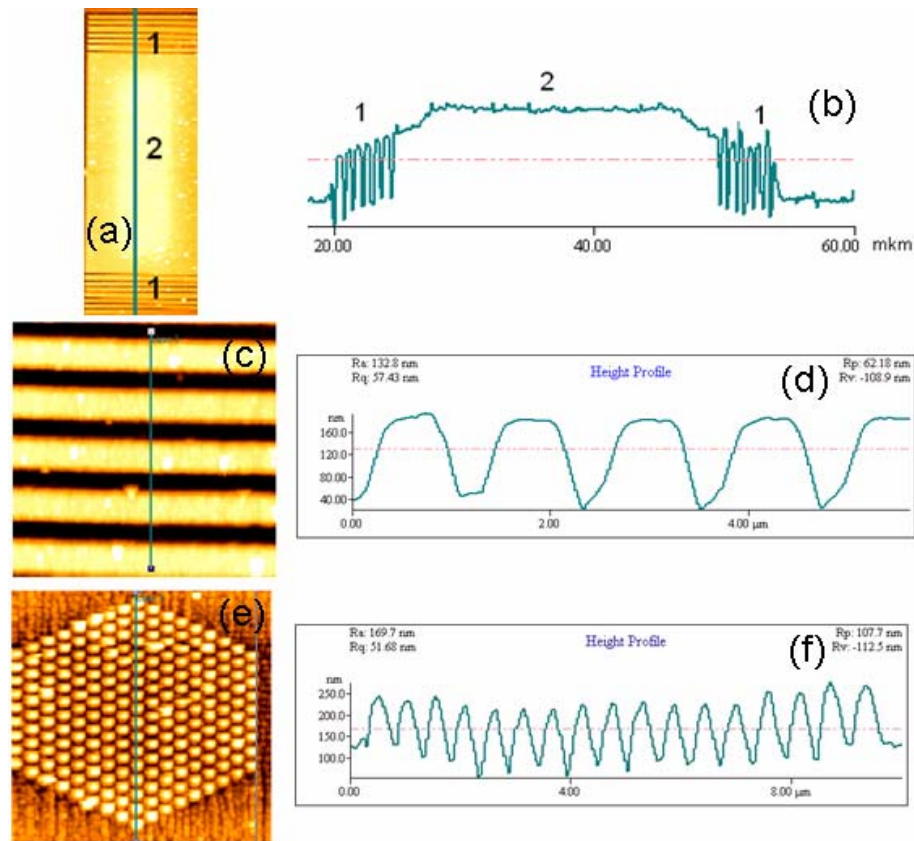
The refractive  $n$  and extinction  $k$  coefficients were obtained by means of fitting of the multilayer model to the reflection coefficient. The refractive index for BST on Si/SRO, Si and Pt is 1.77, 2.16 and 2.03 at 633 nm, respectively. Amorphous films have lower  $n$ , higher band gap energy and more pronounced dispersion of  $n$  than polycrystalline films. The  $n$  value of BST films is lower than those of ceramics. Such difference in optical properties can be due to the strain induced changes in the BST films and lower density of the amorphous structure.

This work was supported by subtask of collaboration Program of fundamental and applied research No. **05.0026.1.**, Latvian Council of Science.

## **DIFFRACTION GRATING LINES ON Si/PMMA BY ELECTRON LITHOGRAPHY**

**R. Krutovostovs, K. Kundzins, I. Aulika, and V. Zauls**

The periodic diffracting grating lines and symmetric hexagons were written in the resistive polymethylmetacrylate (PMMA) thin film using electron beam lithography method together with scanning electron microscope (SEM) EVO 50 XVP. PMMA resist was deposited on Si substrate by spin-coating method. The width and height of diffracting lines and distance between them (Fig. 1.) were detected by atomic force microscope (AFM) and found to be ~ 800, 160 and 400 nm, respectively. The diffracting lines provide the light input and output in the planar wave guide, reflecting from diffracting grating. The width and height of hexagons and distance between them (Fig. 1.) were detected to be ~ 400, 200 and 200 nm, respectively. The optical measurements of PMMA thin-film were performed with a miniature “Ocean Optics” CCD spectrometer, model HR 4000, with fiber optics input under normal incidence angle of the light. Reflective coefficient was detected in the spectral range 250 – 1060 nm (1.17 – 4.95 eV) at room temperature. The thickness of PMMA film was found to 540 nm.



**Fig. 1.** AFM image of diffraction grating lines and fiber (a) written in PMMA by electron lithography method: 1- diffraction grating lines, and 2 – fiber; cross-section (solid green line in (a)) of the sample surface (b) with pronounced diffraction grating lines and fiber; AFM image of diffraction grating lines (c) and its surface cross-section (d); AFM image of hexagons (e) also written in PMMA by electron lithography method and its surface cross-section (f).

## FERROELECTRIC THIN FILMS FOR FUTURE THERMONUCLEAR REACTOR DIAGNOSTICS APPLICATIONS

**V. Zauls, K. Kundzins, I. Aulika, M. Kundzins, and A. Sternberg**

Systematic research and characterization is carried out to develop active components for use in bolometric radiation diagnostics systems of future nuclear fusion reactors based on ferroelectric and antiferroelectric materials. Under modulated thermal irradiation bolometric sensitivity with the range of few milli-Kelvin temperature resolution at 0,2 s time response constant has been demonstrated by thin ferroelectric film capacitive sensor model on thick substrate. Prototype sample measurement system has been developed to be compatible with Wheatstone bridge type bolometric heads measurement concept of *ASDEX* or *Tore Supra* reactor sites for future tests.



## DYNAMICS OF EYE ABERRATION DETECTED BY HIGH-SPEED HARTMANN-SHACK ABERROMETER

Maris Ozolinsh, and Gatis Ikaunieks<sup>1</sup>

<sup>1</sup>*Dept. of Optometry and Vision science, University of Latvia, Latvia*

Significance of eye aberration measurements accuracy increases in the recent decade due to advances in laser refractive eye surgery. Equipment for spatially resolved corneal ablation performed by excimer laser oft includes aberrometer for presurgical corneal refraction mapping. The most used for such purposes Hartmann-Shack waveform sensors are convenient in use and can measure up to the 4<sup>th</sup>-order aberrations. We have studied dynamics of eye aberration within time period including eye blinking and tearfilm breakup events. Results show a sharp increase in wavefront distortion RMS during and after blinking events. Mostly blinking coincides with instinctive eye decentration and an increase of the tilt Zernike. Decentration can cause elimination of some of Hartmann-Shack images from the processing of Zernike terms thus creating alterations in all orders of aberrations. However higher order aberrations (up to the 4th order) show peaks also for events with small eye tilts, obviously caused by the tear film impact on the eye optical quality. Wavefront aberration errors should not be extracted from one single – but „good” measurement representing only one data set of a dynamically changing aberration pattern. That is a matter of great concern for planning of the laser refractive eye surgery. The simulation of the point spread function PSF vs. time using the Zernike term time dependencies before and after eye blinking (compensating defocus and astigmatism) presented in a movie available at: [www.cfi.lu.lv/fer/maris/ocs2005/psf\\_ocs.avi](http://www.cfi.lu.lv/fer/maris/ocs2005/psf_ocs.avi).

### Published in 2006

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2. K. Bormanis, S.A. Satarov, A. Kalvane, A.I. Burkhanov, A.V. Shil'nikov, and M. Dambekalne. Low and Infra-Low Frequency Measurements in Lead Titanate Solid Solutions. *Solid State Phenomena*, Vol. 115, *Mechanical Spectroscopy III (Mechanical Spectroscopy and Relaxation Phenomena in Solids)*, 2006, pp. 229-232.
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5. J.M. Bueno, E. Berrio, M. Ozolinsh, and G. Ikaunieks. Optical Properties of a Polymer Dispersed Liquid Crystal to be Used on Visual Testing. In: *Proc. „ICO Topical Meeting on Optoinformatics / Photonics and Informatics 2006”*, ITMO, St.Petersburg, 2006, pp. 276-278.

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### LECTURES ON CONFERENCES (WITH ABSTRACTS)

#### **100<sup>th</sup> Anniversary of Electro Ceramic Process Symposium. Tokyo, Japan, January 28, 2006.**

1. A. Sternberg. Local Induced Polarization in Modified Ferroelectric Ceramics and Thin Films. Abstracts and Proceedings, 6 pages.

#### **Piezoceramics for end-users II. POLECER International Conference.**

##### **Hafjell, Lillehammer, Norway, March 5-8, 2006.**

1. K. Bormanis, M. Dambekalne, A. Sternberg, M. Antonova, A. Kalvane, N.M. Olekhovich, and J.V. Radjush. High Pressure Production and Properties of PZN Ceramics. Oral and Poster Presentation Abstracts, p. 68.
2. K. Bormanis, A. Sternberg, A.I. Burkhanov, M. Dambekalne, A. Kalvane, and M. Antonova. Dielectric Properties of Layered Perovskite Ceramics. Oral and Poster Presentation Abstracts, p. 69.
3. R. Grigalaitis, J. Banys, A. Brilingas, A. Mikonis, K. Bormanis, A. Sternberg, and V. Zauls. Dielectric spectroscopy and distribution of relaxation times of PMN-PSN ceramics. Oral and Poster Presentation Abstracts, p. 74.
4. S. Kamba, D. Noujni, S. Denisov, A. Sternberg, and J. Petzelt. PMN with Perovskite and Pyrochlore Structure: Comparison of Dielectric Properties. Oral and Poster Presentation Abstracts, p. 71.

#### **2nd Latvian conference „Functional materials and nanotechnologies”, Riga, March 27-28, 2006.**

1. I. Aulika, J. Levoska, M. Tyunina, K. Kundzins, and V. Zauls. Direct Atomic Force Microscopy Analysis of Surface Nanoscale Roughness Effects on Optical Properties of PMN Thin Ferroelectric Film Multilayers. Abstracts, p. 6.
2. M. Dambekalne, M. Antonova, M. Livinsh, M. Kalnberga, A. Kalvane, and K. Bormanis. Ceramics of Lead Containing Heterovalent Niobates – Synthesis, Sintering and Microstructure. Abstracts, p. 16.
3. R. Grigalaitis, J. Banys, A. Brilingas, A. Sternberg, V. Zauls, and K. Bormanis. Polar Nano Regions in Ferroelectric Relaxors. Abstracts, p. 21.
4. E. Klotins Jr. Critical Dynamics in Nanoscale: Copmputing Solutions. Abstracts, p. 30.
5. E. Klotins, and M.Springis. Critical Dynamics in Nanoscale. Abstracts, p. 31.
6. M. Knite, A. Hill, V. Bovtun, V. Teteris, A. Solovjovs, V. Tupureina, G. Shakale, J. Zavickis, I. Aulika, B. Polakovs, S.J. Pas, S. Veljko, I. Klemenoks, J. Zicans,

- D. Erts, J. Petzelt, and A. Fuith. Polymer-Nanostructured Carbon Composite as Multifunctional Sensor Materials – Design, Processing and Properties. Abstracts, p. 32.
7. A. Krumins. Nanomaterials in the New Physics Curriculum at University of Latvia. Abstracts, p. 35.
  8. R. Krutohvastovs, K. Kundzins, and I. Shorubalko. Electron Beam Direct Writing of 2D Structures for Optical Devices. Abstracts, p. 36.
  9. A. Kuznetsov, and A. Bely. Critical Dynamics in Nanoscale: Toward the Inverse Problem of Ferroelectric Hysteresis. Abstracts, p.40.
  10. A. Mishnevs, and E. Ivanovskis. X-ray Line Profile Analysis of Nanostructured Oxytocin. Abstracts, p. 48.
  11. M. Ozolinsh, and G. Ikaunieks. Dynamics of Eye Aberration Detected by High-Speed Hartmann-Shack Aberrometer. Abstracts, p. 54.
  12. A. Pastare, I. Pastare, K. Didrikšone, K. Kundzinsh, J. Svirks, A. Viksna, and D. Erts. Formation of Nanoporous Anodized Aluminium Oxide and Pore Filling. Abstracts, p. 56.
  13. B. Polyakov, J. Prikulis, L. Grigorjeva, D. Millers, V. Zauls, J. Holms, and D. Erts. High Density Arrays of Germanium Nanowire Photoresistors. Abstracts, p. 58.
  14. M. Rutkis, and V. Zauls. Determination of Second Ordered Non-linear Coefficients – Straight Forward Measurement or Complex Optical Investigation? Abstracts, p. 63.
  15. A. Sternberg, and I. Muzikante. National Research Programme of Latvia in Materials Sciences. Abstracts, p. 70.
  16. N. Zaporina, V.N. Timofeev, D. Bocharov, R. Krutohvastov, and J. Grabis. Studies of Multicomponent Nanodisperse Powders by Electron Microscopy's Methods. Abstracts, p. 81.

**LU Cietvielu fizikas institūta 22. Zinātniskā konference. Rīga, 2006.gada 29.-30. marts. 22<sup>nd</sup> Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, March 29.-30., 2006.**

1. I. Aulika, J. Levoska, M. Tyunina, K. Kundziņš, V. Zauls. Uz MgO/LSCO pamatnes lāzeruzputinātu svina magnija niobāta plāno kārtiņu optisko īpašību pētījumi. Optical Properties of PMN Thin Films Deposited by PLD on MgO/LSCO Substrates. Referātu tēzes, 20. lpp.
2. K. Kundzins, V. Zauls, A. Kuzmins, D. Pailharey, F. Jandard. Elektrostatisko pievirsma spēku detektēšanas metode atomspēka mikroskopa pielietojumiem intensīva sinhrotrona starojuma iedarbības apstākļos. Development AFM Electrostatic Force Probe for Use in High Intensity Synchrotron Irradiation Environment. Referātu tēzes, 23. lpp.
3. M. Duce, R. Krutohvastov, K. Kundzins, I. Shorubalko. Skanējošās elektronu mikroskopijas un rentgenstaru enerģijas dispersās Analīzes pielietojumi funkcionālo materiālu pētījumiem. Studies of Functional Materials by SEM and EDX Techniques. Referātu tēzes, 24. lpp.
4. F. Muktepāvela, R. Krutohvastovs, A. Šiško, K. Kravalis, E. Platacis. EUROFER 97 tērauda struktūra un mehāniskās īpašības pēc izturēšanas plūstošā Pb-17Li sakausējumā. Structure and Mechanical Properties of EUROFER 97 Steel Exposed to Flowing Pb-17Li. Referātu tēzes, 32. lpp.
5. V. Zauls, K. Kundzins, I. Aulika, M. Kundziņš, A. Šternbergs. Segnetoelektriskās kārtiņas kodolsintēzes reaktoru diagnostikas pielietojumiem. Ferroelectric Thin Films for Future Thermonuclear Reactor Diagnostics Applications. Referātu tēzes, 35. lpp.

**Annual Meeting of Applied Vision Association – 2006 “Vision in Perception and Cognition”, Bradford University, England, April, 2006.**

1. Maris Ozolinsh, Gatis Ikaunieks, Sergejs Fomins, Michèle Colomb, and Jussi Parkkinen. Perception of Colour Contrast Stimuli in the Presence of Scattering. Abstracts, p. 5.

**Third Annual Meeting COST ACTION P-10 Physics of Risk & Workshop on Complex System Science, Vilnius, Lithuania, May 13 – 16, 2006.**

1. E. Klotins. Critical Dynamics in Nanoscale. Program & Abstracts, p. 58.

**The 8th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity RCBJSF-8. Tsukuba, Japan, May 15-19, 2006.**

1. Andris Sternberg, Vismants Zauls, Karlis Kundzins, Maija Antonova, and Maruta Dambekalne. Local Induced Polarization in Modified Ferroelectric Ceramics and Thin Films. Abstract book, p. 21.
2. Juras Banys, Robertas Grigalaitis, Algirdas Brilingas, Andris Sternberg, Vismants Zauls, and Karlis Bormanis. Anomalous Broad Distribution of Relaxation Times in Mixed PMN-PSN Ceramics. Abstract book, p. 39.
3. Dmitry Pelegov, Vladimir Shur, Genady Lomakin, Oksana Yakutova, Ekaterina Nikolaeva, Ivan Baturin, Evgenii Rumyantsev, Vera Shikhova, and Andris Sternberg. Kinetics and Statics of Nanoscale Domain Structures in Relaxors: PLZT Ceramics and SBN Single Crystals. Abstract book, p. 70.

**The Fourth International Conference on Microwave Materials and Their Applications „MMA – 2006”. Oulu, Finland, June 12-15, 2006.**

1. Maruta Dambekalne, Maija Antonova, Maris Livinsh, Marite Kalnberga, Anna Kalvane, Andris Sternberg, and Karlis Bormanis. Technological Aspects of Producing Ceramics of  $\text{PbB}'_{1/2}\text{Nb}_{1/2}\text{O}_3$  Antiferroelectrics and Binary Solid Solutions with  $\text{PbSc}_{1/2}\text{Nb}_{1/2}\text{O}_3$ . Abstract book, p. 134.
2. Maruta Dambekalne, Maija Antonova, Maris Livinsh, Karlis Bormanis, Marite Kalnberga, Anna Kalvane, and Andris Sternberg. Studies of  $\text{PbB}'_{1/2}\text{Nb}_{1/2}\text{O}_3$  Antiferroelectrics and Binary Solid Solutions with  $\text{PbSc}_{1/2}\text{Nb}_{1/2}\text{O}_3$ . Abstract book, p. 136.
3. K. Bormanis, A.I. Burkhanov, M. Dambekalne, A.V. Alpatov, and A. Kalvane. Peculiarities of Dielectric Response of Ferroelectric Solid Solutions  $(\text{Pb},\text{Sr},\text{Bi})\text{TiO}_3$ . Abstract book, p. 163.

**ELECTROCERAMICS X. Toledo, Spain, June 18-22, 2006**

1. M. Dambekalne, K. Bormanis, M. Antonova, M. Livinsh, M. Kalnberga, and A. Sternberg. Antiferroelectric  $\text{Pb}(\text{B}^{+3}, \text{B}^{+5})\text{O}_3$  and Solid Solutions on Their Bases. Abstracts, CD-version, PDF file, DFPP-P-10.
2. K. Bormanis, A.I. Burkhanov, M. Dambekalne, M. Antonova, A. Sternberg, and A. Kalvane. Dielectric Response of Layered Bi Containing Ceramics. Abstracts, CD-version, PDF file, DFPP-P-12.
3. K. Bormanis, J.V. Radjush, A.I. Burkhanov, M. Dambekalne, A. Sternberg, M. Antonova, A. Kalvane, M. Livinsh, and N.M. Olekhovich. Production and Properties of PZN Ceramics with Perovskite Structure. Abstracts, CD-version, PDF file, DFPP-P-11.
4. D. Kiselev, V. Shvartsman, I. Bdikin, A. Sternberg, K. Bormanis, and A. Kholkin. Local Ferroelectric Properties and Domain Structure in Lead-Based Relaxor Ceramics. Abstracts, CD-version, PDF file, CH-P-06.

5. J. Banys, J. Macutkevic, S. Kamba, A. Pashkin, K. Bormanis, A. Sternberg, and J. Petzelt. Far-Infrared and THz Spectroscopy of PMN-PSN-PZN Relaxors Ferroelectrics. Abstracts, CD-version, PDF file, CH-P-15.
6. R. Grigalaitis, J. Banys, A. Brilingas, A. Sternberg, K. Bormanis, and V. Zauls. Broadband Dielectric Spectroscopy of PSN Ceramics. Abstracts, CD-version, PDF file, COST-O-40.
7. B. Malic, L. Cakare-Samardzija, and M. Kosec. Lead-Free Thin Films Based on Tantalates Prepared by Chemical Solution Deposition. Abstracts, CD-version, PDF file, TTF-P-29.

**Vision in Vehicles, VIV-11, Dublin, Ireland, July 27-29, 2006.**

1. M. Ozolinsh, M. Colomb, J. Parkkinen, G. Ikaunieks, S. Fomins, V. Karitans, and G. Krumina. Different Colour Contrast Stimuli Perception in Fog. Proceedings, VIV-11, p. 12.

**5<sup>th</sup> International Conference Advanced Optical Materials and Devices. Vilnius, Lithuania, August 27-30, 2006.**

1. K. Bormanis, M. Dambekalne, M. Antonova, A. Kalvane, N.M. Olekhnovich, J.V. Radjush, and A. Sternberg. Role of Nanoparticles in High Pressure Production of Ferroelectric Ceramics. Program and Abstracts, p. 68.

**ICOM 2006 conference, Herceg Novi, Montenegro, August 31 – September 2, 2006.**

1. I. Aulika, V. Zauls, K. Kundzins, M. Rutkis, J. Pokorny, and J. Petzelt. Structural and Optical Characterization of  $Ba_{0.8}Sr_{0.2}TiO_3$  Films Deposited by PLD on Various Substrates Using Micro-Raman and Spectral Reflectometry Methods. Abstracts, p. 105.

**Workshop: PATTERNS, Portoroz, Slovenia, September 3-6, 2006.**

1. E. Klotins, and A. Kuznetsov. Critical Dynamics on Quantum – Microscopic Boundary. Program & Abstracts, p. 78.

**E-MRS 2006 conference. Warsaw, Poland, September 4– 8, 2006.**

1. I. Aulika, A. Deyneka, V. Zauls, K. Kundzins, J. Pokorny, and J. Petzelt. Characterization of Structural and Optical Properties of Nanopatterned Polar Thin Films. Abstracts p. 38.

**The Fifth International Seminar on Ferroelastic Physics. Voronezh, Russia, September 10-13, 2006.**

1. А.И. Бурханов, В.Н. Нестеров, Ю.В. Кочергин, К. Борманис, А. Калване, М. Дамбекальне. Особенности низко- и инфранизкочастотного диэлектрического отклика слоистых сегнетоэлектриков. Abstract Book, p. 75.
2. А.В. Алпатов, А.И. Бурханов, К. Борманис, А. Калване, А. Штернберг. Диэлектрические свойства сегнетоэлектрической керамики на основе ЦТС в области морфотропного фазового перехода. Abstract Book, p. 80.
3. А.И. Бурханов, П.В. Бондаренко, К. Борманис, А. Калване, М. Дамбекальне, М. Антонова. Диэлектрический отклик в области сегнето- и антисегнетоэлектрических фазовых переходов в керамике  $(Pb,La)(Zr,Sn,Ti)O_3$ . Abstract Book, p. 93.
4. П.В. Бондаренко, А.И. Бурханов, К. Борманис, А. Калване, М. Дамбекальне, М. Антонова. Влияние смещающих полей на характер диэлектрического отклика в области фазовых переходов керамики  $(Pb,La)(Zr,Sn,Ti)O_3$ . Abstract Book, p. 103.

5. M. Dambekalne, M. Antonova, K. Bormanis, M. Livins, M. Kalnberga, and A. Kalvane. Antiferroelectrics of Lead Containing Rare-Earth Niobates and Solid Solutions on Their Bases. Abstract Book, p. 105.

**Specialized Colloque AMPERE and AvH-Workshop: Advanced Materials as Studied by Spectroscopic and Diffraction Techniques. Vilnius, Lithuania, September 16 - 21, 2006.**

1. A. Katelnikovas, L. Vilciauskas, L. Grigorjeva, D. Millers, V. Pankratov, A. Sternberg, and A. Kareiva. Sol-Gel Chemistry Approach to the Preparation of Nanocrystalline  $\text{CaWO}_4$ . Programme and Abstracts, P14.
2. R. Grigalaitis, J. Banys, A. Brilingas, K. Bormanis, A. Sternberg, and V. Zauls. Dielectric Properties and Distribution of Relaxation Times of Mixed PMN-PSN Ceramics. Programme and Abstracts, P29.
3. K. Bormanis, A.I. Burkhanov, V.N. Nesterov, A. Kalvane, M. Dambekalne, M. Antonova, M. Livinsh, M. Kalnberga, and A. Sternberg. Low and Infra-Low Frequency Dielectric Spectroscopy of Layered Perovskite Ceramics. Programme and Abstracts, P33.

**Baltic Polymer Symposium 2006. Birini Castle, Latvia, September 20-22, 2006.**

1. A. Sternberg, and I. Muzikante. Selected Aspects of Latvian National Research Program in Materials Science. Programme and Proceedings, p. 58.

**ICO Topical Meeting on Optoinformatics/Information Photonics 2006. ITMO, St.Peterburg, Russia, September 2006.**

1. V. Karitans, and M. Ozolinsh. Dynamical Visual Acuity in the Presence of Light Scattering. Proceedings, ITMO, St.Petersburg, pp. 269-270.
2. J.M. Bueno, E. Berrio, M. Ozolinsh, and G. Ikaunieks. Optical Properties of a Polymer Dispersed Liquid Crystal to be Used on Visual Testing. Proceedings, ITMO, St.Petersburg, pp. 276-278.

**Annual Meeting of European Optical Society, Paris, October, 2006.**

1. M. Ozolinsh, G. Ikaunieks, and S. Fomins. Dynamics of Eye Aberration Detected by High-Speed Hartmann-Shack Aberrometer. Proceedings, pp. 92-93.

**Международная научно-техническая конференция «Фундаментальные проблемы радиоэлектронного приборостроения». International Scientific and Technical Conference «Fundamental Problems of Radioengineering and Device Construction» (INTERMATIC – 2006). Москва, Россия, 24-28 октября 2006 г.**

1. П.В. Бондаренко, А.И. Бурханов, К. Борманис, А. Калване, М. Дамбекальне, М. Антонова. Процессы переключения поляризации в области сегнето- и антисегнетоэлектрических фазовых переходов в керамике  $(\text{Pb},\text{La})(\text{Zr},\text{Sn},\text{Ti})\text{O}_3$ . Материалы конференции, Москва: МИРЭА, 2006, часть 1., с. 60-63.

**Международная научно-техническая школа-конференция «Молодые ученые - науке, технологиям и профессиональному образованию в электронике» (МОЛОДЫЕ УЧЕНЫЕ - 2006). International Joint School and Conference «Young Scientists in Electronics: Science, Technology and Education» (YOUNG SCIENTISTS - 2006). Москва, Россия, 5 - 9 декабря 2006 г.,**

1. Ю.В. Кочергин, А.И. Бурханов, В.Н. Нестеров, К. Борманис, А. Калване, М. Дамбекальне. Исследование релаксации поляризации слоистых сегнетоэлектриков. Материалы конференции, Москва: МИРЭА, 2006, часть 2., с. 237-240.



# SEMICONDUCTOR MATERIALS AND SOLID STATE IONICS

Head of Division *Dr.phys. A.Lusis*

## Research Area and Main Problems

### Research areas

- 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, etc.);
- Material preparation methods: thin and thick film technologies, sol-gel process;
- Material characterization by spectroscopic methods (Raman scattering, optical and X-ray absorption, electrical and electrochemical impedance, ESR, etc);
- Solid state ionics:
  - electro-, photo-, chemo- or gaso-chromic phenomena,
  - 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 new nano structured materials for hydrogen storage;
- New measurement technologies and instruments with artificial intelligence;
- Miniaturisation of solid state ionic devices;
- Application specific semiconductor materials and solid-state ionic devices in micro systems for electronic nose.

### Research problems and tasks

1. Stability of materials for electrochemical multi layer systems and electrochromic coatings.
2. Improvements in x-ray absorption spectroscopy methodology and local structural anomalies in the mixed transition metal oxide compounds.
3. Intergrain activity of solid electrolyte layers based on polymer composites.
4. Ion ( $H^+$ ,  $OH^-$ ,  $Li^+$ ) insertion (extraction) in solid electrolytes and electrodes.
5. Components for fuel cells;
6. Hydrogen absorption in composite materials: catalytic activation of molecular hydrogen adsorption and spill-over of hydrogen atoms onto solid surface.
7. Research and development of intelligent sensor systems and application technologies of them:
  - 7.1. Preparation of sensor elements and testing their sensitivity and selectivity;
  - 7.2. Application technologies of electronic nose
8. Air (odour) pollution monitoring methods and instrumentation.

### Scientific staff:

- |                            |                           |
|----------------------------|---------------------------|
| 1. Dr.phys. P.Cikmacs      | 9. Dr.phys A.Kuzmins      |
| 2. Dr.chem. G. Bajars      | 10. Dr.phys. A.Lusis      |
| 3. Dr.phys. V.Eglitis      | 11. Dr.phys. E.Pentjuss   |
| 4. Dr.phys. J.Gabrusenoks  | 12. Dr.hab.phys. J.Purans |
| 5. Dr.phys. R.Kalendarjovs | 13. Dr.phys. V.Ogorodņiks |
| 6. Dr.phys. U.Kanders      | 14. Dr.chem. G.Vaivars    |
| 7. Dr.phys. J.Kleperis     | 15. Dr.chem. A.Vitins     |
| 8. Dr.phys. J.Klavins      | 16. Dr.chem.. Ģ.Vitins    |

### Technical staff:

1. U.Klavins
2. A.Kursitis
3. J.Pinnis
4. M.Purane
5. L.Ļemcovs
6. M.Vanags

### Postgraduate students:

1. L.Grīnberga
2. J. Hodakovska
3. M.Vanags
4. Ģ.Vēveris
5. V.Vorohobovs

### Students:

1. A.Apals
2. J.Blūms
3. D.Brūveris
4. P. Nazarow,
5. L.Tiļuga
6. J. Timošenko

### Laboratories of Semiconductor Material Department

- |                                  |                      |                         |
|----------------------------------|----------------------|-------------------------|
| Laboratory of Solid State Ionics | – Head of Laboratory | Dr. phys. E.Pentjuss    |
| Laboratory of EXAFS Spectroscopy | – Head of Laboratory | Dr. hab. phys. J.Purans |
| Laboratory of Electrophysics     | – Head of Laboratory | Dr.J.Klavins            |
| Laboratory of Sensors            | – Head of Laboratory | Dr.J.Klepers            |

### Cooperation

#### Latvia

1. University of Latvia - Department of Chemistry (Prof. J.Tīliks, Dr. A.Vīksna)
2. University of Latvia, Faculty of Medicine, Riga, Latvia;
3. University of Latvia - Laboratory for Mathematical Modelling of Environmental and Technological Processes (Dr.A.Jakovics).
4. University of Latvia - Departament of Information Technology (Doc. H.Bondars).
5. Riga Technical University (RTU) – Faculty of Electronics and telecommunications (Doc. I.Slaidins, Doc. P.Misans)
6. Riga Technical University - Institute of Inorganic Chemistry (Dr. J. Grabis, Dr. I.Zalite, Dr. A. Dindune).
7. Latvian Academy of Science - Institute of Physical Energetics (Prof. N.Zeltins)
8. Latvian Electroindustry Business Innovation Centre (LEBIC).
9. Certification Centre of Latvian Academy of Science (Prof. J.Matīss)
10. Ulbroka Scientific Institute of Agricultural Machinery of the Latvia University of Agriculture, Ulbrok
11. Riga City Council - Environmental Department.

## **Mobility / visits:**

1. L. Grinberga - Risø National Laboratory, Denmark, February 18 – March 19, 2006
2. L. Grinberga - Risø National Laboratory, Denmark, July 19 – August 19, 2006
3. V. Eglitis - University of Vilnius - Department of Physics – Nov. 19 – Dec. 13, 2006

### **Czech Republic**

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

### **China**

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

### **Denmark**

RISO National Research Center of Denmark (A.S. Pedersen, F.W. Poulsen)

### **Estonia**

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

### **France**

1. CRMC-N, Université de la Méditerranée (Aix-Marseille II) (Marseille, France) - Prof. Y. Mathey, Eng. D. Pailharey, Prof. D. Tonneau.
2. ESRF (Grenoble, France) – Dr. F. Comin.
3. SOLEIL and LURE, National Laboratories of Synchrotron Radiation (Orsay, France) – Prof. D. Raoux, Prof. J.-P. Itié, Dr. Ph. Parent.
4. IPN, Institut de Physique Nucléaire, Orsay, France - Dr. S. Hubert, Dr. B. Fourest

### **Germany**

Tuebingen University – U. Weimar, N. Papamichail

### **Italy**

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

### **Lithuania**

1. University of Vilnius - Department of Physics (Prof. A. Orliukas)
2. Semiconductor Physics Institute (Dr. A. Shetkus)

### **Poland**

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

### **Russia**

1. Joint Institute for Nuclear Research, Dubna (Dr. S.I. Tjutjunnikov)
2. Moscow State Engineering Physics Institute, Moscow (Prof. A. Menushenkov)

### **South Africa**

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

**NEXUS** – Network of excellence in multifunctional microsystems (Dr. A. Lusiš).

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

**Participation in Research Projects:**

**Latvian:**

1. Functional Materials and technologies for Microelectronics, Nanoelectronics, Photonics, Biomedicine and Composites. *State Research Program No. PP-05-15* (2005-2008)
2. Functional materials and technologies for microelectronics and photonics- *Cooperation project of Latvian Science Council SP 05.0005.1.* (2005-2007)
3. “Investigation of Nanostructured and Nanoactivated Glass Fibers” - *Cooperation project of Latvian Science Council SP 05.0026.4.1* (2005-2008) – A.Lusis
4. “Modification physiochemical properties of nanostructured surface of glass fibers for development of new products” - *Cooperation project of Latvian Science Council SP 06.0029.2.10* (2006-2009) – A.Lusis.
5. Physical principles of olfactometry and it modeling with sensor Microsystems. *Grant of Latvian Science Council No. 05.1712* (2005-2008), Manager – J. Kleperis;
6. “Development of new materials and computer managed electro-technology for hydrogen energy systems” *Project from Structural Funds of European Community, Activity No. 2.5.1. “Support to Research in Universities and Institutions”, No. 066/33* (2006-2008), Manager – J. Kleperis;
7. "X-Ray Absorption Spectroscopy with Picometer Accuracy", *Grant of Latvian Science Council No. 05.1714*, 2005-2008 (Head: Dr.hab. J. Purans).
8. "Advanced Spectroscopic Approach to the Study of Nanomaterials Structure", *Grant of Latvian Science Council No. 05.1717*, 2005-2008 (Head: Dr. A. Kuzmin).
9. “Hydrogen Society” *Research Project from Ministry of Education and Science, No. TOP-05-75*, Manager – J. Kleperis;
10. “Research of methods to control pollution from traffic (carbon, TSM and benzene).” *Research Project from University of Latvia*, (Manager Prof. A.Viksna, Dr. J.Kleperis), 2006;
11. “Measurement of breath for different groups of responding people, sportsmen and patients with lung’s diseases” *Research Project from University of Latvia* (Manager Prof. I. Taivans), 2006;
12. “Ozone layer – education demonstrations and activities” *Education and Demonstration Project from Agency of Environment, Geology and Meteorology* (Manager I. Pruse), 2006;

**International:**

- “Removal of Hazardous Substances in Electronics: Processes and techniques for SMEs (GreenRoSE)” *EC FP6 Collective research project № COLL-CT-2003-500225* (Dr. A. Lusis).
- "Nano-scale chemical mapping and surface structural modification by joined use of X-ray microbeams and tip assisted local detection (X-TIP)", *EC FP6 Specific Targeted Research Project NMP4-CT-2003-505634* 2004-2007 (Head: J. Purans).
- “Study of zinc oxide nanofilms for photonics and electronics ” *OSMOSE project 36* within the bilateral collaboration programme between France and Latvia, 2006-2007 (Heads: Dr. hab. J. Purans and Prof. Y. Mathey).

"Lanthanide Chemistry for Diagnosis and Therapy", European COST Action D18, 1999-2006 (Head: Dr. hab. J. Purans).

JET Fusion Technology Programme. Field: Tritium Process and Waste Management.  
Task Title: Investigation on the effect of magnetic field on detritiation of beryllium from JET. Task №: JW6-FT- 2.27. Association: EURATOM – University of Latvia.  
Association: EURATOM – University of Latvia (Prof. Juris Tīliks, Dr.A.Vitiņš).

“Multifunctional percolated nanostructured ceramics fabricated from hydroxylapatite (PERCERAMICS)” EC FP6 Specific targeted research project № STRP504937-1. (RTU: Prof. Dr. habil. phys. Jurijs Dehtjars, ISSP: Dr.A.Vitiņš).

“Integration of advanced hydrogen storage materials and systems into the hydrogen society” Subproject - Integration of electrolytic hydrogen into the hydrogen storage devices. The Nordic Energy Research Project O5493, NERP № 46-02; PhD project 4 (2003-2006) (Dr. J. Kleperis, PhD student L. Grinberga);

8. “Action plans to improve Air quality – local municipalities” Education and Demonstration Project from Baltic Environmental Forum (Manager I. Bremere, Dr.J.Kleperis), 2006.

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

1. Master degree course "Solid State Ionics" (A.Lusis)
2. Master degree Course "Structural Methods in Solid State Analysis" (J.Purans, A.Kuzmin).
3. Master degree Course “Introduction to Cluster Computing” (A.Kuzmin).
4. Master degree course "e-nose" (J.Kleperis)
5. Elaborated and implemented in Faculty of Economics and Management one credit point MS studies course „Ecodesign” (G.Bajars)
6. J. Kleperis
  - Supervisor of PhD studies - L. Grinberga “Ūdeņraža ģenerācija un akumulācija”
  - Supervisor of MS studies - J.Hodakovska „Sensoru selektivitātes īpašības un molēkulu formas reģistrācija”
  - Advance lecture for BS students “Electrocatalyses”
7. L. Grinberga, J. Kleperis – popular about science – lectures and demonstrations for visitors of ISSP, students and school children’s.

### **Renovation of research equipment and facilities**

Purchasing and adaptation of new equipment (thanks to financial support from Structural Funds of European Community and Latvian Government - Ministry of Education and Science):

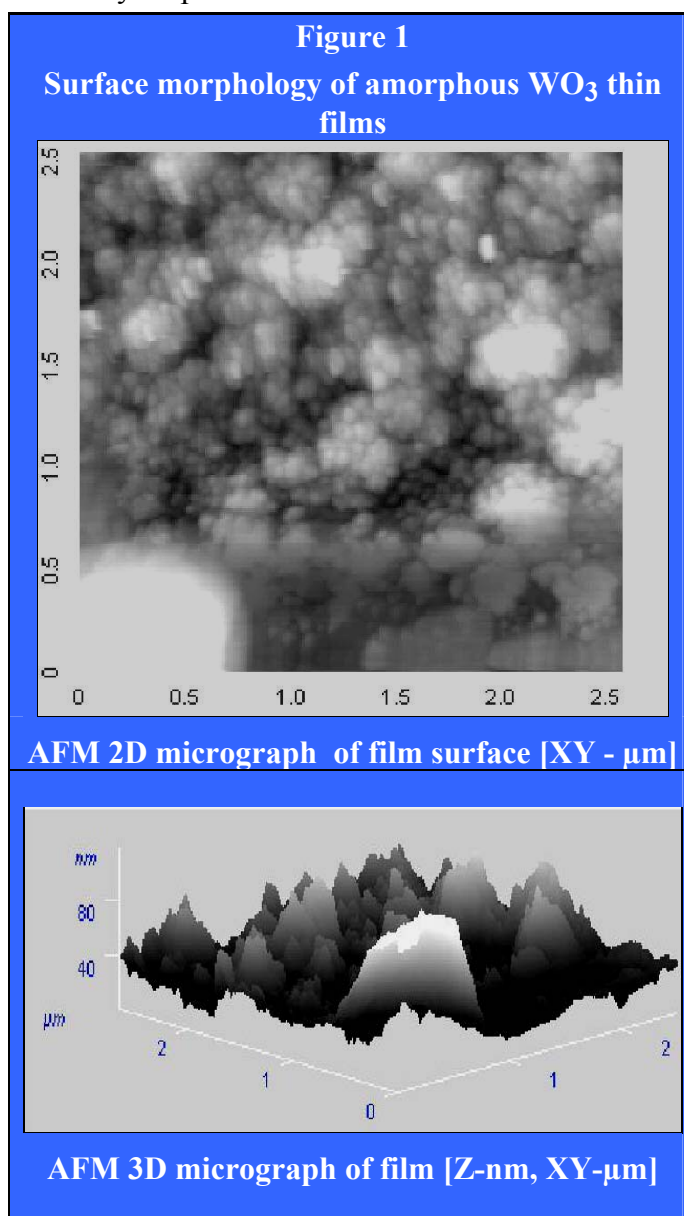
- 1) Raman spectrometer *RAMALOG* have been equipped with new:
  - Ar/Kr laser D-5AK
  - multichannel CCD optical detector JY
  - PC based control systemas well as have been developed new software for data management and collection from photon counting unit.
- 2) Clean Water Production System (Crystal) based on reversible osmoses filtering
- 3) Hydrogen Energy demonstration Kits (Fuel Cell, Solar Battery, PEM Hydrogen Generator with metal hydride storage tank)
- 4) Multiphysics and Electrochemical Engineering modeling tool – COMSOL software.

## Main results

### NANO STRUCTURED AMOURPHOUSS FILMS BASED ON TUNGSTEN OXIDE

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

The model for nanostructured mixed electron-ion conductor thin films have been developed based on thin tungsten oxide films with different microstructure from polycrystalline to amorphous controlled by deposition conditions. Transition metal oxides (TMO) as well as their thin films have applications in different solid-state electronic and ionic devices based on ion insertion/extraction and mixed (ion and electron) conduction phenomenon. The typical representative of such TMO is tungsten oxide, which belongs to group of materials with wide non-stoichiometry. The last is responsible for variety of phases based on  $[\text{WO}_6]$ -octahedron sharing in structural units-particles of pure tungsten oxide with nano dimensions and oxygen deficiency during deposition of thin films with different microstructure. The tungsten oxide is good absorber of atomic hydrogen and proton and can be used as injection or insertion electrode in the hydrogen fuel cells as well as hydrogen storage material. The morphology of tungsten oxide films surface and inner pores are responsible for sorption – adsorption efficiency of hydrogen. The typical morphology of amorphous tungsten oxide film ( $\sim 1 \mu\text{m}$  thick, deposited by thermal evaporation in vacuum chamber) surface is shown in Figure 1. The amorphous tungsten oxide films have nanostructured morphology with particle size 30-50 nm and physical surface and inner pores area more then  $10^6 \text{ cm}^2/\text{g}$ .



# STRUCTURAL STUDIES OF OXIDE MATERIALS BY X-RAY ABSORPTION SPECTROSCOPY, 3D CONFOCAL SPECTROMICROSCOPY AND SCANNING PROBE MICROSCOPY

J. Purans, A. Kuzmin, R. Kalendarev

EXAFS Spectroscopy Laboratory performed the research and development of nano-sized materials, new experimental methods and procedures of x-ray absorption spectra data analysis. We use complex approach based on a combination of modern experimental techniques such as x-ray absorption spectroscopy (EXAFS/XANES) using synchrotron radiation, atomic force microscopy and 3D confocal spectromicroscopy with advanced data analysis methodologies, based on the use of high performance cluster computing.

**Element-Specific Contrast in Local Probe Microscopy via X-Ray Spectroscopy.** The extremely high lateral resolution of the Local Probe Microscopy (LPM) makes them among the most largely used in all the domains of nanoscience. On the other hand, X-ray absorption spectroscopy (XAS) techniques probe the chemical and structural properties of materials. A combination of LPM and XAS techniques realised in collaboration with our colleagues from CRMC-N laboratory (Marseille, France) and IFN-CNR CeFSA (Trento, Italy), has been developed using optical luminescence (XEOL) detection by SNOM in AFM mode.

**Local behavior of negative thermal expansion materials.** Negative thermal expansion (NTE) affects a number of systems. EXAFS can represent a powerful probe of the local behaviour of NTE materials, thanks to the possibility of measuring the expansion of selected inter-atomic bonds and the perpendicular relative atomic displacements. The effectiveness of EXAFS for NTE studies is performed in collaboration with the University of Trento and IFN-CNR CeFSA (Trento, Italy), by a comparison of results obtained on  $\text{ReO}_3$ , germanium,  $\text{CuCl}$  and the cuprites  $\text{Cu}_2\text{O}$  and  $\text{Ag}_2\text{O}$ .

**EXAFS data analysis in disordered solids.** A method based on the simulation of configurationally averaged x-ray absorption spectra was developed to access the local structure around absorbing atom. The approach allows treating correctly arbitrary static and dynamic disorder, which is usually accounted using some simple approximation. The method was successfully applied in collaboration with the University of Trento, IFN-CNR CeFSA (Trento, Italy) and Institute of Physics of the Czech Academy of Sciences, to the study of silver ions environment in silver borate glasses  $g\text{-Ag}_2\text{O}\cdot n\text{B}_2\text{O}_3$  ( $n=2,4$ ) in temperatures range from 77 to 450 K.

**Confocal spectromicroscopy of micro and nano-structured materials.** A Raman confocal spectromicroscopy system Nanofinder-S was used to study in-situ phase composition and surface morphology in amorphous and nanocrystalline pure and mixed tungsten oxide thin films, prepared on silicon and glass substrates by dc magnetron co-sputtering technique. The possible use of these films for the phase-change optical recording was demonstrated using 442 nm He-Cd laser with a variable power of up to 50 mW. The formation of nanocrystalline tungsten trioxide or tungstate phases was observed under the laser irradiation. These nanocrystalline phases show relatively strong Raman activity, which can be used for information reading purposes. A multilayer structure composed of several tungstate films with different chemical composition is proposed as potential write-once optical recording media.

## SOLID STATE IONICS – 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 solid-state 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.

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

J. Kleperis, L. Grinberga, G. Vaivars\*, J. Hodakovska, M. Vanags, V. Nemcevs, J. Blums<sup>1</sup>, D. Bruvers<sup>1</sup>, F. W. Poulsen<sup>2</sup>, A. S. Pedersen<sup>2</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*

<sup>1</sup>*Students from Faculty of Physics and Mathematics of University of Latvia*

<sup>2</sup>*RISØ National Research Centre, Denmark*

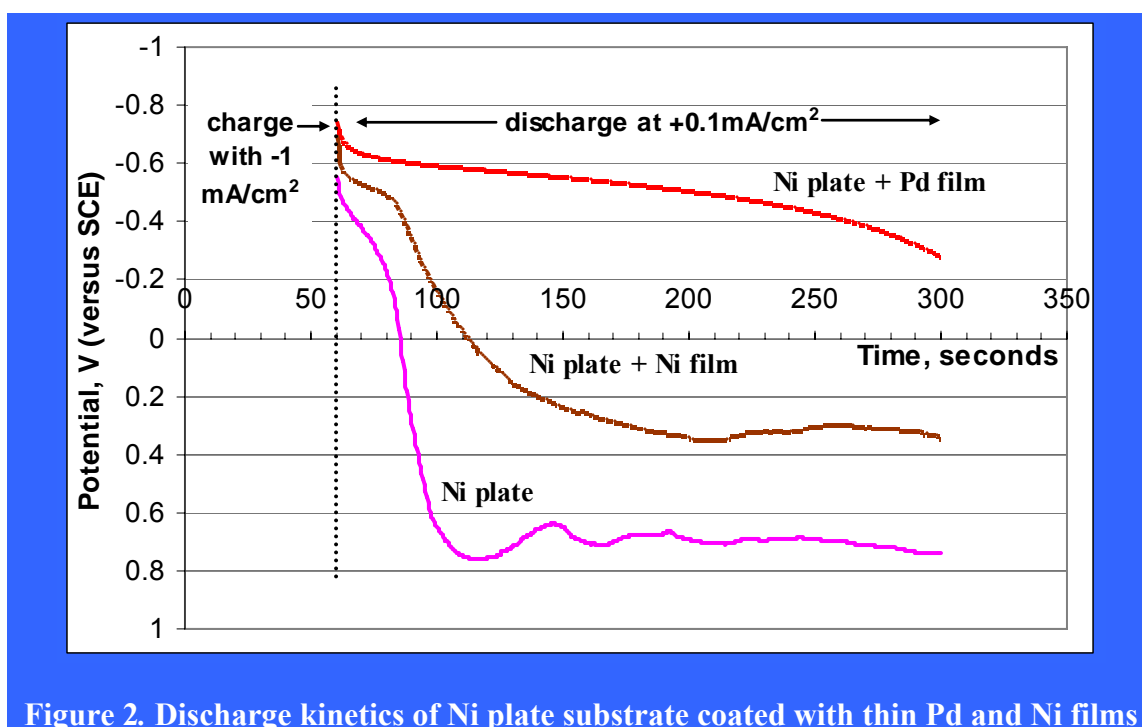
**Amount of absorbed hydrogen as case of the particle size and media.** Nanomaterials are the right key to the catalytic activity and molecular dissociation, necessary for hydrogen storage materials. For the development of efficient hydrogen storage materials, the percentage of stored hydrogen is important, and one way to improve it could be the nanostructuring of traditional materials. Nanomaterials may be produced novel properties that are dominated by surface interactions rather than bulk behavior, and slow hydrogen diffusion processes turned to quick spillover onto developed surfaces. Considerable promise for hydrogen storage could be demonstrated by an approach that exploits hydrogen spill-over effect onto different carriers: nanosize glass particles, nanotubes and zeolites. The amount of absorbed hydrogen was determined in thermogravimetric experiments if the part of metal hydride is substituted with Pyrex glass and particle size is reduced close to nanosize. Unexpected result was observed after hydrogenation of the composite AB<sub>5</sub>+Pyrex glass (C5). The XRD results showed that the diffraction peaks of hydrogenated composite C5 the observed shift of XRD peaks after hydrogenation was even larger than that for hydrogenated AB<sub>5</sub> alloy (Table)! It could be assumed, that the gamma hydride phase ( $\gamma$ ) is forming, when the alloy AB<sub>5</sub> is mixed in composite with Pyrex glass. The mechanism is not clear, who responsible for the more deeply hydrogenation of AB<sub>5</sub> in the presence of glass phase.



**Table: Structural parameters:**

Sample	a, Å	c, Å	V, Å <sup>3</sup>
AB <sub>5</sub>	5,0083	4,0567	88,12
AB <sub>5</sub> hydrogenated	5,326	4,234	104,0
C5 hydrogenated	5,369	4,2754	106,78

**Electrochemical hydrogen storage and usage aspects.** In our work different metals were tested with aim to find materials similar to platinum with activity to initiate hydrogen gas oxidation on different substrates. The conditions of electrochemical formation of nickel hydride were investigated. The electrochemical properties of different nickel based materials were examined to state the hydrogen adsorption/absorption phenomena and possibility to use them as a negative electrode in hydrogen devices (electrolysers, rechargeable batteries, fuel cells). Surface activation of nickel materials were made by electroplating and etching. Thin palladium coating was used to prove the formation of nickel hydride during cathodic charging. Volt-ampere and kinetic measurements showed that not only palladium, but also activated nickel plays important role in the surface activation of electrode materials and promotion of hydrogen absorption in nickel substrate materials. The amount of absorbed hydrogen in different nickel samples (0.5% - plate, 1.2% - electrodeposited, 15% - porous) was estimated accordingly from the amount of hydrogen in the palladium. An experimental result (Figure 2) indicated that the electroplated Ni film partly enhances hydrogen diffusion in a substrate.

**Figure 2. Discharge kinetics of Ni plate substrate coated with thin Pd and Ni films**

**Classical and unconventional aspects of water electrolysis.** Water electrolysis is known from M. Faraday's experiments already 3 centuries, however, investigations, how to split water with a less energy, still are very actual. Nowadays in the market are available different devices for the production of hydrogen gas, mostly based on alkali electrolysis and proton exchange membranes (PEM). Classical electrolysis using alkali has some disadvantages as extra heat, corrosion of vessel material and electrodes, but PEM based devices are expensive due platinum based catalyst used for both electrodes. In our work the pulse electrolysis phenomena in water is investigated. The distilled water is used as electrolyte, and simple steel plates are electrodes, representing capacitor for alternative current (AC). In the serial connection with induction-coil, capacitor forms serial oscillation circuit. The resonance of AC voltage must be observed at certain

frequency. If an oscillation frequency of bias AC is matching with water dipole oscillation frequency, then the resonance in system is reached and rapidly increases absorption of energy supplied by electric field. It is expected, that there will be remarkable water splitting at the resonance frequency, because the bonds between atoms in water molecules can be disrupted and formed gas species evaporate out. Volt-ampere measurements from -15V to +15V DC didn't indicated the presence of oxidation – reduction reactions when distilled water was used as electrolyte. Impedance measurements showed unusual frequency behavior when the AC voltage increased till 0.5V.

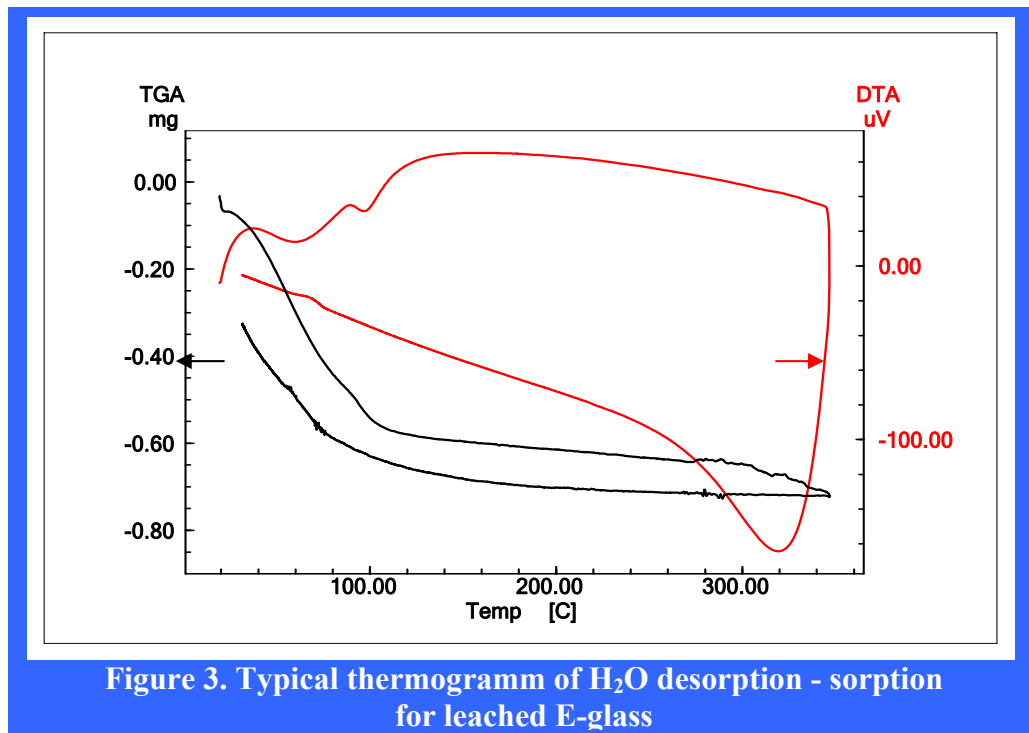
Electrochemical impedance and volt-ampere methods were used to compare an efficiency of water electrolysis for different materials and different electrode configurations. Different nickel and carbon electrodes (plate, porous and textile –type) were used to prove of they effectiveness for usage in an electrolyser device.

## NANOSTRUCTURED MATERIALS FOR SORPTION OF PHYSIOCHEMICAL ACTIVE SUBSTANCES AND HEAVY METALS

V. Eglitis, A.Vitiņš, A. Lusiš, G.Dobele\*, G. Veveris, E.Pentjušs

*\*Institute of wood chemistry*

**Influence of physiochemical treatment of glass fiber on the sorption-desorption properties.** The leaching of sodium aluminosilicate glass fibers have been used as method for modification of substructure of glass fibers. The chemical resistance of alkali and alkali-earth metals glasses is associated with two phenomena - dissolving and leaching of glass in acid media. Although there are many experimental works, the leaching mechanism of alkali silicate glasses is not fully explained. It is accepted that the interaction of alkali silicate glasses with mineral acids and water solutions proceeds in the way of ionic exchange by diffusion mechanism, which is accompanied by chemical reactions. The physiochemical treatment of glass fibers are used to modify leaching process, which have been studied by influence on the sorption - desorption properties. The leached glass fibers have porous substructure. The glass fibers are prepared by leaching of sodium aluminosilicate glass fibers in 1M H<sub>2</sub>SO<sub>4</sub> acid solution at 85-95 °C and stimulated by ultrasonic actuator. The substructures of porous sodium aluminosilicate glass fibers are investigate by AFM, DTA/TG (Figure 3)analyses and by gas isothermal desorption.



The leaching is very sensitive to temperature  $T$ , time  $t$  and ultrasonic power  $Pt$ . These parameters ( $T$ ,  $P$  and  $t$ ) have to be optimised for nanostructuring glass fibers. The data of isothermal analyses are giving the wide pore spectrum in range 3-160 nm. The AFM analyses of surface morphology are giving size of nanopores in range from 2 to 15 nm with depth at least 5 nm. Sodium aluminosilicate glass fibres in the leaching process occur degradation in shape of longitudinal cracks. The total pore volume and surface are 160 cm<sup>3</sup>/g un 0,1 m<sup>2</sup>/g for pore size 10 nm. The optimisation of leaching process is in progress.

**The porous hydroxylapatite (HAP) ceramics had been studied for implementation of the EC FW6 project “PERCERAMICS” on sorption of heavy metals.** Sorption activity of porous hydroxylapatite (HAP) ceramics with respect to Cr(VI), Ni, Cd and Pb was investigated. HAP ceramic tablets covered with immobilized yeast have a low sorption activity with respect to Cd, which is similar to that of as-prepared HAP tablets under the same conditions. Also in solutions with low initial concentrations of Pb  $\leq 1$  mg-Pb / L, the sorption activity of immobilized yeast tablets is similar to that of as-prepared HAP tablets under the same conditions. But in solutions with higher initial concentrations of Pb, 5-20 mg-Pb/L, the sorption activity of immobilized yeast tablets depending on the batch is similar or many times lower than that of as-prepared HAP tablets.

The similar low sorption activity with respect to lead was found also for the immobilized yeast tablets having a very little surface coverage with immobilized yeast of 0.004 mg of dry yeast on 1 tablet, which corresponds to 5% coverage of the surface with immobilized yeast. The authors concluded that for several batches of tablets the immobilization treatment itself considerably decreases the sorption activity of HAP ceramics with respect to lead independently of the amount of immobilized yeast. This result could be explained that little amount of immobilized yeast blocks open pores of HAP ceramics and thus reduces the active inner surface of HAP that could take part in sorption of lead.

From the practical standpoint, though at present HAP ceramics is more expensive than free waste biomass of yeast, HAP ceramics may have several advantages over free waste yeast with respect to sorption of lead. To attain low final concentrations of lead in the

water under treatment and to restore the initial sorption activity of the sorbent, the possibilities to restore the sorption activity of HAP ceramic tablets with respect to lead were investigated. Treatment of the HAP tablets after the lead sorption with 0.01 mol/L HNO<sub>3</sub> for 30 min restored their sorption activity with respect to lead, and caused their weight loss of 0.81%.

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

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

One of quality and reliability problem for solder joints in lead free soldering processes is how to exclude or to reduce formation of intermetallic compounds Cu<sub>6</sub>Sn<sub>5</sub>. For investigation formation of intermetallic compounds Cu<sub>6</sub>Sn<sub>5</sub> on of best method is scanning electron microscopy with microanalyser of chemical elements (Figure 4).

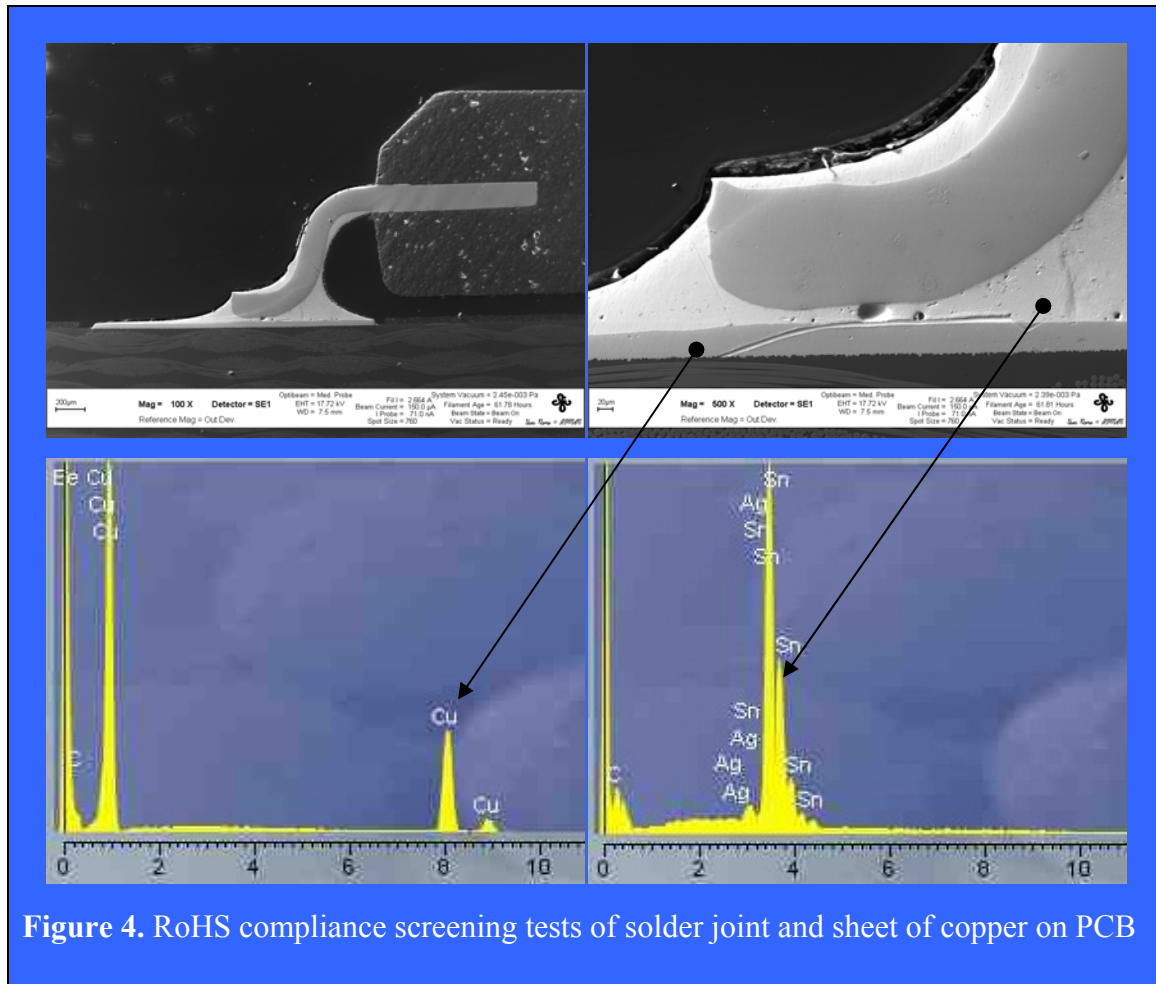


Figure 4. RoHS compliance screening tests of solder joint and sheet of copper on PCB

**ACTIVITIES FOR IMPLEMENTATION OF THE *EURATOM* PROJECT  
 “INVESTIGATION ON THE EFFECT OF MAGNETIC FIELD ON  
 DETRITIATION OF BERYLLIUM FROM *JET*”**

**A. Vītiņš, G. Ķizāne\*, B. Leščinskis\*, J. Tiliks\***

*\*Department of chemistry, University of Latvia*

The experiments on tritium sorption and desorption in samples from beryllium tiles from JET. Beryllium is foreseen as a plasma-facing material in a project of a future experimental fusion reactor ITER. In the ITER-like Wall Project, it is planned to test beryllium as a plasma-facing material of the vacuum vessel of JET. Tritium is localized in beryllium tiles in different ways – thermosorption, impacts of  $T^+$  from plasma, nuclear reactions. All chemical forms of tritium –  $T^0$ ,  $T_2$  and  $T^+$  may occur in plasma-facing beryllium tiles. Tritium release from crystal lattice of beryllium takes place as diffusion of  $T^0$ .  $T_2$  and  $T^+$  may be localized in pores and oxide admixtures of beryllium respectively. The diffusion of  $T_2$  and  $T^+$  may be slower than that of  $T^0$ .

Tritium sorption from gas phase with the tritium partial pressure about 0.1 Pa in samples from an unused beryllium tile under various conditions (temperature 500 °C only, temperature 500 °C with magnetic field of 1.7 T, temperature 500 °C with 5 MeV fast electron radiation of the dose rate 14 MGy/h, and simultaneous action of all these factors) for 3 hours was investigated. Thermo-sorption of tritium doubled in the presence of ionizing radiation. The magnetic field increased the thermo-sorption of tritium by 30%, but the simultaneous action of all the factors increased the thermo-sorption of tritium by 10%, the chemical form was found to be for the most part  $T_2$ .

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

J. Kleperis, V. Ogorodniks, N. Jurks<sup>1</sup>, I. Taivans<sup>1</sup>, L. Tiļuga<sup>2</sup>, A. Apals<sup>2</sup>, A. Osite<sup>3</sup>,  
A. Viksna<sup>3</sup>, E. Vītola<sup>4</sup>, D. Danilāne<sup>4</sup>

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

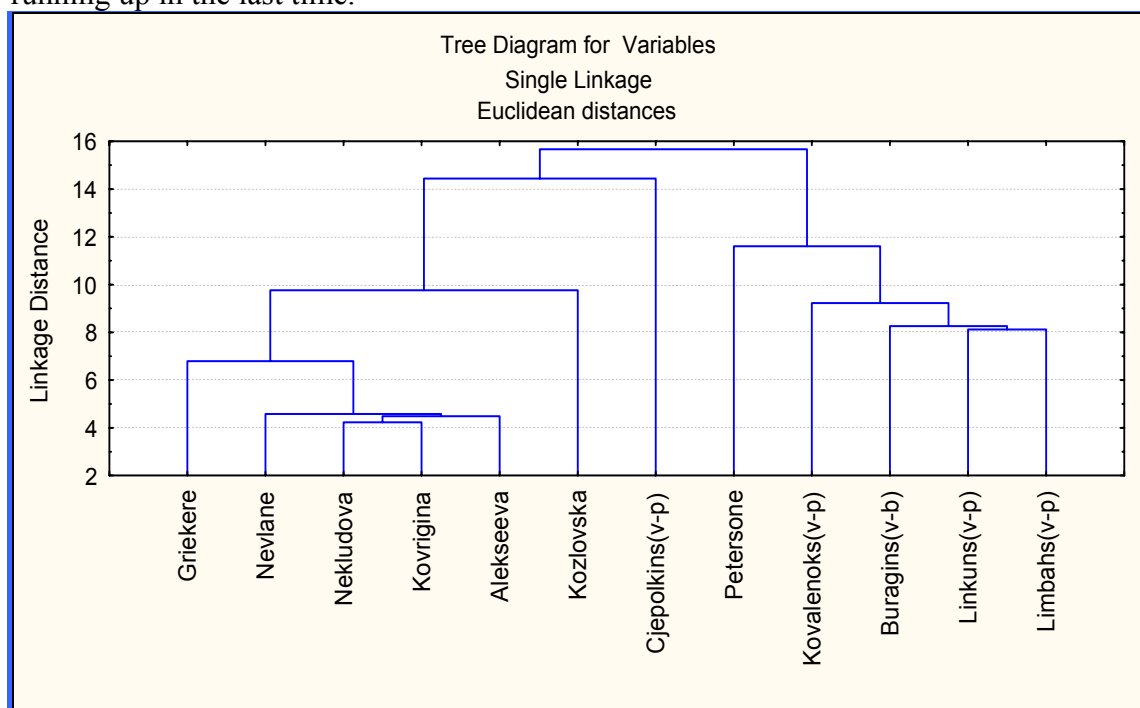
<sup>1</sup>*Medical faculty, University of Latvia;*

<sup>2</sup>*Students from Faculty of Physics and Mathematics of University of Latvia*

<sup>3</sup>*University of Latvia, Chemical Faculty, Kr.Valdemara Str. 48, Riga, LV-1013, Latvia;*

<sup>4</sup>*Department of Environment, Riga City Council, 1 Basteja Boulevard, LV-1050 Riga*

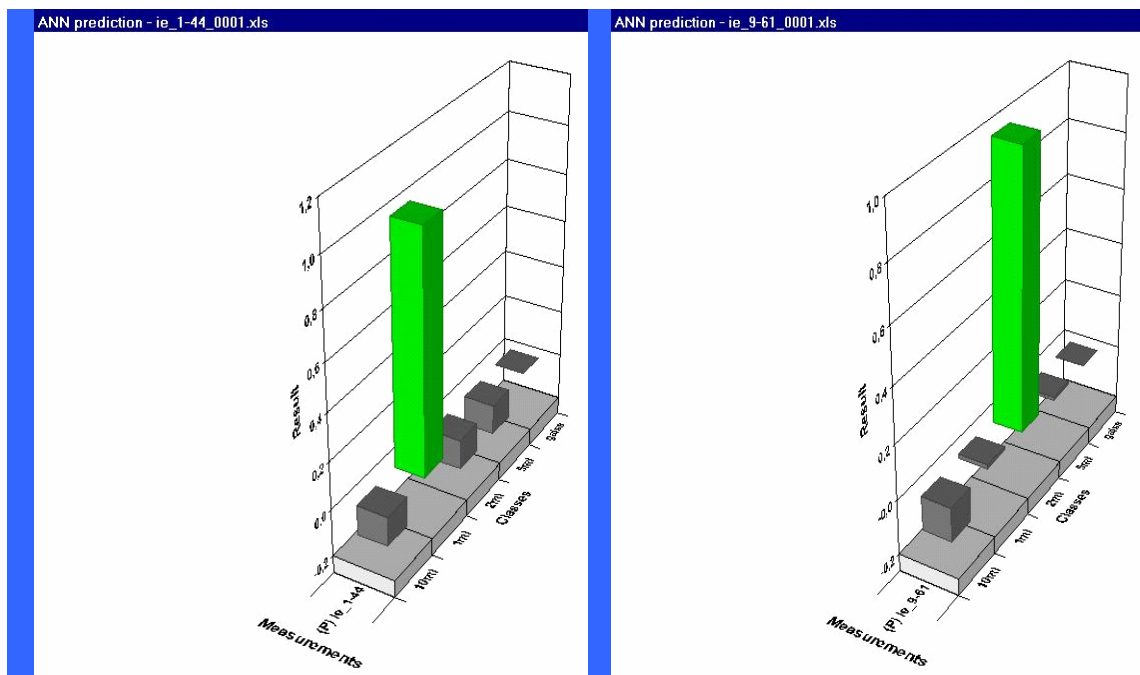
**Diagnostic of lung's diseases patients with the electronic nose.** Quick and exact analysis of lung's disease is an important factor of the recovery. Up-to-date diagnostics methods for lung's disease expect complicated and expensive equipments, long-term analysis and low availability (only few places in Latvia). The interest to the new diagnostics methods (using simple apparatus and complex data analysis founded by aggregate of disease description, its evolution and changes in the therapy process) is running up in the last time.



**Figure 6. Cluster analysis of patients with lung's diseases – second cluster is formed with patients having lung's cancer, the first cluster - patients with another lung's diseases.**

Also the request for online diagnostics methods is urgent nowadays. The expiration from lung's disease patients have been investigated in our work. The samples of expired air were investigated by artificial odour instrument (electronic nose) and fast gas chromatograph. The aim of an investigations were to find the typical odours of lung's diseases (asthma, pneumonia, cancer of lung and others) and to develop online diagnostics methods of lung's diseases guided by odours data base. Breath samples from different patients were investigated by statistical methods: cluster analysis, analysis of covariance and correlation (Figure 6).

**Breath evaluation with electronic nose.** Electronic nose and quick gas chromatograph were used to test the breath for different groups – accidentally selected peoples and sportsmen.



**Figure 7. Breath analysis accordingly concentration of lactose in the blood – good recognition results for sportsmen No. 1.**

During Science Night 2006 there were made measurements of breath for different people with aim to differ fresh and stale breath. Separate objects were snuffed in laboratory with Electronic Nose and reference class was made to compare with measured breath samples. Comparisons showed that it is possible to differ between different peoples and to characterize them accordingly the freshness of their breath. Next classes of respondents were sportsmen from National selection. Our task was to test possibility to determine the concentration of the lactic acid from the breath of sportsmen under the load. sportsmen are under the load, it is known, that the lactic acid is produced from glucose in an organism. The concentration of lactose is an indicator that the training must be stopped. Nowadays only method determining the lactic acid in the blood is used, but it is disagreeable process for sportsman and can't be used to monitor the load during trainings. We used the breath control to find the lactic acid in an expired air. The reference class was made from synthetic lactic acid solution in water in different concentrations and measured at temperature +36°C. The breath samples from sportsmen were compared with constructed class of concentrations and obtained results compile with standard concentrations determined from the analysis of the blood. First results showed that direct measurement of the lactose in gas phase is not possible with current gas sensor system (Figure 7). New measurements are planned to test the presence of lactic acid in the sweat.

*Particle pollution and monitoring analysis in Riga.* The EU reference methods for fine particles PM<sub>10</sub> and PM<sub>2.5</sub> are based on samplers that collect the PM material with subsequent weighing in a laboratory. There are many problems associated with this approach, including the considerable time delay in obtaining results. There are many "automatic" analyzers in the marketplace, including TEOMS, beta-attenuation, and optical laser instruments, giving reliable hourly data necessary for online public information. These new instruments and methods have many advantages. But the main problem is that the PM concentration measured using these automatic analyzers may not (and if fact usually does not) compare well with the EU reference method and only one existing guideline – average daily concentration. Hot discussion arises last year about the smog in the city center in connection with new Riga development plan. Can high buildings in Lucavsala screen the city center from prevailing winds usually cleaning city from smog? Is the smog found in Riga? Driving cars are main air polluting sources in



Riga nowadays. Every day the motor vehicles emit tons of pollutants into the air. In many urban areas, motor vehicles are the single largest contributor to ground-level ozone, a major component of smog. The smog with high levels of ground-level ozone is the most serious air pollution problem in the large cities. In this work the photochemical smog formation conditions and possible case were analyzed from monitoring data. Long time monitoring results in Riga don't reveal high ozone concentrations in Riga during sunny working days, when high pollution with nitrogen and carbon oxides, hydrocarbons.

## **BUILDING ENERGY EFFICIENCY AND HEAT LOSSES REDUCTION POTENTIAL USING DIFFERENT TYPE OF FACADE'S GLAZING**

**U.Kanders, J.Kļaviņš, N.Zeltiņš**

Recent findings concerning buildings' energy efficiency are taking a new look at high-performance glass facades as key in creating buildings with improved access to daylight, better indoor air quality and improved energy efficiency. But a facade that helps improve a building's interior environment and limits its loss of energy is highly necessary for Latvian climate zone. A building's skin should be a power generator rather than an energy liability. Even glass curtain walls are becoming more and more thermally efficient. The goal of creating an energy-conserving facade is one of diminishing returns. All the building facades, clad entirely in photovoltaic (PV) panels, could generate 40-50% of the building's electricity requirements. Unfortunately, despite the fact that many recent high-profile projects consider PV panels as facade elements more detailed research show that they generate only a small portion of buildings total power requirements.

Scientists and manufacturers in Latvia and Europe are also looking beyond photovoltaics to the next generation of variable materials. These so-called "smart" glazings dynamically respond to exterior conditions to control daylighting and solar heat gain. The most promising of such switchable technologies for use in buildings is electrochromic glazing, which undergoes a reversible change in optical properties when exposed to light. But an energy-efficient building envelope isn't just about the materials. Limiting solar and thermal transfer requires integrating the facade system with the lighting, mechanical, heating and cooling systems.

## **ACADEMIC KNOWLEDGE ASSESSMENT SYSTEMS APPLIED AT UNIVERSITIES AND THEIR METROLOGICAL FUNDAMENTALS**

**U.Kanders, J.Kļaviņš**

The research report deals with academic knowledge assessment systems widely used in schools and universities to account students' academic achievements. The main attention has been paid the well known 10-grade assessment system. Academic knowledge assessment systems used in several European countries have critically been analyzed and compared with that used in Latvia. The grading mark data being analyzed within the research project have been collected during time period 1998-2003 by Entrance board of the university. The collection contains about 120000 grading marks of 7000 applicants' secondary schools certificates prepared and presented during more than 30 years - 1972-2003. The applicants' population has been split into several samples depending on the students' enrolment year, study program or study form as full time or part time studies. Frequency distributions of the samples show that the grade "7" is their mode in all the cases treated within the research. The small grading marks as "1-2-3" have seldom been employed: usually not for knowledge assessment but for punishment purposes. The researches results allow derive a symmetric natural grading scale with the



zero-level in the scale center. The zero-level corresponds with a specific academic knowledge level called as erudition quota (EQ). All the 10-grade assessment systems have been derived from the natural grading scale.

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2. A. Kuzmin, G. Dalba, P. Fornasini, F. Rocca and O. Šipr, X-ray absorption spectroscopy of strongly disordered glasses: local structure around Ag ions in  $g\text{-Ag}_2\text{O}\cdot n\text{B}_2\text{O}_3$ , *Phys. Rev. B* 73 (2006) 174110:1-12.
3. A. Kuzmin, R. Kalendarev, A. Kursitis and J. Purans, Confocal spectromicroscopy of micro and nano-structured materials, *Latvian J. Phys. Tech. Sci.* 2 (2006) 66-72.
4. J. Purans, A. Kuzmin, R. Kalendarev, E. Cazzanelli and M. Castriota, Structural characterization of mixed Ta-Re oxide films, *Solid State Ionics* 177 (2006) 1887-1891.
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6. S. Hubert, J. Purans, G. Heisbourg, P. Moisy and N. Dacheux, Local structure of actinide dioxide solid solutions  $\text{Th}_{1-x}\text{U}_x\text{O}_2$  and  $\text{Th}_{1-x}\text{Pu}_x\text{O}_2$ , *Inorg. Chem.* 45 (2006) 3887-3894.
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### Abstracts

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11. G. Vaivars, M.M. Nkosi, A. Nechaev, V. Linkovs, J. Kleperis. Template synthesis of nanomaterials – nickel nanowires. Abstract Nr. PO-19 in ABSTRACTS of FM&NT-2006, 2nd Latvian conference “Functional materials and nanotechnologies” Riga, March 27-28, 2006.
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21. J.Kleperis, E. Vitola. Development plan of Riga – action plan to improve air quality. Abstracts of International conference “EcoBalt 2006”, May 11-12, 2006, Riga (Latvia), p. 26-27.

### **Participation in Conferences**

#### **1. 22th Scientific Conference of Physics of Institute of Solid State Physics of University of Latvia**

- 1) J. Kleperis “Hydrogen absorption and adsorption characteristics in materials” – oral.
- 2) L. Grinberga “Influence of glass phase to the thermogravimetric characteristics of lanthanum rich mischmetal” – oral.
- 3) E.Pentjuss, G.Bajars, A.Lusis, J.Smilga (2006) Readiness of Latvian electrical and electronics industry to restrict hazardous substances in their products – oral.
- 4) G.Bajars, A.Lusis, E.Pentjuss (2006) Raising eco-design awareness for small and medium sized enterprises of the electrical and electronics sector – oral..
- 5) V.Ogorodnikovs “Detection and analyses of signals from muscles and their mental analogies” – oral.
- 6) J. Hodakovska “Non-destructive optical surface research methods” – oral.
- 7) U.Kanders, J.Kļaviņš, N.Zeltiņš, Building energy efficiency and heat losses reduction potential using different type of facade’s glazing, (oral).
- 8) U.Kanders, J.Kļaviņš, Academic knowledge assessment systems applied at universities and their metrological fundamentals, -oral.

#### **2. The 2nd Latvian conference "Functional materials and nanotechnologies", March, 27-28, 2006, Riga, Latvia.**

- 1) A.Kuzmin "Application of cluster computing in materials science" - oral;
- 2) A.Kuzmin "Confocal spectromicroscopy of micro and nano-structured materials" (oral).
- 3) J. Kleperis, M.M.Nkosi, A.Nechaev, V.Linkovs, G.Vaivars “Template synthesis of nanomaterials – nickel nanowires” – poster: PO-19
- 4) L. Grinberga, Xin Wang, S.Naidoo, G.Vaivars, V.Linkov “Optimization of the synthesis of Pt – Ru/C fuel cell anode catalyst” – poster: PO-20
- 5) L. Grinberga, P.Ndungu, N.Onyegbule, A.Nechaev, V.Linkov “A simple route for synthesis of carbon nanotubes using LPG as a carbon source” – poster: PO-21

- 6) G. Veveris, V.Eglitis, A. Lūsis, E. Pentjuss. “Leaching as method for surface nanostructuring of sodium aluminosilicate glass fibres” - poster: PO-5
- 3. The 4th International Conference Information Technologies and Management, 2006, ISMA, Riga, Latvia, April 11-12.**  
A.Kuzmin “Load-balancing technology in cluster computing” - oral.
- 4. The 10<sup>th</sup> Int.Conf. on Structure of Non-Crystalline Materials (NCM10), Praga, Czech Republic, September 18-22, 2006.**  
A.Kuzmin “Confocal spectromicroscopy of amorphous and nanocrystalline tungsten oxide films” - oral.
- 6. International conference “EcoBalt 2006”, May 11-12, 2006, Riga (Latvia)**
- 1) J. Kleperis “Particle monitoring in Riga today and perspectives, - oral.
  - 2) J. Kleperis “Development plan of Riga – action plan to improve air quality” - oral.
  - 3) J. Kleperis “Can you find the smog in Riga?” - oral.
  - 4) G.Bajārs, A.Lūsis, Ē.Pentjušs. „Ecodesign drivers and tools in electrical and electronics sector” – poster.
  - 5) G.Bajārs, A.Lūsis, Ē.Pentjušs, J.Smilga. „Implementation of RoHS directive in electrical and electronics sector of Latvia” – poster.
- 7. VIII Meeting “Fundamental problems of Solid State Ionics”, June 13–16, 2006, Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia**  
J. Hodakovska “Electrochemical hydrogen – storage and usage aspects, VIII Meeting “Fundamental problems of Solid State Ionics” - poster.
- 8. NORSTORE conference/workshop, May 29–31, 2006, Jyllinge, Denmark**
- 1) L. Grinberga, “Studies of Sorption Properties of Metal Hydride Electrodes” - oral.
  - 2) J. Kleperis, “The ways how hydrogen could be implemented in Latvia – phantom from Latvian Hydrogen Association” - oral.
- 9. 4<sup>th</sup> International JTET Conference „Sustainable development, culture and education”. University of Helsinki, May 31-June 3, 2006**  
G.Bajārs, A.Lūsis. “Turn from the restrictions to benefits: an ecodesign study course for sustainable development” – oral.
- 10. 11<sup>th</sup> International Exhibition „Baltic Industry 2006” and 3<sup>rd</sup> International Scientific and Research Exhibition „Research & Innovation”. Riga, October 18-21, 2006.**  
G.Bajārs, A.Lūsis, E.Pentjuss. “Implementation of RoHS EC Directive in practice“ – oral.

#### **Lectures on ISSP seminar**

1. L. Grinberga, Reality and challenges of development of hydrogen energy in Latvia, Iceland and South Africa. Scientific Seminar of ISSP University of Latvia, November 16 2005, Riga, Latvia - oral
2. J. Kleperis. Electronic nose – situation today and development in future. Scientific Seminar of ISSP University of Latvia, November 23 2005, Riga, Latvia. - oral

## **Theses**

- Dmitrijs Bocharovs, "Quantum chemical interpretation of x-ray absorption spectra in perovskite-type compounds", M.Sc. Thesis, Latvian University, Riga, 2006.

## **Popular Scientific Articles**

1. M. Vanags, Kāpēc ūdeņraža enerģija ir tik dārga, *Enerģija & Pasaule*, 2 (37), Aprīlis-Maijs, 2006, 3 lpp
2. M. Vanags, Ūdeņraža enerģijas laboratorija Latvijā, *Enerģija & Pasaule*, 2 (37), Aprīlis-Maijs, 2006, 1 lpp
3. J.Kleperis, Elektriskā lauka mīlas dziesma, *Terra*, Septembris-Oktobris, 2006, 4 lpp.
4. L. Grīnberga, Stikls kā pierādījums, *Terra*, Septembris-Oktobris, 2006, 3 lpp.
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# NONLINEAR PROCESSES IN SOLIDS

**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 and nanostructures;
- thermodynamics of advanced materials: bulk, surface, interface;
- stochastization of magnetic field lines in magnetized fusion plasma;
- gyrotron development.

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

### Scientific staff

1. Dr. hab. E. Kotomin
2. Dr. hab. V. Kuzovkov
3. Dr. hab. J.R. Kalnin (left in September)
4. Dr. O. Dumbrajs
5. Dr. Yu. Zhukovskii
6. Dr. A. Popov
7. Dr. R. Eglitis
8. Dr. G. Zvejnieks
9. Dr. S. Piskunov
10. Dr. D. Gryaznov

### PhD students

11. V. Kashcheyevs
12. Yu. Mastrikov
13. D. Bocharov

### Scientific visits abroad

Dr. hab. E. Kotomin, EC Institute of Transuranium Elements, Karlsruhe, Germany (10 months), Max Planck Institute for Solid State Research, Stuttgart, Germany (3 weeks), Imperial College, London, UK (1 week).

Dr. O. Dumbrajs, Max Planck Institute for Plasma Physics, Garching, Germany (3 months).

Dr. Yu. Zhukovskii, Northwestern University, Evanston, USA (10 weeks), Max Planck Institute for Solid State Research, Stuttgart, Germany (7 weeks), National Laboratory of Frascati, Italy (5 weeks), St. Petersburg State University, Russia (1 month), EC Institute of Transuranium Elements, Karlsruhe, Germany (1 week), Uppsala University, Sweden (1 week).

Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (10 months), National Laboratory of Frascati, Italy (1 month).

Dr. R. Eglitis, University of Osnabrück, Germany (8 months), Sung Kyun Kwan University, Suwon, Korea (3 months).

Dr. G. Zvejnieks, Institute of Semiconductor Physics, Vilnius, Lithuania (1.5 months).



- Dr. S. Piskunov, Forschungszentrum Jülich, Germany (6 months), Northwestern University, Evanston, USA (4 months).
- Dr. D. Gryaznov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (9 months), EC Institute of Transuranium Elements, Karlsruhe, Germany (2 months).
- V. Kashcheyevs, Tel Aviv University, Israel (8 months), [Ben-Gurion University of the Negev, Beer-Sheva, Israel](#) (3 months).
- Yu. Mastrikov, Max Planck Institute for Solid State Research, Stuttgart, Germany (11 months).

### **International Cooperation**

- |                  |  |
|------------------|--|
| <b>Austria</b>   | 1. Institute of Chemical Technologies and Analytics, Vienna University of Technology, Vienna (Prof. Dr. J. Fleig)      |
| <b>Estonia</b>   | 2. Institute of Physics, Tartu University (Prof. A. Lushchik)  |
| <b>Finland</b>   | 3. Helsinki University of Technology (Dr. T.M.J. Ikonen)   |
| <b>France</b>    | 4. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre)   |
|                  | 5. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. van Uffelen),  |
|                  | 6. Institut für Hochleistungsimpuls & Mikrowellentechnik, Karlsruhe (Dr. B. Piosczyk)                                  |
| <b>Germany</b>   | 7. Institut für Werkstoffe und Verfahren der Energietechnik, Forschungszentrum Jülich (Prof. Dr. E. Spohr)             |
|                  | 8. Max Planck Institut (MPI) für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)                                   |
|                  | 9. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm)  |
|                  | 10. Technische Universität Braunschweig (Prof. Dr. W. von Niessen)   |
|                  | 11. Universität Osnabrück (Prof. Dr. G. Borstel)   |
| <b>Greece</b>    | 12. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. Y. Kominis) |
| <b>Israel</b>    | 13. School of Physics and Astronomy, Tel Aviv University (Prof. A. Aharony)  |
|                  | 14. Ben Gurion University of the Negev, Beer Sheeva (Prof. D. Fuks)  |
| <b>Italy</b>     | 15. Laboratori Nazionali di Frascati (Dr. S. Bellucci)   |
| <b>Japan</b>     | 16. FIR Center, University of Fukui (Prof. T. Idehara)   |
| <b>Korea</b>     | 17. Sung Kyun Kwan University, Suwon (Dr. J.C. Lee)  |
| <b>Lithuania</b> | 18. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)  |
| <b>Romania</b>   | 19. University of Craiova (Dr. D. Constantinescu)  |
| <b>Russia</b>    | 20. St. Petersburg University (SpbU) (Prof. R.A. Evarestov)  |
| <b>Spain</b>     | 21. University of Barcelona (Prof. F. Illas)   |
| <b>Sweden</b>    | 22. Uppsala University (Prof. K. Hermansson)   |
|                  | 23. Imperial College London (Prof. R.W. Grimes)  |
| <b>UK</b>        | 24. King's College London (Prof. L. Kantorovich)   |
|                  | 25. University College London (Profs. A.M. Stoneham and A. Shluger)  |
| <b>Ukraine</b>   | 26. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)  |
|                  | 27. Northwestern University, Evanston, Illinois (Prof. D.E. Ellis)   |
| <b>USA</b>       | 28. <i>University of Maryland, College Park (Dr. G.S. Nusinovich)</i>  |
|                  | 29. California Institute of Technology, Pasadena (Dr. E. Heifets)  |

## Main Results

### RANDOM WALK APPROACH TO THE ANALYTICAL SOLUTION OF DISORDERD SYSTEMS WITH MULTIPLICATIVE NOISE – THE ANDERSON LOCALIZATION PROBLEM

**V. Kuzovkov,**

**W. von Niessen** (*Braunschweig Technical University, Germany*)

Understanding fundamental properties of low-dimension disordered systems continue to attract great attention. *In collaboration with Technische Universität Braunschweig, Germany*, we developed a new analytical random walk approach for calculating the phase-diagram of spatially extended systems with multiplicative noise. We study the *Anderson localization* problem as an example. The transition from delocalized to localized states was treated as a generalized diffusion with a noise-induced first-order phase transition. The generalized diffusion manifests itself in the divergence of averages of wave functions (correlators) controlled by the Lyapunov exponent, which is the inverse of the localization length. The appearance of the generalized diffusion arises due to the instability of a fundamental mode corresponding to correlators. The generalized diffusion could be described in terms of a signal theory, which operates with the concepts of input and output signals and the filter function. Delocalized states correspond to the bounded output signals whereas localized states to unbounded output signals, respectively. The transition from bounded to unbounded signals is defined uniquely by the filter function.

### CO OXIDATION AT Pd(111) SURFACE

**V. Kuzovkov and G. Zvejnieks,**

**V. Petrauskas and E. Tornau** (*Semiconductor Physics Institute, Vilnius, Lithuania*)

Catalytic surface reactions still remain an actual research topic, which is supported by both search of effective catalysts in automotive industry and challenges for applicability of theoretical methods. *In collaboration with the Semiconductor Physics Institute (Vilnius)*, the model has been proposed to simulate numerically the reaction  $O + CO \rightarrow CO_2$  and occurring phase transitions on Pd(111) surface. We calculated the phase diagram for this system by means of the kinetic Monte Carlo method. We have shown existence of the phase transitions  $p(2 \times 2)_O \rightarrow \sqrt{3} \times \sqrt{3} R 30^\circ_O$  and  $p(2 \times 2)_O \rightarrow \sqrt{3} \times \sqrt{3} R 30^\circ_O \rightarrow p(2 \times 1)_O$  with increase of CO coverage for room and intermediate temperatures, respectively, while in the low temperature limit the direct  $p(2 \times 2)_O \rightarrow p(2 \times 1)_O$  phase transition is observed. We demonstrated that the reaction rate is the crucial factor determining the occurrence of the  $p(2 \times 1)_O$  phase and vanishing of the  $\sqrt{3} \times \sqrt{3} R 30^\circ_O$  with temperature decrease. The results of correlation function analysis indicated that the reaction proceeds inside both the  $p(2 \times 2)_O$  and  $\sqrt{3} \times \sqrt{3} R 30^\circ_O$  phases, but on the perimeter of the domains of  $p(2 \times 1)_O$  structure.

### STOCHASTIC PROCESSES IN ASDEX UPGRADE TOKAMAK

**O. Dumbrajs and G. Zvejnieks,**

**V. Igochine, H. Zohm and A. Flaws** (*MPI für Plasmaphysik, Garching, Germany*),

**D. Constantinescu** (*University of Craiova, Romania*)

One of major problems in fusion tokamak is plasma stability. *In collaboration with Max Planck Institute, Garching*, the diffusion coefficient was determined (by means of the mapping technique) for stochastic field lines arising in fast reconnection phenomena in magnetized fusion plasma during the frequently interrupted regime of

neoclassical tearing mode (FIR-NTM), as well as in non-complete Sawtooth reconnection in ASDEX Upgrade tokamak in ASDEX Upgrade tokamak. Solution of the non-stationary diffusion equation with variable diffusion coefficients predicts that the temperature profile during the FIR-NTM event is shifted towards the plasma boundary within 30  $\mu s$  and during the Sawtooth reconnection within 10  $\mu s$ . Phenomena of non-complete Sawtooth reconnection in ASDEX Upgrade tokamak are associated with internal kink mode which does not vanish after the crash phase (as would be the case for complete reconnection). It was shown that higher harmonics play an important role during the Sawtooth crash phase. To model incomplete Sawtooth reconnection, we employed the Hamiltonian formalism and reconstructed perturbations. It was demonstrated that stochastization appears due to excitation of low-order resonances. The central safety factor value is always less than unity in case of non-complete Sawtooth reconnection. Stochastic model agrees well with experimental observations and can be proposed for explanation of the Sawtooth reconnection.

The role of stochastization of magnetic field lines in fast reconnection phenomena occurring in magnetized fusion plasma was analyzed *in collaboration with the MPI, Garching, Helsinki University of Technology, and University of Craiova*. A mapping technique was applied to trace the field lines of toroidally confined plasma where the perturbation parameter is expressed in terms of experimental perturbation amplitudes determined from the ASDEX Upgrade tokamak. It was found that fast reconnection observed during amplitude drops of the neoclassical tearing mode instability in the frequently interrupted regime can be related to stochastization. It was also shown that stochastization can explain the fast loss of confinement during the minor disruption. This demonstrates that stochastization can be regarded as a possible cause for different MHD events in ASDEX Upgrade.

## GYROTRON DEVELOPMENT FOR ITER

**O. Dumbrajs,**

**B. Piosczyk and G. Dammertz** (*Forschungszentrum Karlsruhe, Germany*),

**Y. Kominis and K.A. Avramides** (*National Technical University of Athens, Greece*),

**G.S. Nusinovich** (*University of Maryland, College Park, USA*)

The development of high-power high-frequency gyrotrons is strongly driven by the needs of fusion technology. Gyrotrons are superior to other rf sources in the frequency range relevant for electron cyclotron resonance heating (ECRH), or about 170 GHz for ITER. To make an ECRH system cost-effective, the output power of a single gyrotron should be around continuous 2 MW power. Coaxial cavity gyrotrons have the potential to fulfil this requirement as has been experimentally demonstrated within the development program performed as an *ITER task at Forschungszentrum Karlsruhe (FZK)*. In proof of principle experiments carried out at FZK Karlsruhe on a 165 GHz coaxial cavity gyrotron during the last years, the feasibility of manufacturing a 2 MW, CW coaxial gyrotron at 170 GHz has been demonstrated and information necessary for a technical design has been obtained. Based on these results and on the experience acquired during the development of the 1MW, CW, 140 GHz gyrotron for W7-X, the technical feasibility of a 2 MW, CW, 170 GHz coaxial cavity gyrotron has been studied before EFDA has placed a contract with Thales Electron Devices (TED) for procurement of a first industrial prototype of such a coaxial gyrotron tube. The development work is done in cooperation between European research centers together with TED, the main European tube manufacturer. Experimental operation of the gyrotron could start in summer 2007.

Our laboratory *in collaboration with Forschungszentrum Karlsruhe, National Technical University of Athens, and University of Maryland, College Park*, actively participates in this development. Most recently, the effect of microwave reflections in

gyrotrons with radial output and consequences for the ITER coaxial gyrotron was studied, azimuthal instability in gyrotrons with overmoded resonators was investigated, feasibility of coaxial super power (4 MW) was examined, Hamiltonian map description of electron dynamics in gyrotrons was proposed, eigenvalues and ohmic losses in coaxial gyrotron cavity were reexamined by means of a novel method.

## UNIVERSAL DESCRIPTION OF ELECTRONIC CORRELATIONS IN DOUBLE QUANTUM DOTS

**V. Kashcheyevs,**

**A. Aharony and O. Entin-Wohlman** (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),

**A. Schiller** (*Hebrew University of Jerusalem, Israel*)

Quantum dots are very important for the optoelectronic applications. *In collaboration with Ben Gurion University of the Negev, Ber Sheeva, and Hebrew University of Jerusalem*, we have put forward a theoretical framework for accurate characterization of strongly correlated states in double quantum dots. Such systems consist of two nanoscale objects with discrete electronic states that are coupled to two leads. In strong magnetic fields only one non-degenerate electronic state dominates the transport in each dot. Strong Coulomb repulsion between the dots can force the two-level system into the regime of a single occupancy, where it effectively becomes a charge qubit. Recently a number of intriguing phenomena in this system have been identified: level population inversion and oscillations, transmission phase lapses and sharp transmission resonances.

Our work presents a unified quantitative explanation for these phenomena in terms of coherent dynamics of the pseudo-spin, and identifies the relevant physical mechanism, namely competition between the polarizing effect of the effective magnetic field and the Kondo-screening by the coherent environment. By a proper rotation of the quantum-mechanical representation for the charge states on the dots and in the leads, we map the system exactly onto a generalized Anderson impurity model. For the most general case of interest we develop a quantitative pseudo-spin description (Kondo type Hamiltonian), which reveals renormalization of the effective magnetic field and anisotropy of the exchange couplings. Exploiting the exact Bethe *ansatz* solution of the Kondo model, we have put forward very accurate expressions for the occupation numbers and the linear conductance. Our analytical results are in a very good agreement with advanced numerical renormalization group calculations, and call for an experimental test.

## REVISITING CLASSICAL GRAIN BOUNDARY DIFFUSION MODELS

**D. Gryaznov,**

**J. Fleig** (*Vienna University of Technology, Vienna, Austria*),

**J. Maier** (*MPI for Solid State Research, Stuttgart, Germany*)

Prediction of transport properties of nanomaterials is of great interest. This study was performed *in collaboration with the Max Planck Institute for Solid State Research, Stuttgart, and Vienna University of Technology* and completed on 20 September 2006 by a successful defense of PhD Thesis at *Stuttgart University*. The main scope of present study was to analyze limitations of classical grain boundary diffusion models (Fisher's model, Whipple's solution, Le Claire's relation) used to find the grain boundary diffusivity from measured diffusion profiles. The classical grain boundary diffusion models are based on different approximations, supposing sufficiently high temperatures and/or long diffusion times. However, nanocrystalline materials impose new conditions, *i.e.* short diffusion times and low temperatures. To find the grain boundary diffusivity we have established special procedure, which gives accurate values for bi- and

polycrystals at short and long diffusion times if orientations of the grain boundaries can be ignored. It was also estimated that the latter effect underestimates the grain boundary diffusivity by using the standard Le Claire relation. The analytical dependence for the maximum of the diffusion profile derivative not only gives an alternative procedure for deducing the grain boundary diffusivity but also sufficiently improves determination of the grain boundary diffusivity in ionic materials.

## FIRST PRINCIPLES ATOMISTIC MODELLING OF NUCLEAR FUELS

**E. Kotomin, Yu. Zhukovskii, Yu. Mastrikov, and D. Gryaznov,  
P. Van Uffelen** (*EC Joint Research Center, Institute for Transuranium Elements,  
Karlsruhe, Germany*)

Actinide nitrides are promising as advanced nuclear fuels for future fast reactors, since they exhibit higher thermal conductivity and higher metal density over the oxides, most commonly used to fabricate commercial nuclear fuels so far. To predict fuel performance under different operation conditions and understand the evolution as spent fuel over long times in a repository, it is necessary to study the defect-induced processes caused by material self-irradiation and the accumulation of fission products. *In collaboration with Institute for Transuranium Elements, Karlsruhe*, we have performed DFT plane-wave calculations on perfect and defective UN *fcc* crystal using VASP computer code. Neutral vacancies were modelled by removing a U (N) atom from the supercell, the Frenkel and Schottky defect pairs were also modeled. Nitrogen Frenkel defects were described by moving a N atom from a regular site into the interstitial position in the cube center. Results of our calculations reproduce quite well the basic properties (lattice constant  $a_0$ , bulk modulus and cohesive energy) of pure UN. The calculated effective (Bader) atomic charges indicate the complex chemical bonding, with covalency contributions due to U *5f* and N *2p* orbital hybridization. We calculated defect formation energies, changes of the macroscopic lattice parameter and local lattice distortions. The formation energies for intrinsic Frenkel and Schottky defect pairs inside a  $4 \times 4 \times 4$  supercells were found to be 4.6 eV and 3.8 eV, respectively.

Handling and disposal of new nuclear materials, including uranium nitride, require a deeper knowledge of the surface reactivity. *In collaboration with Institute for Transuranium Elements, Karlsruhe*, we have performed DFT calculations of the atomic and electronic structure of perfect and defective UN substrate as well as the early stages of surface oxidation. We have focused on a study of (i) (001) substrate relaxation, (ii) basic properties of surface point defects and adsorbed oxygen (including dissociation of  $O_2$  molecules at surface), and (iii) modification of substrate properties as a result of defect formation or oxygen adsorption. The lattice relaxation energy of 1.35 eV calculated for the surface N vacancies ( $V_N$ ) at the 0.25 ML concentration is twice as larger as that in the bulk (0.7 eV) whereas the formation energy of the surface vacancy is smaller than in the bulk. This indicates that vacancies should segregate to the UN grain boundaries. Due to metallic-covalent chemical bonding in UN, we observe high affinity of atomic oxygen towards the (001) substrate: the *binding energies* are found to be 8.1 and 7.1 eV *per* adatom atop surface U or N atoms, respectively. We found also that O adatom atop surface U and N ions transforms into  $O_{ads}^-$  ion, which determines an initiation of the oxidation process.

## DEFECTS, SURFACES, SOLID SOLUTIONS, AND REACTIVITY OF ADVANCED PEROVSKITES

**E. Kotomin, Yu. Zhukovskii, S. Piskunov, R. Eglitis, and Yu. Mastrikov**  
**R.A. Evarestov** (*St. Petersburg University, Russia*)  
**D.E. Ellis** (*Northwestern University, Evanston, Illinois, USA*)  
**E. Heifets** (*California Institute of Technology, Pasadena, USA*)

**J. Felsteiner** (*Technion, Haifa, Israel*) and **A. Gordon** (*Haifa University, Tivon, Israel*)

**G. Borstel** (*Osnabrück University, Germany*)

**J. Maier** (*MPI for Solid State Research, Stuttgart, Germany*)

Understanding perovskites surface properties of is important for catalysis, growth of high  $T_c$  materials, and optoelectronics. *In collaboration with Northwestern University, Evanston, and California Institute of Technology, Pasadena, we have studied the atomic and electronic structures as well as thermodynamic stability of three double-layered (DL) SrTiO<sub>3</sub>(001) surfaces: (i) SrO-terminated, (ii) TiO<sub>2</sub>-terminated, and (iii) TiO<sub>2</sub>-terminated with (2×1) substrate reconstruction. A thermodynamic stability diagram obtained from our DFT calculations using hybrid B3PW exchange-correlation functional have shown that regular TiO<sub>2</sub>- and SrO-terminated surfaces are the energetically most stable. Due to nearly perfect agreement of calculated and experimental formation energies we have determined boundaries of stability for different crystals very well. The stability regions of (2×1) DL TiO<sub>2</sub>- and DL SrO-terminated surfaces lie beyond the precipitation lines of SrO and TiO<sub>2</sub> compounds and, thus, are less stable than regular SrTiO<sub>3</sub>(001) surfaces. Precipitation of strontium and titanium oxides occurs much earlier, than any of studied DL terminations can be formed. We suppose that the SrO or TiO<sub>2</sub> oxide films would grow preferably on SrTiO<sub>3</sub> perovskite through cluster formation rather than layer-by-layer deposition. When partial pressure of O<sub>2</sub> gas decreases at a constant temperature, either TiO<sub>2</sub> precipitation or Ti atom reduction occurs, which precipitate to metallic particles. Sr precipitation on SrTiO<sub>3</sub> surface will not occur. Increase of Sr chemical potential leads to SrO precipitation.*

*In collaboration with Osnabrück University and California Institute of Technology, Pasadena, we have also calculated relaxation of BaTiO<sub>3</sub> and PbTiO<sub>3</sub> perovskite (001) surfaces and surface rumpling for two different terminations (BaO&PbO and TiO<sub>2</sub>) as well as relaxation of BaTiO<sub>3</sub> and PbTiO<sub>3</sub> (110) surfaces for three different terminations (Ba&Pb, TiO<sub>2</sub>, and O). The O-terminated A-type BaTiO<sub>3</sub>(110) polar surface possesses a surface energy close to that for the (001) surface, which indicates that both (110) and (001) BaTiO<sub>3</sub> surfaces can exist simultaneously in perovskite ceramics. The energetically most unfavorable, and thereby most unstable are found to be metal (Ba or Pb) terminated BaTiO<sub>3</sub> (3.24 eV) or PbTiO<sub>3</sub> (2.03 eV) (011) surfaces. The surface energies for the O terminated, A type BaTiO<sub>3</sub> and PbTiO<sub>3</sub> (011) surfaces practically coincide (1.72 eV).*

Due to its antiferroelectric behavior, PbZrO<sub>3</sub> (PZ) is technologically important for many applications including actuators and high-energy storage devices. PbZrO<sub>3</sub> is also a parent compound of PbZr<sub>1-x</sub>Ti<sub>x</sub>O<sub>3</sub> solid solutions, which are of high technological interest for their ferroelectricity and piezoelectricity, observed over a wide range of compositions. The structural and electronic properties of pure cubic and low-temperature orthorhombic PbZrO<sub>3</sub> (antiferroelectric phase), as well as cubic PZ containing single  $F$  centers (neutral oxygen vacancies) have been simulated *in collaboration with Northwestern University, Evanston.* The band gap obtained for PZ bulk (cubic phase) is in good agreement with the experimental data (3.7 eV). The electronic charge

redistribution calculated for a cubic PZ bulk confirms a notable Pb-O bond covalency, which considerably increase in the orthorhombic phase. We have also found a strong increase of the Zr-O bond covalency near the ZrO<sub>2</sub>-terminated (001) surface as compared to the PZ bulk. Formation of an *F* center in cubic PZ is accompanied by a substantial displacement (0.25 Å) of the nearest Pb atoms towards the vacancy. The *F* center forms a defect level in the middle of the band gap (1.72 eV below the conduction band bottom) unlike the shallow *F* level found in SrTiO<sub>3</sub> (0.5 eV). Thus, the point defects affect both atomic polarization in PZ and its ferroelectric properties.

Understanding and control of surface properties of pure and Sr-doped LaMnO<sub>3</sub> is important for applications in fuel cells, magnetoresistive devices, and spintronics. We have compared the atomic, electronic, and magnetic structures of LaMnO<sub>3</sub> bulk as well as the (001) and (110) surfaces calculated *in collaboration with Max Planck Institute for Solid State Research, Stuttgart, and St. Petersburg University*, using two *ab initio* approaches – hybrid B3PW functionals with optimized LCAO basis set and GGA-PW91 functional with plane wave basis set. Combination of non-local exchange and correlation used in hybrid functionals allows us to reproduce the experimental *magnetic coupling constants*  $J_{ab}$  and  $J_c$  as well as the optical gap much better than using other methods. Calculations performed by both methods using slab models show that the anti-ferromagnetic (AFM) and ferromagnetic (FM) (001) surfaces have lower *surface energies* than the FM (110) surface. Both AFM and FM surfaces reveal considerable atomic relaxations, up to the fourth plane from the surface, which reduce the surface energy by about a factor of two, being typically one order of magnitude larger than the energy difference between different magnetic structures.

## FIRST-PRINCIPLES CALCULATIONS AND THERMODYNAMIC STUDY ON SURFACE REACTIVITY OF LIGHT METAL OXIDES AND FLUORIDES

**Yu. Zhukovskii, E. Kotomin, and R. Eglitis**

**D. Fuks** (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),

**D.E. Ellis** (*Northwestern University, Evanston, Illinois, USA*)

**P. Balaya and J. Maier** (*MPI for Solid State Research, Stuttgart, Germany*)

**G. Borstel** (*Osnabrück University, Germany*)

Understanding the metal adhesion and growth mode of thin metallic films is important for micro- and nanoelectronics. In collaboration with *Northwestern University, Evanston and Ben Gurion University, Ber Sheeva*, we have performed *ab initio* calculations (using hybrid B3LYP method) and thermodynamic study of Ag and Cu adhesion onto defective MgO(001) substrate. We observe a strong change of the bonding between the metal adatoms and substrate in the vicinity of the surface  $F_s$  centers (neutral O vacancies), which affects the thermodynamic conditions and the morphology of the growing metallic layer. For a perfect MgO surface we confirm the experimentally observed submonolayer growth of *metallic islands*. However, the surface  $F_s$  centers weaken the trend toward metal atom aggregation and above some critical surface concentration lead to formation of *disordered* 2D metallic films; *i.e.*, the island formation mode is changed for the layer-by-layer growth mode. For silver films, the effect of the  $F_s$  centers is less pronounced than for copper: substantially higher atomic fraction of defects (at least 35-40 per cent) is needed for the growth of uniform Ag film, which is substantially larger than that for Cu (<10 per cent).

*Ab initio* calculations on H<sub>2</sub>O and O<sub>2</sub> molecules adsorbed on different Al<sub>2</sub>O<sub>3</sub> substrates, namely the Al terminated (0001) surface of crystalline corundum, and amorphous-like (Al<sub>2</sub>O<sub>3</sub>)<sub>n</sub> clusters with n=2-7 formula units, have been performed *in collaboration with Osnabrück University*. Two types of first-principles computer codes,



CRYSTAL and SIESTA, have been used for the calculations on periodic slabs and clusters, respectively. We have performed complementary research of adsorption and dissociation of water on  $(\text{Al}_2\text{O}_3)_n$  amorphous-like clusters with  $n = 2-7$ . We have also calculated the binding energy of an  $\text{O}_2$  molecule on  $\alpha\text{-Al}_2\text{O}_3$  (0001) substrate. Our results point to a large contribution of Coulomb correlations and relaxation effects for the energies of  $\text{H}_2\text{O}$  and  $\text{O}_2$  molecule adsorption on alumina surfaces and clusters.

To clarify the mechanism of lithium storage anomaly in LiF nanocomposites in the context of lithium batteries, we have performed comparative DFT hybrid calculations on the atomic and electronic structure of the non-polar Cu/LiF(001) and model Li/LiF(001) interfaces, *in collaboration with Max Planck Institute for Solid State Research, Stuttgart*. For this aim, we have modeled the extra Li atoms incorporated at several possible sites of the Me/LiF interface, including the free surface of the substrate slab and interstitial sites inside a slab. Increase of Li concentration at the substrate side of interfaces is accompanied by an increased electron charge transfer from the extra Li atoms towards the transition metal adlayers, in agreement with a proposed mechanism of interfacial charge storage. Interfacial stability and charge transfer depends on the number of extra Li atoms and Me adatoms *per* LiF(001) surface unit cell. The Li diffusion on the interface is found to be energetically much easier than Li penetration into the bulk.

### **FIRST PRINCIPLES SIMULATION OF ELECTRONIC STRUCTURE FOR PERFECT AND DEFECTIVE $\text{BaF}_2$ AND $\text{CaF}_2$ : BULK AND SURFACE**

**R. Eglitis,**

**H. Shi and G. Borstel** (*University of Osnabrück, Germany*)

In collaboration with *Osnabrück University*, we have performed *ab initio* calculations on technologically important barium and calcium fluorides (perfect and defective bulk and densely-packed surfaces).  $\text{BaF}_2$  is important as a candidate material for high-temperature batteries, fuel cells, chemical filters and sensors.  $\text{CaF}_2$  has been identified as a prime candidate for windows operating at chemical laser wavelengths due to very low bulk absorption and exceptionally small thermal tensing coefficients. The hybrid B3PW method was used as implemented into the *CRYSTAL'03* code, which provides the best agreement with experiment for the band gap. When comparing the results of calculations on  $\text{CaF}_2$  (111), (110), and (100) surfaces, we have confirmed that the  $\text{CaF}_2$ (111) surface is the most stable one, in agreement with the experiment, the same is true for the  $\text{BaF}_2$ (111) surface. The charge density map of the *F* center in  $\text{CaF}_2$  shows that the charge is well localized inside the vacancy: the spin density on the *F* center has been found to be  $0.716 e$ . The relaxation of atoms around defect is rather small. Our results for defect level position suggest a possible mechanism for absorption in  $\text{CaF}_2$ . We also calculated the aggregates of two *F* centers (*M* center) for both  $\text{BaF}_2$  and  $\text{CaF}_2$ .

### **EXPERIMENTAL AND THEORETICAL STUDIES OF NANOSTRUCTURED MATERIALS**

**A. Popov and Yu. Zhukovskii**

**C. Balasubramanian, S. Bellucci, M. Cestelli Guidi, A. Grilli, and M. Piccinini,**  
(*National Laboratory of Frascati, Italy*),

**I. Bolesta, S. Velgosh, and I. Karbovnyk** (*National University of Lviv, Ukraine*)

**V. Baranov, V. Biryukov, Yu. Chesnokov, and V. Maishev**  
(*Institute for High Energy Physics, Protvino, Russia*)

*In collaboration with Laboratori Nazionali di Frascati (LNF) at Synchrotron Radiation Facility using both XANES (X-ray absorption near edge spectroscopy) and FTIR (Fourier transform infrared spectroscopy) techniques, we have studied different AlN nanosystems using spectroscopic methods, in order to investigate both tribological and electronic properties of nanostructured materials. III group nitrides nanostructures*



attract enhanced attention of both experimentalists and theorists, due to numerous technological applications in nanoengineering. Comparison has been performed between measurements by standard X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) at the K-edge of Al, sensitive to the local order and correlated to the local and empty density of states of wide band-gap semiconductor. Preliminary XAS simulations were also performed. Correlations between XRD and XAS have been drawn. Using infrared (IR) absorption both in the mid- and in the far-IR ranges we have compared parameters of different AlN samples: powders, nanoparticles and nanotubes. Our results clearly show difference between their electronic properties and optical phonon modes.

*In collaboration with LNF, Frascati*, we have also analyzed the effect of N vacancies created on AlN single-walled (SW) nanotubes (NT), on both the electronic and structural properties of NTs. For this aim, we construct 1D periodic models of armchair- and zigzag-type chiralities and perform their DFT calculations using the *CRYSTAL-03* code taking into account structural reconstruction around each point defect on AlN NTs. To achieve the limit of single vacancy for both nanotube chiralities, we have considered three sets of inter-defect distances repeated along the axes of these nanotubes. The Mulliken charges on the *F* centers are found to be  $-2 e$ , close to the effective charges on N ions. However, the electron charge density re-distributions around the *F* center are substantial for both chiralities. They remain well localized along NT axis and disturb the electron density on the nearest atoms across NTs. N vacancies results induce one-electron energy levels in the NTs band gaps with main contributions from  $3p$  and  $3s$  atomic orbitals of the nearest Al atoms. The larger is the inter-defect distance on AlN SW NTs, the smaller dispersion of defect levels.

*In collaboration with National University of Lviv and LNF, Frascati*, we have studied an influence of  $(Cd_i)_n$  metallic clusters on the optical absorption and phonon spectra of  $CdI_2$  crystals, to understand a role of Cd nano&micro-clusters in context of  $CdI_2$  crystal application as possible scintillator material and very promising materials for second harmonic generation. Metallic clusters of spherical shape were formed during the growth of non-stoichiometric crystals. Radii of clusters fall in the range from 10 to 500 nm, according to scanning electron microscopy (SEM) data. The density of clusters was estimated from fractal dimension calculations. Both spectral and size dependencies on extinction coefficients have been calculated using Mie theory. The experimentally obtained spectra show that metallic clusters are responsible for the bands in the transparency region of  $CdI_2$  crystals (360–430 nm) and peaks in mid-infrared absorption spectra, which are not present in those for cadmium iodide. The nature of this additional optical and infrared absorption is concerned with bulk and surface plasmons and surface phonon modes of metallic clusters, respectively. Transmittance in the far-IR (50 to 600  $cm^{-1}$ ) and mid-IR (600 to 1300  $cm^{-1}$ ) regions was measured at the infrared station of the Synchrotron Radiation facility of LNF. The activation of crystals by diffusion during/after growth does not have any significant effect on their far IR spectra. Relative intensity of IR peaks varies depending on the impurity. This result is in a good agreement with SEM analysis and optical data.

Recently invented technique of crystal bending has been applied to produce samples with a high curvature. *In collaboration with LNF, Frascati, and Institute for High Energy Physics, Protvino*, we have investigated the deflection of a positron beam with energies of 400–700 MeV, available in the beam test facility (BTF) of LNF, by means of bent silicon crystals. This technique was successfully applied for crystal undulator production. We have observed positron bending by a crystal lattice, presumably being guided by a channeling phenomenon, deflecting the beam by about 10 milliradian over a 1 mm length of silicon. This technique may result in the use of the channeling effect for steering particle beams at energies below 1 GeV for the purpose of producing beams of low emittance with enhanced stability for medical and biological applications. By giving to nanotubes a controlled bending of a few milliradian, we could

deflect the channeled particles out of the incident beam. Carbon nanotubes (CNT) proposed for particle channelling have been synthesized at LNF and then have been characterized there by SEM, TEM and AFM to obtain ratio and dimensions of the CNTs. SEM images show that the ratio of NTs is very high (more than 70%). Single-wall-CNTs have an average diameter 1.3 nm and a length of several microns.

#### D. Bocharov **and** QUANTUM CHEMICAL INTERPRETATION OF X-RAY ABSORPTION SPECTRA IN ABO<sub>3</sub> COMPOUNDS

A. Kuzmin (*EXAFS Laboratory, ISSP, Riga, Latvia*)

X-ray absorption spectroscopy (XAS) provides experimentalists with unique information on electronic, atomic and dynamic structure of materials. At the same time, quantum chemistry allows us to simulate reactivity, chemical properties, atomic and electronic structure of crystalline solids. In this work, we have interpreted experimental O K-edge XAS in perovskite-type WO<sub>3</sub> and AWO<sub>3</sub> compounds (A is the first group ion: H, Li, Na, K, Rb, Cs) using both DFT method as implemented in *CRYSTAL-2003* code and conventional multiple-scattering approach realized in *FEFF-8.2* code. Our calculations performed using both codes show qualitative agreement with available experimental data.

*FEFF* multiple-scattering calculations of XANES region allow us to obtain spectra qualitatively close to experimental ones. Calculated XAS have energy scale, which is non-linearly compressed. The position of the Fermi level was estimated with an accuracy of about  $\pm 2-4$  eV. Since XAS is sensitive to the position of the Fermi level, its correction is required to achieve reasonable agreement with the experiment. A cluster size of 6.5-7.5 Å around absorbing oxygen atom allows one to reproduce qualitatively experimental curves. The accuracy of *CRYSTAL* program for description of unoccupied electron states was tested for AWO<sub>3</sub> systems. Several optimized basis sets give similar results for our compounds in the region up to 15 eV above the Fermi level, whereas strong deviation of calculated results for higher energies indicates *CRYSTAL* code limitations. Our calculations make it possible to estimate bonds covalency in AWO<sub>3</sub> compounds: O-H bond is strongly covalent, W-O may be described in terms of both ionic and covalent contributions whereas O-A bonds are either pure ionic (A = K, Cs, Rb) or ionic with almost negligible covalency.

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#### ***PhD Thesis*** (*Defended on 20<sup>th</sup> September 2006, at Stuttgart University, Germany*)

Denis Gryaznov, Simulation of diffusion in nanocrystalline materials: continuum approach.

#### ***Master Thesis*** (*Defended on 31<sup>st</sup> May 2006, at University of Latvia, Riga*)

Dmitry Bocharov, Quantum chemical interpretation of X-ray absorption spectra in ABO<sub>3</sub> compounds.

### Presentations at Conferences

#### ***The workshop on Interactions and Dynamics in Low Dimensional Quantum Systems (Rehovot, Israel, January, 2006).***

1. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, "Applicability of the equations-of-motions technique for quantum dots".

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7. A. Gopejenko and S. Piskunov, "Electronic structure of pure and defective PbZrO<sub>3</sub>: first-principles calculations". Abstracts: p. 17.
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34. Yu.F. Zhukovskii, E.A. Kotomin, R.A. Evarestov, and D.E. Ellis, "Periodic quantum chemical simulations of point defects in metal oxides". Abstracts: p. 116.

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35. S. Illy, B. Pioszyk, T. Rzesnicki, G. Dammertz, O. Dumbrajs, G. Gantenbein, J. Jin, O. Prinz, W. Leonhardt, G. Michel, M. Schmid, and M. Thumm, "2 MW, CW, 170 GHz Coaxial Cavity Gyrotron - results obtained with an experimental pre-prototype". Abstracts: p. 29.

**XX. Joint 31<sup>st</sup> International Conference on Infrared and Millimeter Waves and 14<sup>th</sup> International Conference on Terahertz Electronics IRMMW -THz 2006 (Shanghai, China, September, 2006).**

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**XXI. 7<sup>th</sup> International Workshop Nanoscience&Nanotechnology (Frascati, Italy, November, 2006).**

39. S. Bellucci, I. Bolesta, M. Cestelli Guidi, I. Karbovnyk, V. Lesivtsiv, P. Piccinini, A.I. Popov, and S. Velgosh, "Micro- and nanosized metallic clusters in cadmium iodide layered crystals: the influence on the optical properties". Abstracts: p. 9.

40. Yu.F. Zhukovskii, C. Balasubramanian, and S. Bellucci, "Influence of point defects on properties of AlN single-walled nanotubes". Abstracts: p. 61.

41. V. Savchyn, A.I. Popov, C. Balasubramanian, and S. Bellucci, "Luminescence from AlN nanotube/CsI pellets under electron beam excitation at 80-300 K". Abstracts: p. 72.



# OPTICAL RECORDING

**Head of Laboratory Dr. J.Teteris**

## **Research Area and Main Problems**

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

### **Scientific Staff**

1. Prof. Dr.hab. A.Ozols
2. Dr. M.Reinfelde
3. Dr. J.Teteris
4. Dr. K.Jefimovs

### **PhD Students**

O.Balcers  
A.Gerbreders  
E.Sledevskis

### **Technical Staff**

1. J.Gurovs
2. D.Popele

### **Students**

1. T.Bernots
2. U.Gertners
3. A.Zeipiņš
4. J.Aleksejeva

### **Scientific visits abroad**

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

### **Cooperation**

#### **Latvia**

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

#### **Finland**

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

#### **USA**

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

## Lithuania

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

### Main Results

#### EFFECTS OF POLARIZATION, GEOMETRICAL FACTORS AND IMPURITIES ON THE HOLOGRAPHIC RECORDING IN LiNbO<sub>3</sub> CRYSTALS

A.Ozols, M.Reinfelde

Holographic grating recording by He-Ne laser (633 nm) in LiNbO<sub>3</sub>:Fe, LiNbO<sub>3</sub>:Cu, LiNbO<sub>3</sub>:Fe+Ca, LiNbO<sub>3</sub>:Fe+Ti crystals has been experimentally studied depending on their oxidation degree, on the recording and readout light polarization as well as on the recording geometry ( $\mathbf{K} \parallel \mathbf{P}_s$  or  $\mathbf{K} \perp \mathbf{P}_s$ ,  $\mathbf{K}$  being the holographic grating vector,  $\mathbf{P}_s$  – spontaneous polarization). The crystals were kept about 20 years at room temperature before the first recording. The second recording was performed after the annealing at 200°C. Annealing considerably improved the diffraction efficiency  $\eta$  and specific recording energy  $W$  in all cases except LiNbO<sub>3</sub>:Fe at  $\mathbf{K} \perp \mathbf{P}_s$  case. The  $\mathbf{K} \parallel \mathbf{P}_s$  geometry was much more efficient than  $\mathbf{K} \perp \mathbf{P}_s$  one. The best results were obtained for LiNbO<sub>3</sub>:Cu crystals ( $\eta_{oomax} = 40\%$ ,  $W_{oomax} = 6.8 \text{ J}/(\text{cm}^2\%)$ ; indices denote the recording and readout polarization). Recording efficiency of crystals decreases in the following order: LiNbO<sub>3</sub>:Cu, LiNbO<sub>3</sub>:Fe, LiNbO<sub>3</sub>:Fe+Ca, LiNbO<sub>3</sub>:Fe+Ti. The recording efficiency polarization dependence of LiNbO<sub>3</sub>:Cu crystals markedly differed from the known polarization dependence of LiNbO<sub>3</sub>:Fe crystals. The obtained results can be explained regarding the influence of possible defects on the absorption and photogalvanic effect.

#### SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

Mara Reinfelde and Janis Teteris

Thin films of amorphous chalcogenide semiconductor As<sub>2</sub>S<sub>3</sub>, As-Se and As-S-Se systems were used for recording of refractive index and surface-relief modulated gratings. Amorphous chalcogenide semiconductors are high index materials with refractive index in the range 2.2 – 3.5, depending on the film composition and light wavelength. The photoinduced changes of refractive index down to  $\Delta n \approx 0.15 - 0.5$  are observed in these systems.

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

The recording of the subwavelength gratings with a period of 0.15  $\mu\text{m}$  – 1  $\mu\text{m}$  was performed by holographic method. The fringe period for two intersecting light beams in a media with high refractive index  $n$  can be expressed as  $\Lambda = \lambda_0 / 2n \sin\theta$ , where  $\lambda_0$  is the wavelength of laser light in vacuum,  $n$  is refractive index of the resist and  $\theta$  is the half-angle between the laser beams inside the resist. The right angle prisms with  $n = 1.8 - 2.6$  were used to increase the value of  $\theta$ . The grating period and profile after chemical etching was measured by AFM. The transmission, reflection and polarization properties of the obtained gratings were studied.

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

## IMMERSION HOLOGRAPHIC LITHOGRAPHY IN AMORPHOUS CHALCOGENIDE THIN FILMS

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

### Scientific Publications

1. A.Ozols, K.Ozols, G.Ivanovs. *Phase conjugation properties of As-S-Se films*. Proc. SPIE, 2006, vol.6180, pp.618010-1 – 618010-6.

2. A.Ozols, Dm. Saharovs, M.Reinfelde. *Holographic recording in amorphous As<sub>2</sub>S<sub>3</sub> films at 633 nm*. Journ. Non-Cryst.Solids, 2006, vol.352, pp.2652 – 2656.
3. Dm. Saharov, A.Ozols, V.Kampars, V.Kokars, J.Kreicberga, S.Ratyeva. *Influence of chromophore group concentration on the holographic properties of spin-coated azobenzene oligomers*. Latv. J.of Phys. and Techn. Sciences, 2006, No2, pp.59 – 65.
4. J.Teteris and M.Reinfelde, *Solid immersion holographic recording in amorphous chalcogenide thin films*, Microsyst.Technol. 6 (2006) 164-169.
5. K. Jefimovs, J. Laukkanen, T. Vallius, T. Pilvi, M. Ritala, T. Meilahti, M. Kaipainen, M. Bavdaz, M. Leskela, J. Turunen, *Free-standing inductive grid filter for infrared radiation rejection*, Microelectronic Engineering 83 (2006) 1339-1342.
6. O.Balcers and J.Teteris. *Luminescence study of detergent optical brighteners in the context of developing optical environmental sensors for water quality control*. Journ. of Environmental Engineering and Landscape Management 14 (Nr 3) (2006) 121-125.

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1. A.Ozols,Dm.Saharov, V.Kampars, V.Kokars, J.Kreicberga, S.Ratyeva. *Holographic properties of azobenzene oligomers with differently bonded chromophore groups*. Phys. Stat.Sol.(c), 2007.
2. A.Ozols, M.Reinfelde, Dm.Saharov, K.Kundzins, V.Kampars, V.Kokars. *Holographic recording of surface relief gratings in tolyle-based azobenzene oligomers*. Thin Solid Films, 2007.
3. A.Ozols, Dm.Saharov. *Sub-bandgap light hologram recording in amorphous chalcogenides*. Proc. SPIE, 2007.
4. J.Porins, A.Ozols, P.Onufrijevs. *Nanosecond and picosecond pulse transmission in optical fibres*. Proc. SPIE, 2007.

### Lectures on Conferences

#### **22th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, March 29 – 30, 2006.**

A.Ozols. *Microobjective studies of dynamic holographic gratings*. Abstracts, p13.

J.Teteris. *Application of amorphous chalcogenide semiconductors in optical technologies*. Abstracts, p.12.

M.Reinfelde, J.Teteris. *Reflected holograms in arsenic chalcogenide films*. Abstracts, p.14.

#### **10th Europhysical Conf. On Defects in Insulating Materials, Milano, Italy, July 10-14, 2006**

A.Ozols,Dm.Saharov, V.Kampars, V.Kokars, J.Kreicberga, S.Ratyeva. *Holographic properties of azobenzene oligomers with differently bonded chromophore groups*. Abstracts, p.317.

#### **10th European Conf. On Organised Films, Riga, Latvia, August 20-24, 2006.**

A.Ozols, M.Reinfelde, Dm.Saharov, K.Kundzins, V.Kampars, V.Kokars. *Holographic recording of surface relief gratings in tolyle-based azobenzene oligomers*. Abstracts, p.72.

#### **5th Int. Conf. „Advanced Optical Materials and Devices“, Vilnius, Lithuania, August 27-30, 2006.**

A.Ozols, Dm.Saharov. *Sub-bandgap light hologram recording in amorphous chalcogenides*. Abstracts, p.101.

J.Porins, A.Ozols, P.Onufrijevs. *Nanosecond and picosecond pulse transmission in optical fibres*. Abstracts, p. 83.

# LABORATORY OF OPTICAL MATERIALS

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;
- design of the model eye with externally controllable light scattering (electrooptic PLZT ceramics, polymer dispersed liquid crystals PDLC);
- 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;
- vision ergonomics and behavioural optometry;
- evaluation of accommodation/convergence mechanisms reading print materials and for regular computer users.

### Scientific Staff

1. Prof. I.Lācis
2. Prof. M.Ozolins
3. Dr. G. Krūmiņa
4. Dr. J.Dzenis

### PhD Students

1. M.Sc. A.Švede
2. M.Sc. G.Ikaunieks
3. M.Sc. R.Paeglis
4. M.Sc. S.Fomins

### Graduate Students

1. B.Sc. V. Karitāns

### Partners abroad

#### Italy

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

#### Sweden

Lund University (Prof. S.Svanberg)  
Department of Clinical Science of Karolinska Institute (Dr. H. Richter)

#### Norway

Chalmers TH, Sweden (Prof. L.Komitov)  
Buskerud Høgskolan, Institutt for optometri (Prof. J.R.Bruehich).

#### England

Bradford University (Prof. D.Whittaker)

#### Spain

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

<b>Scotland</b>	Psychology Department, University of Glasgow, Scotland (Dr.D.Simmons)
<b>Finland</b>	Colour Research Laboratory, University of Joensuu (Prof. J.Parkkinen)
<b>Germany</b>	<b>Institut für Arbeitsphysiologie an der Universität Dortmund</b>
<b>The Netherlands</b>	Utrecht University (Prof. R. van Ee)
<b>France</b>	Laboratoire Régional des Ponts et Chaussées de Clermont- Ferrand (Dr.M.Colomb)

## MAIN RESULTS

### PERCEPTION OF COLOUR CONTRAST STIMULI IN THE PRESENCE OF SCATTERING

**Maris Ozolinsh<sup>1</sup>, Gatis Ikaunieks<sup>2</sup>, Sergejs Fomins<sup>1</sup>, Michèle. Colomb<sup>3</sup>,  
Jussi Parkkinen<sup>4</sup>**

<sup>1</sup>*Inst. of Solid State Physics, University of Latvia;*

<sup>2</sup>*Dept. of Optometry, University of Latvia;*

<sup>3</sup>*Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand;*

<sup>4</sup>*Color research laboratory, University of Joensuu*

Visual acuity and contrast sensitivity were studied in real fog conditions (fog chamber in Clermont-Ferrand) and in the presence of light scattering induced by light scattering eye occluders. Blue (shortest wavelength) light is scattered in fog to the greatest extent, causing deterioration of vision quality especially for the monochromatic blue stimuli. However, for colour stimuli on a white background, visual acuity in fog for blue Landolt-C optotypes was higher than for red and green optotypes. The luminance of colour Landolt-C optotypes presented on a screen was chosen corresponding to the blue, green and red colour contributions in achromatic white stimuli. That results in the greatest luminance contrast for the white-blue stimuli, thus improving their acuity. Besides such blue stimuli on the white background have no spatial modulation of the blue component of screen emission. It follows that scattering which has the greatest effect on the blue component of screen luminance has the least effect on the perception of white-blue stimuli comparing to white-red and, especially, to white-green stimuli. Visual search experiments were carried out with simultaneous eye saccade detection. Red, green and blue Landolt-C stimuli were blurred using a Gaussian filter to simulate fog, and were shown together with distractors. Studies revealed two different search strategies: (1) for low scattering - long saccades with short total search times; (2) for high scattering, shorter saccades and long search times. Results of all experiments show better recognition of white-blue comparing to white-green colour contrast stimuli in the presence of light scattering.

### SEARCH EXPERIMENTS WITH BLURRED COLOUR STIMULI

**S. Fomins<sup>1</sup>, J. Parkkinen<sup>2</sup>, M. Ozolinsh<sup>1</sup>, V. Karitans<sup>1</sup>**

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

<sup>2</sup>*Department of Computer Science, University of Joensuu*

'C' letter optotype stimuli on white screen background were presented to observers with the task of finding a diagonally oriented gap letter between vertically oriented similar

distractors. The stimuli presented consisted of the sum of the clear stimulus and the blurred contribution. Blurring was applied through digital filtering with a Gaussian. Michelson contrast ratio of the luminance modulation along the gap region was chosen as a measure of the blur depth. The stimuli subtended 0.37, 0.75, and 1.5 deg. Blue and green stimuli were presented to three observers and thirty trials were run for the each of the search sets. The search time and the search object notification distance, were analysed. Two distinct searching behaviours were found. In the case of the low contrast and highly blurred sets the search behaviour is characterised by small step saccades mostly to the neighbouring distractor. Many backwards steps were made to compare the current stimulus with the previous one. With the high-contrast sets more typical for blue stimuli, large rapid saccadic movements along the task field were dominant. The fit of the search behaviour to the salience-based method of attention and object recognition model is applied.

### **SCATTERING-INDUCED LUMINANCE AND COLOUR CONTRAST DECREASE IN VISUAL PERCEPTION**

**M. Ozolinsh<sup>1</sup>, M. Colomb<sup>2</sup>, J Parkkinen<sup>3</sup>, G. Ikaunieks<sup>4</sup>, S. Fomins<sup>1</sup>,  
V. Karitans<sup>1</sup>, G. Krumina<sup>4</sup>**

*<sup>1</sup>Inst.of Solid State Physics, University of Latvia;*

*<sup>2</sup>Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand;*

*<sup>3</sup>Color research laboratory, University of Joensuu;*

*<sup>4</sup>Dept.of Optometry, University of Latvia*

The main impact of light scattering on vision tests is a deterioration of visual performance due to the decrease of luminance and colour contrasts of retinal images. We showed earlier that lowering of visual acuity and contrast sensitivity by scattering in the monochromatic case has the greatest effect on the perception of shorter-wavelength blue ^ black stimuli. For polychromatic stimuli, however, both luminance and colour contrast changes should be taken into account. Here, we present results of subsequent experiments on the perception of various polychromatic stimuli: high-contrast or isoluminant stimuli under different scattering conditions, such as natural fog; obstacles with various scattering degrees and spectral dependences; and digital simulation of scattering on presented stimuli. For the two latter cases, attenuation of the transmitted light was taken as a measure of the degree of scattering. Studies revealed that the extent of decrease of static and dynamic visual acuity and contrast sensitivity, and increase of the visual-search time due to scattering were greatest when distinguishing green stimuli on a white background, with no spatial modulation of the blue contribution over all areas of presentation of polychromatic stimuli.

### **TRAINED TO ANIMALS: SACCADE DIFFERENCES TO CLASSIFY IMAGES**

**R.Paeglis<sup>1</sup>, A. Podniece<sup>1</sup>, A. Pikulins<sup>1</sup>, I. Lacis<sup>2</sup>**

*<sup>1</sup>Dept.of Optometry, University of Latvia;*

*<sup>2</sup>Inst.of Solid State Physics, University of Latvia*

Psychologists, neurobiologists, and computer vision experts agree that the human visual system can classify objects ultrarapidly. It does so even without foveating or paying attention. We explored saccadic parameters as image categorisation tools. The voluntary response of the observer comes from the oculomotor system that overlaps the perceptual system. Ten subjects were asked to make a saccade towards a peripheral image if it contained a target, or else make an antisaccade. The control is then not transferred to a

different motor system, ie hand movement. Two synchronised computers with an iView X eye tracker were tuned to present a series of images for 300 ms each. With image recognition beyond 80%, eye movements as object recognition tools equip the researchers with additional knowledge about the classification process. Variability of saccadic velocities, amplitudes, and targets has been used as characteristics of image classification. We have studied regressive equations that describe gaze fixation 100 ms prior the movement launched. Fixations and saccadic velocity are tightly bound to the features of the briefly presented stimulus.

## **NO AVERAGE READER: PROFESSIONAL READERS EMPLOY A DIFFERENT FIXATIONAL STRATEGY**

**I.Lacis<sup>1</sup>, R. Paeglis<sup>2</sup>, K. Bagucka<sup>2</sup>**

*<sup>1</sup>Inst. of Solid State Physics, University of Latvia;*

*<sup>2</sup>Dept. of Optometry, University of Latvia*

Ability to read efficiently is an increasing challenge in the modern society. Malformed reading practices are to blame for insufficient academic accomplishments of students. In eye-movement recordings, properties of fixations emerge as predictors of text comprehension and word skipping. We extend the concept of a skilled reader to a person whose professional duties consist of text analysis and reviewing. 'Reading professionals' demonstrated their fixational length and saccadic velocity pattern (iViewX). As compared to students of various fields, 'professionals' exhibited higher word-grouping selectivity and information retention. Their pattern cannot be extrapolated from the common skilled reading. To test the effect of educational practice, 5 'non-professionals' were subjected to a speed-reading training for two months. After the training, the reading speed, number of fixations, and quality of text retention testified to higher processing efficiency. However, the reading pattern diverges from that of 'professionals'. We also stress that reading efficiency is language-specific. Fluent readers fixate about 60% more when reading in a second language, as compared to the native one. Eye movements in reading are specific to language and depend on education. Experimental data lend support to the conclusion that the concepts of 'average reader' and 'skilled reader' should be used with caution.

## **DYNAMICS OF EYE ABERRATION DETECTED BY HIGH-SPEED HARTMANN-SHACK ABERROMETER**

**Maris Ozolinsh<sup>1</sup>, Gatis Ikaunieks<sup>2</sup>, and Sergejs Fomins<sup>1</sup>**

*<sup>1</sup>Inst. of Solid State Physics, University of Latvia;*

*<sup>2</sup>Dept. of Optometry, University of Latvia*

Significance of the eye aberration measurements accuracy increases in the recent decade due to advances in the laser refractive eye surgery. Dynamic eye wavefront errors obtained with a high speed (30 frames/sec) Hartmann-Shack lenslet sensor aberrometer "MultiSpot 2500" providing measurements with 20 sec epoch time. Statistical analysis of measurement data was performed in time and frequency domains to estimate and characterize artefacts due to eye blinking and the tear film break-up in the 3rd and 4th order Zernike terms



# LIGHT SCATTERING EFFECT ON CENTRAL AND PERIPHERAL VISUAL ACUITY

G. Ikaunies<sup>1</sup>, M.Ozolinsh<sup>2</sup>

<sup>1</sup>*Dept. of Optometry, University of Latvia;*

<sup>2</sup>*Inst. of Solid State Physics, University of Latvia*

To assess the effect of light scattering on central and peripheral visual functions the visual acuity thresholds were measured at the fovea and at the different retinal eccentricities (0.5 – 4 degree) inducing different levels of light scattering. Black Landolt C optotypes with different colors backgrounds (grey, red, green and blue) were used as stimuli. The luminance contrast for all stimuli presented on computer screen was the same (60%). Stimuli were viewed using the best refraction correction. In order to generate different levels of light scattering the electrically controllable PDLC polymer dispersed liquid crystal eye occluders were applied. For black stimuli on grey background the visual acuity thresholds were significant different for two cases with and without light scattering occluders only within 2 degrees of the central fovea. Similar data however for word acuity thresholds are reported previously where contrast changes were applied directly to stimuli presented on computer screen. Results are compared with results of stimuli on red, green and blue backgrounds. Main factors which cause reduction of visual acuity with PDLC eye occluders for colored and achromatic stimuli are discussed.

## Scientific publications

### Published in 2005

1. S.Fomins, J.Parkkinen, M.Ozolinsh, V.Karitans, Search experiments with blurred colour stimuli, *Perception*, **35**, p. S171-2 (2006).
2. M. Ozolinsh, M. Colomb, G. Ikaunieks and V. Karitans, Colour stimuli perception in presence of light scattering, *Visual Neuroscience* **23**, pp. 597–601 (2006).
3. R. Paeglis, K. Bagucka, N. Sjakste, I. Lacis, Maximizing reading: pattern analysis to describe points of gaze. *Proc. SPIE*, Vol.**6315**, p.6515OR-7 (2006).
4. I.Lacis, R. Paeglis, K. Bagucka, No average reader: Professional readers employ a different fixational strategy, *Perception*, **35**, p. S87 (2006).
5. G.Ikaunieks, M.Ozolinsh, Light scattering effect on central and peripheral visual acuity, *Perception* **35**, S129 (2006).
6. M.Ozolinsh, M.Colomb, J.Parkkinen, G.Ikaunieks, S.Fomins, V.Karitans and G.Krumina, Scattering-induced luminance and colour contrast decrease in visual perception, *Perception* **35**, S136 (2006).
7. M. Ozolinsh, M. Colomb, G. Ikaunieks and V. Karitans, Colour stimuli perception in presence of light scattering, *Visual Neuroscience* **23**, pp. 597–601 (2006).
8. V.Karitans, M. Ozolinsh „Dynamical Visual Acuity in the Presence of Light Scattering”, In: Proc.ICO „*Photonics and Informatics*”, ITMO, St.Petersburg, pp.269-270 (2006).
9. M. Ozolinsh, G. Ikaunieks, and S. Fomins „Dynamics of eye aberration detected by high-speed Hartmann-Shack aberrrometer,” *Proc. Eur. Opt.Soc. Annual.*, Paris, pp.92-93 (2006).
10. J. M. Bueno, E. Berrio, M. Ozolinsh and G. Ikaunieks, „Optical properties of a polymer dispersed liquid crystal to be used on visual testing”, In: „*ICO Topical Meeting on Optoinformatics/Information Photonics 2006*”, ITMO, St.Petersburg, pp.276-278(2006).
11. R.Paeglis, A. Podniece, A. Pikulins, I. Lacis, Trained to animals: Saccade differences to classify images, *Perception* **35**, p. S87-88 (2006).

### **Reports in conferences**

1. Int. Student conference on Development in Optics and Photonics 2006, Riga.
2. 2nd Latvian conference “Functional materials and nanotechnologies”, 2006, Riga, Latvia
3. Eur. Conference on Visual Perception 2006, St.Peterburg, Russia.
4. Mathematics of Data/Image Pattern Recognition, Compression, and Encryption with Applications IX, SanDiego,2006.
5. Annual EOS-2006, Paris,2006.
6. Vision in Vehicles-11, Dublin, Ireland, 2006
7. ICO Annual „Photonics and Informatics-2006”, St.Peterburg, 2006.

# WIDE BAND GAP MATERIALS

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

## Research Area and Main Problems

Interests of the Laboratory of Wide Band Gap Materials are focused on the spectral research of compounds from the III, IV and V group elements such as AlN, BN, diamond, and some other related materials, which are promising for the various applications including optoelectronics and dosimetry. The special interest is focused on nanomaterials which could present some new features compared to those of their macro-sized forms. The properties of each material strongly depend on its defect structure possessing its own spectral characterization. Therefore, the spectral investigations performed in this laboratory and based on luminescence studies (photoluminescence (PL) and its excitation (PLE), optically stimulated luminescence (OSL) and thermoluminescence (TL)), can give the essential information about the defects and the optical properties of the material, including 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. Part of the investigations was performed together with the collaboration partners from abroad.

### Scientific Staff

1. Dr. Hab.Phys, Assoc. Prof. B.Berzina
2. Dr. L.Trinkler
3. J.Sils
4. A. Auziņa

### Students

1. V.Korsak
2. D.Kasjane
3. G.Ošeniēks
4. E.Tjutjunnika

### Visitors from abroad:

1. Prof. R.Tomasiunas, Institute of Material Science and Applied Research, Vilnius University, Lithuania (5 days).

### Scientific Visits Abroad:

1. B.Berzina, Wake Forest University, USA (5 days).
2. J.Sils, University of Osnabruk, Germany (11 month)

### Collaborations

#### Latvia

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

#### 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).

## **Taiwan**

National Taiwan University, (Prof. Li-Chyong Chen)

## **Lithuania**

Vilnius University, Vilnius, (Prof. R. Tomasiunas).

## **Romania**

National Institute for Material Physics in Solids, Bucharest, (Prof. S.Nistor)

## **Main results**

### **SPECTRAL CHARACTERIZATION OF h-BN NT/h-BN MIXED MATERIAL AND h-BN MACRO-SIZED PARTICLES**

**B. Berzina, L.Trinkler, V.Korsak, R.T.Williams<sup>1</sup>, B.Ucer<sup>1</sup>, D.Carroll<sup>2</sup>, E.Shishonok<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> *Institute of Solid State Physics and Semiconductors, Belarus Academy of Sciences, Belarus*

The spectral characteristics – photoluminescence (PL) spectra and its excitation spectra (PLE) were studied and compared using two types of h-BN materials. They were: *i*) the mixed material - nt-BN/h-BN consisting of BN nanotubes (mixture of single-walled and multi-walled tubes with diameters  $\geq$  to 5 nm) and a very small part of a raw material - h-BN macro-size powder, which is synthesized in the Center of Nanotechnologies, Wake Forest University, USA, and *ii*) h-BN macro-size powder obtained in Belarus Academy of Sciences.

The main results obtained are the following.

*i*) In the case of the nt-BN/h-BN material it was found that the BN nanotubes are responsible for the 390 nm wide PL band with the appropriate 260 nm excitation band. The mechanisms of this luminescence based on the excitonic processes were proposed and discussed.

*ii*) In macro-size h-BN powder the PL of the nano-arches, which are formed at the edges of the main h-BN sheets by dangling  $sp^2$  bounds, and which can be considered as a half of a nanotube was found (a wide PL band at 390 nm with excitation at 260 nm).

*iii*) The mechanisms of the exciton relaxation and self-trapping in the case of h-BN nanotubes were proposed and discussed.

# AlN FOR APPLICATION IN UV-LIGHT DOSIMETRY

**L.Trinkler, B.Berzina**

Dosimetric characteristics of AlN ceramics synthesized in Institute of Inorganic Chemistry, Riga Technical University were studied in this laboratory for a long time with the aim to elaborate a new sensitive material for application in the UV-light dosimetry. It was found that the main dosimetric properties of AlN keep up with such widely used materials as Al<sub>2</sub>O<sub>3</sub>:C and doped LiF and even overcome them, however, in the case of AlN the UV light-induced information, which is accumulated in the material on basis of the oxygen-related defects with 400 nm luminescence, is not stable at room temperature and decays with time presenting the so called fading. It was found that another luminescence band at 480 nm, which is also observed in the different types of AlN structures (ceramics, nanopowder, nanotips) is more stable at room temperature and therefore could be more prospective for the dosimetric application.

## OPTICAL PROPERTIES OF AlN NANOMATERIALS: NANOTIPS AND NANOPOWDERS

**L.Trinkler, B.Berzina, A.Auzina, D.Kasjane, E.Tjutjunnika, G.Ošeniēks, J.Grabis<sup>1</sup>, I.Šteins<sup>1</sup>, L.C. Chen<sup>2</sup>, S.C.Shi<sup>2</sup>**

<sup>1</sup> *Institute of Inorganic Chemistry, Riga Technical University, Latvia*

<sup>2</sup> *Center of Condensed Matter Sciences, National Taiwan University, Taiwan*

The UV light-induced luminescence properties have been studied for the AlN nanopowder with the grain size of 20 – 80 nm performed in the Institute of Inorganic Chemistry, RTU, Latvia and for the AlN nanotips (~1200 nm long with the diameter of 10 nm at the top and 100 nm at the base of the tip) synthesized in National Taiwan University, Center of Condensed Matter Sciences.

*i)* In the AlN nanopowder the main luminescence band is located at 480 nm with its excitation at 280 nm. The well known luminescence at 400 nm (250 nm excitation) of the oxygen-related centers, being predominant in the bulk material (AlN ceramics) is weak in comparison with that of the 480 nm in the nanopowder. The analysis of the luminescence properties allows us to conclude that 480 nm luminescence could be caused by luminescence centers located at the surface of the AlN grains.

*ii)* It was found that in the case of the AlN nanotips the well-pronounced 480 nm luminescence with its own photo excitation at 280 nm also appears besides the well-known luminescence at 400 nm caused by the oxygen-related defects. In the case of nanotips the main luminescence (at 400 nm and 480 nm) excitation is realized through the band-to-band transitions.

### Scientific Publications

1. B.Berzina, L.Trinkler, V.Korsak, R.Krutohvastov, D.L.Carrol, K.B.Ucer and R.T.Williams. "Exciton luminescence of boron nitride nanotubes and nano-arches", *phys. stat. sol.(b)* 243, No 14, 3840-3845 (2006).

2. S.-C. Shi, C. F.Chen, S. Chattopadhyay, K.-H. Chen, B.-W. Ke, L.-C. Chen, L. Trinkler and B. Berzina. „Luminescence properties of wurtzite AlN nanotips”. Appl. Phys. Lett. **89**, 163127-163127 (2006).
3. L.Trinkler, B.Berzina, A.Auzina, M.Benabdesselam, P. Iacconi. “UV light energy storage and thermoluminescence in AlN ceramics”. Accepted for publication in phys. stat. sol. (c) (Proceedings of EURODIM 2006).
4. L.Trinkler, B.Berzina, A.Auzina, M.Benabdesselam, P. Iacconi. “Use of aluminum nitride for UV radiation dosimetry”. Accepted for publication in Nuclear Instruments and Methods in Physics Research A. (Proceedings of ISRP-10).
5. R.T.Williams, K.B.Ucer, D.L.Carroll, B.Berzina, L.Trinkler, V.Korsak, and R.Krutohvostov. „Photoluminescence of self-trapped excitons in boron nitride nanotubes”. Accepted for publication in the Journal of Nanoscience and Nanotechnology.
6. B.Berzina, L.Trinkler, J.Grabis, I.Steins. „Photoluminescence in AlN macro-size and nano-powder”. Accepted for publication in phys. stat. sol. (c) (Proceedings of EURODIM 2006).

#### Lectures on Conferences

#### **22. LU Scientific Conference of Institute of Solid State Physics, University of Latvia, March 29-30, 2006, Riga, Latvia**

1. A.Auzina, L. Trinkler, B.Berzina. *Influence of oxygen ion implantation on photoluminescence of AlN ceramics*. Abstracts, p.11 (oral).

#### **2<sup>nd</sup> Latvian conference “Functional materials and nanotechnologies”, March 27-28, 2006, Riga, Latvia**

1. B.Berzina, L.Trinkler, A.Auzina, L.C.Chen, S.C.Shin, K.H.Chen, J.Grabis, I.Steins. *Luminescence processes in AlN: macrosized and nanomaterials*. Abstracts, p.11 (oral).

#### **10<sup>th</sup> Europhysical Conference on Defects in Insulating Materials EURODIM 2006, July 10-14, 2006, University of Milano-Bicocca, Italy**

1. L. Trinkler, B.Berzina, A.Auzina, M. Benabdesselam, P. Iacconi. *UV light energy storage in AlN ceramics.*, Abstracts, p 370 (poster).
2. B.Berzina, L.Trinkler, A.Auzina, L.C.Chen, S.C.Shin, K.H.Chen, J.Grabis, I.Steins. *Light-induced processes in AlN: macrosized and nanomaterials*. Abstracts p 186 (poster).

#### **10<sup>th</sup> International Symposium on Radiation Physics ISRP-10, September 17-22, 2006, Coimbra, Portugal**

1. L.Trinkler, B.Berzina, M. Benabdesselam, P. Iacconi. *Use of aluminum nitride for radiation dosimetry*. Abstracts, B-94 (poster).

#### **7<sup>th</sup> International Conference on Excitonic Processes in Condensed Matter EXCON 2006, June 26-30, Winston\_Salem, NC, USA**

1. B.Berzina, L Trinkler, R.Krutohvostov, V.Korsak, R.T.Williams, B.Ucer, D.Carroll. “*Photoluminescence on boron nitride nanotubes and nano-arches*”. Abstracts, p 53 (oral).

# **SURFACE PHYSICS**

**Head of Laboratory *Dr. hab. phys. J.Maniks***

## **Research Area and Main Problems**

The research interests of the laboratory cover materials for application in micro/nano-technologies, optics and tribology.

Research topics:

- micromechanical properties of surfaces, interfaces and thin films;
- obtaining of nanostructured materials, adhesion and related processes on phase boundaries and interfaces in heterogeneous and nanostructured materials;
- Surface modification by irradiation with swift heavy ions.

### **Scientific staff**

1. Dr.hab. J.Maniks
2. Dr. I.Manika
3. Dr. F.Muktepavela

### **Technical staff**

1. A.Petersons

### **Students**

1. G.Bakradze

## **Cooperation**

### **Latvia**

1. AS Sidrabe (Dr.V.Kozlovs).
2. Riga Technical University (Prof.V.Mironovs).
3. Daugavpils University (Dr. E.Tamanis).
4. Institute of Physics, University of Latvia (Dr.A.Shishko).

### **Germany**

GSI, Darmstadt (Prof.K.Schwartz).

### **Israel**

Technion, Haifa (Dr.S.Stolyarova).

### **Russia**

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

## Main Results

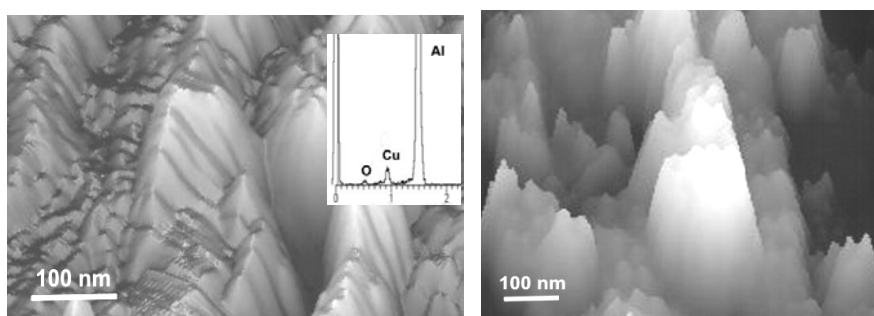
### OBTAINING, MECHANICAL PROPERTIES AND THERMAL STABILITY OF NANOSTRUCTURED METAL/OXIDE COATINGS

F. Muktepavela, G. Bakradze, E.Tamanis<sup>1</sup>, S.Stolyarova<sup>2</sup>

<sup>1</sup>Daugavpils University, Latvia

<sup>2</sup>Technion, Solid State Institute, Haifa, Israel

Nanostructured metals obtained by severe plastic deformation exhibit a good complex of mechanical properties due to the formation of dislocation-disclination substructure with the grain size of 10-100 nm. However, such nanostructure is not thermally stable. We elaborated a microtribological method for deposition of nanostructured coatings on different substrates. During such procedure performed in air atmosphere, small metal particles are cut out from a bulk metal specimen by means of rotating wire brush and transferred to the substrate under conditions of severe dynamic shear deformation and intensive oxidation which favor the formation of oxidized interlayers and ensure the thermal stability of nanostructures.



The AFM images and EDX spectrum of Al coatings on Cu (a) and glass (b).

The structure, surface morphology and microhardness of nanostructured Al, Zn, Cu, Sn, Pb and Cd coatings on glass and metal substrates obtained by the microtribological method were investigated. Coatings show strong adhesion to the substrates because of shear stress induced formation of reaction zone on the metal/substrate interface. Microhardness of obtained coatings is by a factor of 3-10 higher than that for the source metals due to the presence of oxidized interlayers in coatings. The annealing in vacuum leads to oxygen redistribution along oxidized interlayers as barriers for grain growth. Al/glass system is more stable in wide interval of temperatures, than the Al/Cu system, in which a possibility of different oxides ( $\text{Cu}_2\text{O}$ ,  $\text{CuO}$ ,  $\text{Al}_2\text{O}_3$ ) formation exists in the accordance with thermodynamics of metal-oxygen interaction. The method may be recommended for surface hardening, improving the wear-resistance and renovating the surfaces of the machinery elements.

This work was carried out in the framework of the National program of Latvia in Materials Science, project “Perspective inorganic materials for optoelectronics and microelectronics, and modern methods for the structure studies”.

### HEAVY-ION- INDUCED DAMAGE AND REDUCTION OF DISLOCATION MOBILITY IN LiF SINGLE CRYSTALS

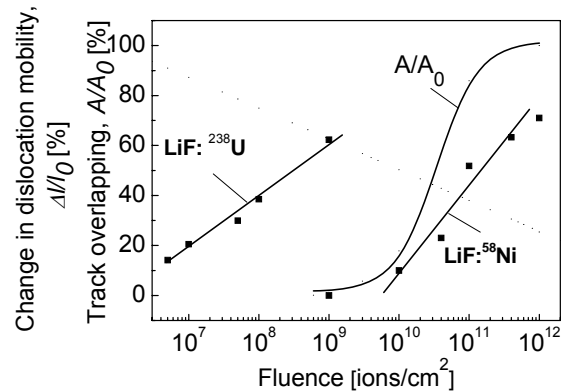
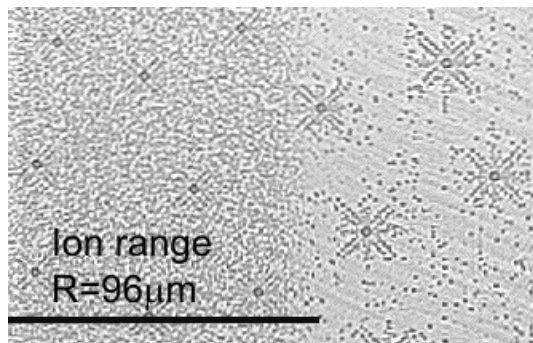
I.Manika, J.Maniks, K.Schwartz<sup>1</sup>

<sup>1</sup>GSI, Planckstrasse 1, D-64219 Darmstadt, Germany

Ion-induced reduction of dislocation mobility in LiF crystals irradiated with swift heavy (U) and light (Ni) ions of a specific energy of 11 MeV per nucleon at fluences between



$10^6$  and  $10^{11}$  ions/cm<sup>2</sup> was studied. The results show that irradiation with U ions reduces the dislocation mobility at comparatively low threshold fluences (above about  $10^6$  ions/cm<sup>2</sup>) were individual tracks as strong obstacles for dislocations play a dominating role. For lighter Ni ions, which create no track core damage, the reduction of dislocation mobility is observed only at high-fluence irradiations (above  $10^9$  ions/cm<sup>2</sup>) where the tracks overlap and the single defects can saturate and transform to more complex  $F_n$ -centers, alkali colloids, vacancy and halogen clusters.



For U ions, markedly stronger modifications of structure and dislocation mobility were observed on irradiated surface compared to those in the deeper layers. Generally, the results show that deep (up to 100 μm) implantation with fast heavy ions is suitable for nanoscale structuring and improving of micromechanical properties of materials.

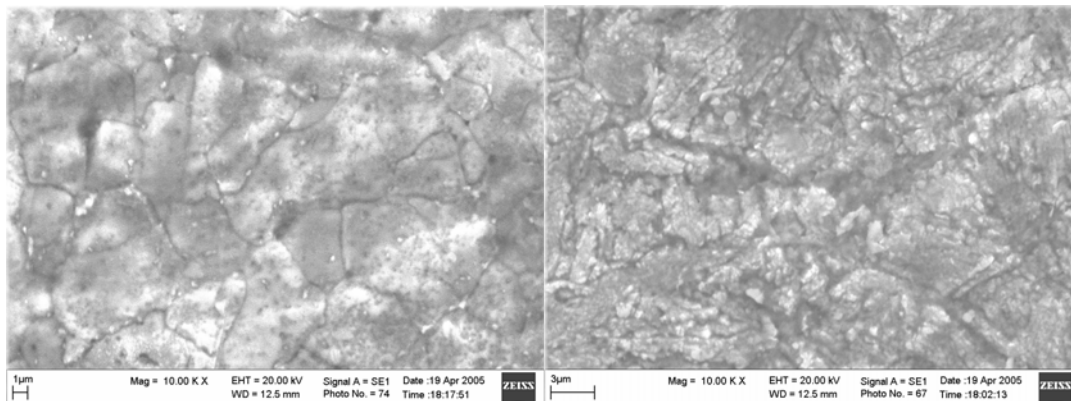
The work was supported by the grant No.05.1705 and Collaboration project No.05.0026.01 of the Latvian Council of Science.

## INFLUENCE OF MAGNETIC FIELD ON THE STRUCTURE AND MECHANICAL PROPERTIES OF EUROFER STEEL EXPOSED TO LIQUID Pb17Li ALLOY

**F. Muktepavela, I. Buceniaks<sup>1</sup>, E. Platacis<sup>1</sup>, A. Shishko<sup>1</sup>, K. Kravalis<sup>1</sup>**

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

EUROFER 97 steel as structural material in liquid metal blankets for fusion reactors should meet high stability of structure and mechanical properties under conditions of neutron irradiation, high temperature, magnetic fields and attack of liquid Pb-17Li alloy. The aim of presented work was the experimental investigation of magnetic field (B=1.7T) effect on corrosion processes of EUROFER 97 steel exposed to Pb-17Li eutectic alloy flow having mean velocity 2.5÷ 5 cm/s at  $T_{\max} = 550$  °C in specially for this purpose designed liquid metal loop. Optical and electron microscopy studies of surfaces exposed to liquid metal showed that dissolution of surface without magnetic field occurs uniformly both for ferrite and for martensite grains.



SEM structure of steel surface after contact with PbLi alloy without magnetic field (a) and with magnetic field (b), x10 000

At the presence of the magnetic field, a crushing of martensite phases and fast dissolution of interphase volumes is observed. Microhardness values of surfaces after corrosion in the presence of magnetic field have decreased by a factor of about two. EDX analysis of surfaces showed that the magnetic field promotes dissolution of Cr, Fe and W, that is in agreement with the results of microindentation. Obtained results testify the distinctions in corrosion mechanisms of EUROFER 97 steel in Pb-17Li flow with and without magnetic field.

The investigations were performed in the framework of EUROATOM project.

## EVALUATION OF THE MECHANICAL PROPERTIES OF SINGLE CRYSTALS IN SUB-MICROMETER VOLUMES

**J.Maniks, I.Manika**

The indentation size effect (ISE) in Au, Ag, Cu, Al and LiF single crystals has been investigated using Vickers microindentation test. The microhardness data and reference data of static nanoindentation of Au, Ag, Cu, Al and LiF crystals for a wide range of indentation depth fit a linear  $\log H - \log h$  relationship. This has allowed us to perform extrapolations and estimate the hardness for sub-micrometer deformed volumes. The estimated hardness values at the surface approach the theoretical shear strength of the material. The results confirm the complex nature of the ISE. Localization of the deformation, strain gradients in the deformation zone and effect of free surface are considered as primary factors responsible for the ISE. A substantial contribution from the non-dislocation mechanisms based on the mass-transport by the point defects (e.g. crowdional plasticity) is also suggested.

The work was supported by the grant No.05.1705 of the Latvian Council of Science.

### Scientific publications Published in 2006

1. I.Manika, J.Maniks. Size effects at micro- and nanoscale indentation. *Acta Materialia*, 2006, vol. 54, Issue 8, pp.2049-2056.
2. I.Manika, J.Maniks. Evaluation of the mechanical properties of single crystals in sub-micrometer volumes. *Latvian Journal of Physics and Technical Sciences*, 2006 No2 (II), pp.75-82.
3. I.Manika, J.Maniks. Ion-induced hardening in LiF: energy loss and fluence effects. *Nuclear Instruments and Methods B*, 2006, vol.245, Iss.1, pp.260-263.
4. F. Muktepavela, G. Bakradze and S. Stolyarova. Effect of Mechanoactivation on Interfacial Interaction in Metal/Oxide Systems. *Defect and Diffusion Forum*, Trans.

- Tech. Publications, Ed. B.S. Bokstein and B.V. Straumal, 2006, vol 249, p.263-268.
5. Ф.Муктепавел, Г.Бакрадзе, С.Столярова, Особенности твердофазного взаимодействия на границе раздела металл/оксид в условиях пластической деформации металла, Известия РАН, Серия: Физическая, 2006, vol. 70, N9, p.1384-1387.
  6. G.Bakradze, F.Muktepavela, S.Stolyarova, E.Tamanis. Mechanical properties and thermal stability of Al-Cu-O nanostructured coatings obtained by the microtribological method. Latvian Journal of Physics and Technical Sciences, 2006, No2 (II), pp.141-148.
  7. I. Bucenieks, R.Krishbergs, E.Platacis, G. Lipsbergs, A.Shishko, A.Zik, F.Muktepavela. Investigation of corrosion phenomena in EUROFER steel in Pb-17Li stationary flow exposed to a magnetic field. J. Magnetohydrodynamics, 2006, vol.42, No.2-3, pp. 237-251.
  8. V.Mironov, V.Lapkovskis, F.Muktepavela. Property and structure changes of sintered powder materials by treatment in the pulse magnetic field. Proceedings of the 5th International Conference of DAAM Baltic (ed.R.Kyttner), Tallin, Estonia, 2006, pp.78-80.
  9. F.Muktepavela, G.Bakradze, S.Stolyarova. Investigation of the role of metal deformation processes and nanostructure state in solid-state adhesion between s-p metals and oxides at 293K. RTU Zinātniskie raksti . Materiālzinātne un lietišķā ķīmija, 2006, 10. sējums, lpp. 133-142.

#### Lectures on Conferences

##### **22th Scientific Conference of Institute of Solid State Physics, University of Latvia, February 6-9, 2005, Riga, Latvia**

1. F.Muktepavela, R.Krutohvastovs, A.Shishko, K.Kravalis, E.Platacis. Structure and mechanical properties of EUROFER97 steel exposed to flowing Pb-17 Li. Abstr.p.32
2. **A.Shishko, I.Bucenieks, E.Platacis, G.Lipsbergs, R.Krishbergs, F.Muktepavela Influence of MHD Phenomena on steel corrosion in Pb-Li flow. Abstr. p.31.**
3. V.Skvortsova, N.Mironova-Ulmane, V.Silinevich, G.Bakradze. Effect of impurities on optical and micromechanical properties of magnesium oxide. Abstr.p.10.

##### **10th Europhysical Conference on Defects in Insulating Materials, EURODIM 2006, July 10-14, Milano, Italy**

4. **F. Muktepavela, G. Bakradze, S. Stolyarova Nanostructured me/oxide coatings. Abstr, p.273**

##### **2nd Latvian conference “Functional materials and nanotechnologies”, March 27-28, 2006, Riga, Latvia**

5. G.Bakradze, F.Muktepavela, S.Stolyarova, E.Tamanis. Thermal stability of Al-Cu-O nanostructured coatings obtained by the microtribological method. Abstr. p. 9.
6. I.Manika, J.Maniks. Evaluation of the mechanical properties in submicron volumes. Abstr.p.44.
7. A.Medvids, P.Onufrijevs, D.Grabovskis, F.Muktepavela, G.Bakradze. Low -K SiO<sub>2</sub> layer formation on Si by YAG:Nd laser radiation..Abstr. p. 46.

**International Conference “Advances in Nanostructured Materials, Processing-Microstructure-Properties”, Nanoved 2006- Nenamat, May 14-17, 2006, Stara Lesna, Slovakia**

8. F. Muktepavela, G. Bakradze, S. Stolyarova, E. Tamanis, R.Krutohvastov.  
Nanostructured Al coatings obtained by microtribological method Abstr. p.110

**Петербургские чтения по проблемам прочности,  
14-16 марта 2006, С-Петербург, Россия**

9. F.Muktepavela, G. Бакрадзе. Формирование и микромеханические свойства межфазных границ ме/оксид в условиях сдвиговых деформаций металла. Тезисы, стр 183.

**International Workshop on Liquid Breeder Blankets,  
June 7-9, 2006, St.Petersburg, Russia**

10. F.Muktepavela, I.Buceniaks, E.Platacis, A.Shishko, K.Kravalis Results of experimental investigations of the magnetic field influence on the corrosion of Eurofer stell in the Pb17Li flows at 550C. Abstr. P.30.

**5th International Conference of DAAM Baltic, Industrial Engineering - Adding Innovation Capacity of Labour Force and Entrepreneurs,  
20-22 April, 2006, Tallin, Estonia**

11. V Mironov., V. Lapkovskis, F. Muktepavela Property and structure changes of sintered powder materials by treatment in the pulse magnetic field.

**International Conference „Advanced Optical Materials and Devices”, AOMD-5,  
27-30 August, 2006, Vilnius, Lithuania**

12. I.Manika, J.Maniks, K.Schwartz. Heavy ion induced damage and reduction of dislocation mobility in LiF single crystals. Abstr. p.59.

# LABORATORY OF RADIATION PHYSICS

Head of laboratory Dr. hab. J.Berzins

## Research Area and Main Problems

The Laboratory consists of four groups – the nuclear spectroscopy and theory, applied nuclear physics, oxide physics and high temperature superconductivity. 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;
- application of the liquid scintillation methods for monitoring tritium content in surface and underground waters;
- the magnetic ions exchange interaction in the antiferromagnetic oxides MeO - MgO solid solutions were studied using of optical absorption, luminescence, EPR and Raman spectroscopies;
- exchange interaction between radiation defects and transition metals ions in the dielectric crystals with the transition metals ions;
- develop electron paramagnetic resonance (EPR) dosimetry to measure accumulated doses of ionising radiation absorbed by individuals;
- investigations of magnetic hysteresis loops for ensembles of single domain particles
- development of gamma spectrometric methods for investigation of radionuclides, its migration in the soils and ground waters in the most potentially polluted regions of Latvia.
- application of the liquid scintillation methods for monitoring tritium content in surface, underground and drinking waters.
- study on possibility to use Salaspils cyclotron for activation analysis.

The systematic investigations of hyperdeformation in the  $A \approx 100-130$  mass region were performed in the framework of the cranked relativistic mean field theory.

The magnetic ions exchange interaction in the antiferromagnetic oxides MeO-MgO solid solutions were studied using of optical absorption, luminescence, EPR and Raman spectroscopies.

The values of magnetic parameters of fine magnetic particles are the result of complicated 'game' of different kinds of anisotropies, their magnitudes and distribution of particles in the ensembles; in the case of oxidized Co particles uniaxial anisotropy arising from dipole-dipole interaction should be taken into account.

## Scientific Staff

- |                             |                            |
|-----------------------------|----------------------------|
| Dr.hab. J.Berzins           | 10. Dr. D.Riekstina        |
| Dr.hab. M.Balodis           | 11. Dr. V.Skvortsova       |
| Dr.hab. V.Bondarenko        | 12. Dr. O.Veveris          |
| Dr.hab. A.Afanasjevs        | 13. Dr. A.Petrovs          |
| Dr. hab. U.Ulmanis          | 14. Dr. J. Ruza            |
| Dr.hab. N.Mironova - Ulmane | 15. Dr. G. Smilskalne      |
| Dr. hab. J. Tambergs        | 16. Dr. Ing. A.Pavlenko    |
| Dr. L.Simonova              | 17. Mag. sc.I. Motmillere  |
| Dr. T. Krasta               | 18. Mag. sc. J. Proskurins |
|                             | 19. Mag. sc. A. Polakov    |

### Technical Staff

1. S.Afanasjeva
2. L. Neiburgs
3. A. Sotaks

### Students

1. Bach. sc. A. Andrejevs
2. R. Sadauskis

### Scientific visits abroad

- Dr. hab. A.Afanasjev Mississippi University, Mississippi, USA (10 month).  
Dr. hab. J. Berzins European Commission Euratom, Brussels, Belgium (10 days).  
Dr. hab. J. Berzins European Commission Workshop on Quality of measurements, Geel, Belgium  
Dr. hab. J. Berzins 35th European Cyclotron Progress Meeting (ECPM 2006) Nice (France) 2.-4.11.  
Dr. hab. J. Berzins Cyclotron Networking Meeting, Ispra, Italy, 22-22 November.  
Mag.sc. J.Proskurins, 56th International Conference „NUCLEUS-2006” on Problems of Nuclear Spectroscopy and Structure of Atomic Nucleus. Sarov, Russia, 4-8 September, 2006  
Dr. D.Riekstina, 3<sup>rd</sup> International Conference in Lithuania “Metals in The Environment”, Lithuania, Vilnius (4 days),  
Dr. D.Riekstina, International Symposium In Situ Nuclear Metrology as a Tool for Radioecology, Turkey, Kusadasi (3 days).  
Dr. hab. N.Mironova-Ulmane, Institute of Physics Tartu Estonia (1week +1 week)  
Dr. hab N.Mironova-Ulmane, Kyonggi University, Seoul, Korea (1week)  
Dr. V. Skvortsova Krakov, Poland, (1week) .  
Dr. V. Skvortsova, Coimbra, Portugal. (1week)

## Cooperation

### Latvia

1. Medical Academy of Latvia ( Dr. hab., Prof. M.Eglite, Dr. hab. Prof. I. Cema, Dr.T.Zvagule).
2. Hazardous Waste Management State Agency “BAPA”.
3. Radiation Safety Center (A.Skujina)
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.Dehtjar,).

### USA

1. Lawrence Livermoor National Laboratory, California (Prof. R. W. Hoff).
2. Brookhaven National Laboratory, Upton (Prof. R.F. Casten).
3. New-York University Stony Brook, Stony Brook (Prof. D. Fossan).
4. Notre Dame University, Notre Dame, USA (Prof. S. Frauendorf).

### Brasil

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

**Lithuania**

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

**Canada**

Department of Astronomy and Physics, Saint Mary's University, Halifax  
(Mg.A.Aleksejevs)

Department of Physics, Acadia University, Wolfville (Mg.S.Barkanova)

**Germany**

Technische Universität München (Prof. T von Egidy, Dr. H.-F. Wirth)

**Czech Republik**

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

2. Department of Nuclear Physics, Charles University (Prof. J. Kvasil).

**France**

1. Institute Laue-Langevin, Grenoble (Prof. H. Börner).

**Estonia**

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

**Italy**

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

2. Dipartimento di Scienze Geologiche, Università Roma Tre, Rome ( M. Piccinini)

3. INFN and Dipartimento di Fisica, Università di Trento, Povo (Trento)( G.Mariotto)

4. INFN and Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (Cosenza) (E.Cazzanelli)

**Ukraine**

1. State University “ Lvivska Politechnika” , Lvov ( prof. A.Matkovskii).

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

3. 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 Physics, PAS, Warsaw ( Dr. A.Suchocki).

**Russia**

1. Ural State University, Ekaterinburg (Prof. A. Nikiforov).

2. Ural Technical University, Ekaterinburg (Prof. B.Shulgin)

5. Institute of Chemical Physics, Chernogolovka, Russia (prof.V.Petinov)

6. St.Petersburgh Nuclear Physics Institute, Gatchina (Dr.V.Bunakov)

**Austria**

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

2. IAEA (Dr. A. Shakashiro)

## Denmark

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

## Kazakhstan

1. Eurasian national university , Astana (Prof. K. Dombaev )

## MAIN RESULTS

### THE ORIGIN OF THE NEW ISOMER IN $^{187}\text{W}$

**V. Bondarenko\*\* , J. Honzátko\* , I. Tomandl\* , J. Bērziņš\*\* ,**

An evidence for the unknown short-lived activity in  $^{187}\text{W}$  isotope has already been reported in our previous work [1]. As was established for the first time, the decay slope for the pair of 273-474 keV transitions belonging to  $^{187}\text{W}$  was almost constant in comparison to the slope of the well known 134-479 keV isomeric pair in the daughter  $^{187}\text{Re}$  with  $T_{1/2}=555(2)$  ns. These preliminary data gave the lifetime of the unknown isomeric state greater than 1  $\mu\text{s}$ . To determine more precisely this value the available time range in the new measurements was increased by a factor two. Representative timing spectra created by selected pairs of  $\gamma$ -transitions are shown in Fig. An analysis of the experimental data points belonging to the delayed events gives the weighted averaged  $T_{1/2}=1312(80)$  ns that is determined relative to the decay slope of the  $^{187}\text{Re}$  isomer.

A firm placement in the level scheme and the origin of the new isomer become clear only when the whole analysis of the prompt level populations in the (n, $\gamma$ ) and (d,p) reactions has been completed. The new isomer is now localized at 410.1(5) keV excitation energy and this state is associated with the  $11/2^+[615]$  Nilsson state which existence at low energies was expected but not found previously [2].

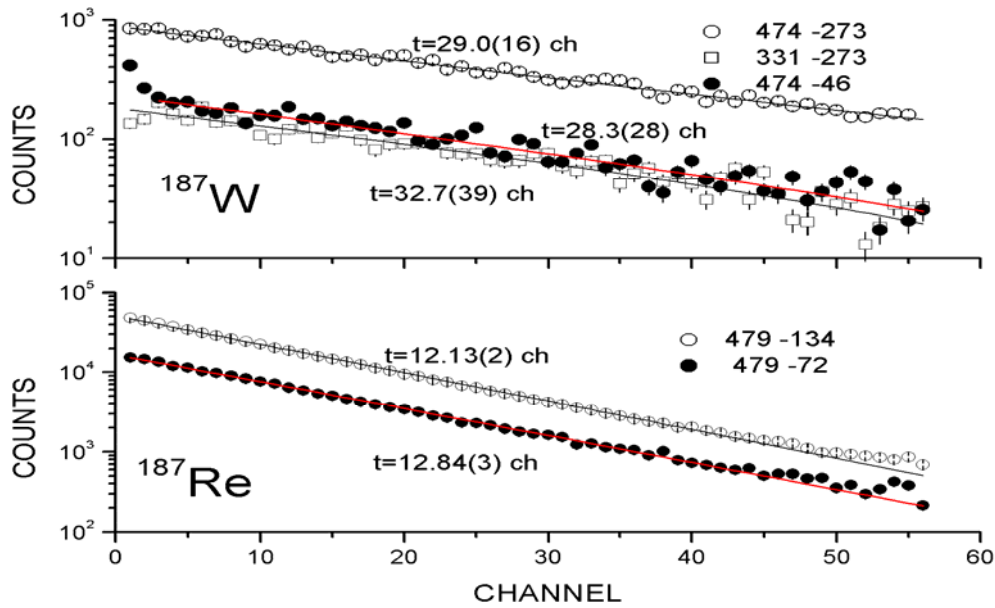
\*Nuclear Physics Institute, 250 68 Řež, Czech Republic,

\*\*Institute of Solid State Physics, University of Latvia, Rīga, LV-1063, Latvia,

[1] I. Tomandl, J. Honzátko, V. Bondarenko, J. Bērziņš, Proceedings of the workshop on Neutron Measurements, Evaluations and Applications (NEMEA-1), Nov. 2003 Budapest, ed. A. Plompen, EUR Report 21100 EN.

[2] V. Bondarenko, A.V. Afanasjev, T. von Egidy, L. Simonova, J. Bērziņš, I. Kuvaga, W. Schauer, J. Ott, P. Prokofjevs, R. Georgii, M. Kessler, T. Körbitz and W. Schott, Nucl. Phys. A 619 (1997) 1.





## STRUCTURE OF $^{194}\text{Ir}$ VIA GEOMETRIC AND ALGEBRAIC MODELS

*M. Balodis, H.-F. Wirth<sup>1</sup>, G. Graw<sup>1</sup>, R. Hertenberg<sup>1</sup>, J. Bērziņš, N. Krāmere, J. Jolie<sup>2</sup>, S. Christen<sup>2</sup>, O. Moeller<sup>2</sup>, D. Tonev<sup>2</sup>, and T. von Egidy<sup>1</sup>*

Model interpretation needed for a complete picture of the studied  $^{194}\text{Ir}$  nuclear structure is shortly described. A revised interpretation via Nilsson configurations (see our earlier publications) and associated rotational bands is obtained. New rotational levels is an important result.. Most low energy levels belong to negative parity, and they are grouped into nine bands: three with  $K=0$ , three –  $K=1$ , two –  $K=2$ , one –  $K=3$ . The high spin isomer  $K=11^-$  also is a band head. Positive parity levels are interpreted via four bands resp. band heads with  $K=2, 3, 4$ , and  $5$ .

From all bands expected at low energies, only those with  $K=6,7^+$  could not be identified, because of too high spin values.

Today's interpretation is thought to be essentially better, although an approach is traditional. One should note that  $^{194}\text{Ir}$  is the heaviest rare earth region nucleus interpreted in detail via prolate-deformed nuclear shape. Main configurations are attributed for generally highly mixed band structures. Algebraic model of supersymmetry for  $^{194}\text{Ir}$  and the neighbouring nuclei is analyzed by our coauthors Jan Jolie et al. (Univ. Koeln (Cologne)) in their recent conference reports.

1 Physik-Department, Technische Universität München, D-85748 Garching, Germany.

2. Institute of physics, University of Köln, Germany.

## STUDIES OF $^{188}\text{Re}$ STRUCTURE

**V. Bondarenko, I. Simonova, J. Berzins**

$^{188}\text{Re}$  has been studied using the prompt  $\gamma$ - $\gamma$  coincidences from thermal neutron capture in  $^{187}\text{Re}(n,\gamma)^{188}\text{Re}$  reaction at the LWR-15 reactor in Rež (Czech Republic). Secondary

gamma transitions were recorded in the energy range 60 – 2230 keV. 99 gamma spectra were calculated in gamma-gamma coincidences for high and low energy gates (5808-4619 keV and 63-394 keV) and 37 new levels were established in the the energy range 700 – 2150 keV. The data evaluation is in progress.

### **STUDIES OF CLASSICAL ENERGY LIMIT OF INTERACTING BOSON MODEL IN THE CASE OF THREE-BODY INTERACTIONS**

**J.Proskurins, A.Andrejevs, T.Krasta, L.Neiburgs, J.Tambergs**

In presented study of the classical energy limit of Interacting Boson Model two ways of inclusion of the three-body interaction terms have been considered.

In the first case, it has been found that the energy minimum for triaxial nuclear shape at the triaxiality parameter  $\gamma=30^\circ$  is ensured by all cubic d-boson interaction terms with momenta  $L=0,3,4,6$  together. This conclusion is opposite to the exclusive role of  $L=3$  term only, stressed in other authors studies before.

Alternatively, the classical energy minima for two recently proposed (G.Thiamova, P.Cejnar, 2006) simple Interacting Boson Model versions with cubic  $O(6)$  symmetric quadrupole operator interaction terms have been considered via a detailed study of solutions of corresponding quartic algebraic equations for energy minima conditions. The analysis of spherical-prolate-oblate shape phase transitions have been given on the basis of obtained results.

### **APPLICATION OF A LIQUID SCINTILLATION SPETROMETRIC METHOD FOR MONITORING TRITIUM IN GROUND WATERS**

**D. Riekstina, O. Veveris, A. Skujina, A. Zalkalne**

The monitoring of tritium concentration level in the wells around the shut-down nuclear research reactor Salaspils and the radioactive waste depository has been carried out for the period of 7 years. The increased concentration of tritium was detected in three wells of the reactor territory and in one well of the radioactive waste repository. The periodic changes of tritium concentration level was observed in some wells of the reactor territory. In the territory of radioactive waste repository, the increased concentration of tritium was observed in one well in the direct vicinity of the waste basin. The tritium concentration in this well is more than 10 times lower than that according to the 1997 year data. The H-3 concentration in the rest of this territory wells is within 2-18 Bq/l limits during last 5 years.

### **ASSESSMENT OF RADIUM-226 POLLUTED TERRITORY OF A SHUT DOWN MEDICAL INSTITUTION**

**D. Riekstina, J. Malnacs, O. Veveris, J. Berzins, A. Grivite**

The aim of presented study was to assess the extent of pollution by radium and its decay products in the rooms (walls, floors) of the former medical object, as well as the migration of this pollution in the soils of territory, surrounding the object. For many years, this object incorporated a complex of radon production facility, where radon was produced from radium salts and used for the treatment of patients. The overall territory of the object was 2600 m<sup>2</sup>, and there were 6 buildings.

The presence of natural radionuclide U-238, which is in equilibrium with its decay products Ra-226, Bi-214, Pb-214, was established in all samples of soil. In upper layers, Cs-137 (global pollution) was detected as well. Difference in the concentrations of Ra-226 radioactivity and that of other U-238 decay products allow one to assess the pollution level with Ra-226. In some separate places concentration of Ra-226 exceeds natural background 100 times. Pollution of soil was established in the depths up to 3 m. Obtained data enable one to work out a strategy for the recovery of investigated territories.

### **ESTIMATION OF INTERNAL AND EXTERNAL EXPOSURE IN RETROSPECTIVE DOSIMETRY**

**N. Mironova-Ulmane, A. Pavlenko**

Individual dose reconstruction by Electron Paramagnetic Resonance (EPR) has been performed for group of Latvian inhabitants participated in Chernobyl reactor accident clean-up activities. The total EPR dose including exposure from internal/external beta and gamma radiations was significantly higher, when officially documented dose where only external gamma exposure was registered. The internal component of total EPR dose has been verified by activity concentration measurements on teeth enamel. The radioactivity of the teeth was measured in the low-background equipment, placing above the sample the Al filter that fully absorbs beta-particles from  $^{90}\text{Sr}$ , but partly - from  $^{90}\text{Y}$ . Hence we avoid the error caused by the self-absorption of low energy beta particles of  $^{90}\text{Sr}$  in the investigated sample. The radioactive standard of  $^{90}\text{Sr}$  plus  $^{90}\text{Y}$  was measured in the same way. The results demonstrated correlation between external and internal exposure for one part of liquidators. The other part having no records on external exposure had significant dose from internally incorporated nuclides.

### **UNCERTAINTIES OF ABSORBED DOSE RECONSTRUCTION ON TOOTH ENAMEL**

**N. Mironova-Ulmane, A. Pavlenko**

Retrospective assessment of individual dose by Electron Paramagnetic Resonance (EPR) utilized human teeth enamel as a radiation detector. Ionizing radiation creates stable  $\text{CO}_3^{3-}$  radicals in enamel which latter on are measured by EPR. The amplitude of EPR signal is proportional to the amount of inserted radicals and to absorbed dose. The EPR method was applied for assessment of individual radiation dose for the survivors of the atomic bomb explosion in Japan, nuclear workers in South Ural, Chernobyl reactor accident liquidators. Results of these studies confirmed possibility to use EPR method for dose reconstruction done to 30 mGy level. However, for evaluation of such low level exposure the special precautions should be taken. The given paper is focused on evaluation and analysis of possible uncertainties arising during dose reconstruction on teeth enamel by EPR method. The contribution of different factors (equipment and sample related, radiation sensitivity calibration, signal processing) to the combined standard uncertainty of EPR method analyzed.

### **CALCULATIONS OF HYSTERESIS LOOPS FOR COBALT FINE PARTICLES WITH EXCHANGE ANISOTROPY**

**A. Petrovs, I. Kudrenickis**

To explain the observed difference in the magnitude of the coercitive force  $H_c$  between the ensembles of particles cooled respectively in the magnetic field and without one it is

reasonable to suppose that in the latter case the crystallographic direction [111] is the ease one both for the uniaxial and exchange anisotropies and the exchange anisotropy is randomly distributed over the ensembles of the particles.

#### Calculation Data for Hysteresis Loop Changes

$K_{\text{exch}}, \text{erg/cm}^2$	$c$	$\delta D_c$	$\delta M_r$	$\delta H_c, \text{Oe}$
0.14	-0.4	0.15	0.02	130
0.23	-0.7	0.33	0.05	280
0.28	-0.83	0.37	0.07	320

$D_c$  – relative coercitive force,  $D_c = (M_s H_c) / K_{\text{uniaxial}}$ ,  $\delta D_c$  – the change of  $D_c$

$\delta M_r$  – the change of the relative remanent magnetization,

$c = K_{\text{exch}} S / K_{\text{uniaxial}} V = 3(K_{\text{exch}} / K_{\text{uniaxial}}) / R$ ,  $R$  – radius of particle

$\delta H_c$  – the change of coercitive force  $H_c$ ,

the values of  $K_{\text{uniaxial}} = 1.3 \cdot 10^6 \text{ erg/cm}^3$  and  $M_s = 1450 \text{ G}$  are taken to determine  $c$  and  $\delta H_c$ .

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2. A. V. Afanasjev, Superheavy nuclei: a Relativistic Mean Field Outlook, Physica Scripta T125 (2006) 62-67.
3. A.O. Evans, E. S.Paul, ... K.Starosta, C.Vaman, A.V.Afanasjev, and I. Ragnarsson et al, Magnetic properties of smooth terminating dipole bands in  $^{110,112}\text{Te}$ , Physics Letters B636 (2006) 25-30.
4. A.O.Evans, E.S.Paul, A.J.Boston, A.V.Afanasjev, and I. Ragnarsson et al, Magnetic properties of deformed dipole bands in  $^{110,112}\text{Te}$ , Physica Scripta T126 (2006) 192.
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Smooth terminating bands in  $^{112}\text{Te}$ : particle-hole induced collectivity, Physical Review C 75 (2007) 014308: 1-10.
7. P.J.Davies, AV.Afanasjev, R. Wadsworth, et al, Identification of the g 9/2 proton and neutron band crossing in the N=Z nucleus  $^{76}\text{Sr}$  Physical Review C, in press.
8. M. Balodis, H.-F. Wirth, G.Graw, R. Hertenberger, J. Berzins, N.Kramere,J.Jolie, T. von Egidy, transfer and neutron capture reactions to  $^{194}\text{Ir}$ , Nucl. Phys., in press.
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#### **22-th Scientific Meeting of Institute of Solid state Physics, University of Latvia, Riga, March 29-30, 2006.**

1. M. Balodis, J. Berzins, Study of the  $^{192}\text{Ir}$  nuclear level scheme using the geometric rotor-plus-particle model, p. 28.

2. V. Bondarenko, I. Tomandl, J. Honzatko, H.-F. Wirth, J. Berzins, Evidence for a new isomer in  $^{187}\text{W}$ , p. 29.

3. J.Proskurins, A.Andrejevs, T.Krasta, J.Tamberg. Studies of Classical Energy Limit of Interacting Boson Model in the Case of Triaxial Deformations, 2006, p. 27.

4. V.Skvotsova, N.Mironova-Ulmane, V.Silinevich, G.Bakradze. Effect of impurities on optical and micromechanical properties of magnesium oxide. Abstracts p.10.

5. D. Riekstina, O. Veveris, Diffusion of  $^3\text{T}$  and  $^{137}\text{Cs}$  in water from cement compound, p. 34.

#### **56th International Conference „NUCLEUS-2006” on Problems of Nuclear Spectroscopy and Structure of Atomic Nucleus, 4-8 September, 2006, Sarov, Russia**

1. J.Proskurins, A.Andrejevs, T.Krasta, L.Neiburgs, J.Tamberg. Studies of Classical Energy Limit of Interacting Boson Model in the Case of Three-Body Interactions p 111-112.

#### **XXII Baltic Conference on the History of Science Vilnius, October, 5-6, 2006.**

J.Tamberg. History of Theoretical Nuclear Physics in Latvia (1936-2006). Abstracts, Vol.1, p.35-36.

#### **3<sup>rd</sup> International Conference in Lithuania “Metals in The Environment”, Vilnius, Lithuania, April 26-29, 2006**

1. D. Riekstina, O. Veveris, J.Berzins, J.Alksnis, A. Skujina, Evaluation of radionuclides accumulation in soil around the shut-down nuclear reactor and radioactive waste repository of Latvia, p. 102-103.

#### **International Conference “EcoBalt’2006”, Riga, May 11-12, 2006**

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#### **International Symposium In Situ Nuclear Metrology as a Tool for Radioecology, Kusadasi, Turkey, September 06-08, 2006**

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V. Skvortsova, N. Mironova-Ulmane, A. Kuzmin, U. Ulmanis, I. Sildos, Growth and Optical Properties of Transition Metal Oxides Single Crystal Solid solution, p. 205.

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V. Skvortsova, N. Mironova-Ulmane, U. Ulmanis. Radiation defects and transition ions interaction in magnesium oxide, p. C-17.

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N. Mironova-Ulmane, A. Pavlenko. Estimation of Internal and External Exposure in Retrospective Dosimetry. Proceeding of ISSN 1727-1983 ISBN 3-540-36839-6 Springer Berlin Heidelberg New York pp.2026 – 2028.

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1. N. Mironova-Ulmane, A. Kuzmin, V. Skvortsova, U. Ulmanis, I. Sildos, The role of phonons and magnons in formation of optical absorption fine structure in MnO, pp. 96 - 99.

2. N. Mironova-Ulmane, A. Kuzmin, V. Skvortsova, U. Ulmanis, I. Sildos, Optical properties of solid solution  $Ni_cMg_{1-c}O$  International conference, pp. 93- 95.

3. V. Skvortsova, N. Mironova-Ulmane, U. Ulmanis, Defects in gadolinium gallium garnet single crystals irradiated by neutrons, pp.149 - 151.

**International Symposium on Spin Waves in Magnetics, June 28 – July 1, 2005, Sankt-Petersburg, Russia May 2006.**

1. A. Petrovs, I. Kudrenickis, Calculations of Hysteresis Loops for Cobalt Fine Particles with Exchange Anisotropy. Symposium Abstracts, page 39.

**6<sup>th</sup> International Conference on Fine Particles Magnetism(ICFPM) “ New trends in nanoparticle magnetism”, Rome, October 9-12, 2007**

1. A. Petrov, I. Kudrenickis, Exchange Anisotropy in cobalt fine particles, theses

**VIII Latin American Workshop on Magnetism, Magnetic Materials and their Applications, 12-16 August, 2007, Rio de Janeiro, Brazil**

1. A. Petrov, I. Kudrenickis, Calculations of Hysteresis Loops for Cobalt Fine Particles with Exchange Anisotropy, theses.

**Popular scientific papers**

V. Gavars. J. Bērziņš, Investigation of possible implementation of joint Baltic nuclear power plant, EU Forum, 2006.

*Didactic work*

University of Latvia

1. Master degree course „Basic principles of general relativity and cosmology” (J. Tambergs).

2. Lecture courses „Science and religion” (J. Tambergs).

3. J. Tambergs

- Supervisor of PhD studies – J.Proskurins, „Theoretical study of quantum chaos and phase transitions in nuclear models”;
- Supervisor of BS studies – J.Dinsbergs „Bell’s inequalities in the classical and quantum mechanics”;

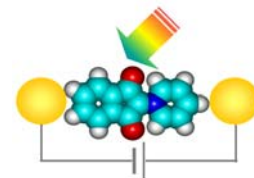
J. Berzins

- Supervisor of BS studies – R.Sadauskis „Determination of radionuclide concentration in soils and water by gamma spectroscopic methods”

Riga Technical University

1. Lectures „Nuclear and elementary particle physics” (J. Berzins).

# LABORATORY OF ORGANIC MATERIALS



Head of Laboratory Dr. I.Muzikante

## Research Area and Main Problems

### Scientific Staff

Inta Muzikante	Dr.habil.phys.	Leading researcher
Lilīta Gerca	Dr.chem.	Leading researcher
Egils Fonavs	Dr.phys.	Leading researcher
Mārtiņš Rutkis	Dr.phys.	Leading researcher
Oskars Viliītis	Dr.phys.	Emeritus

### Engineers

Rorijs Dobulāns	Bc.phys., master student
Elīna Laizāne	Bc.phys., master student
Jānis Latvels	Bc.phys.
Andrejs Tokmakovs	Bc.chem., master student
Aivars Vembris	Bc.phys., master student

### Technicians

Edgars Nitišs	bachelor student
Jurģis Sīpols	bachelor student

### Scientific projects of the Latvian Council of Sciences

05.0005.1	<b>Functional Materials and Technologies for Microelectronics and Photonics</b> - Organic Materials for Microelectronics
05.0026.5	<b>Nanomaterials and nanotechnologies</b> - Nanostructured thin layers of organic molecules and polymer for molecular electronics

### National Research Program in Materials Science, Project No.3

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

### International projects

Projects of Joint France-Latvian Scientific Program Osmose 2006-2007:

1 P.M.Curie University, Paris ISSP UL	Gas sensitive molecular diode based on metal phthalocyanines
2 Angers University, Angers ISSP LU	Non – linear optical investigation of molecular orientation in thin organic films and their interfaces

EU COST Action P8 project "Materials and Systems for Optical Data Storage and Processing"

### Cooperations

#### **Latvia:**

1. Department of Material Science and Applied Chemistry, Riga TU (Prof. V.Kampars).



- Latvian Institute of Organic Synthesis (Dr. E.Markava).
- Institute of Chemical Physics, University of Latvia, (Dr. D.Erts).
- Institute of Physical Energetics, Latvian Academy of Sciences (Dr. I.Kaulach).

#### Lithuania:

- Institute of Physics (Prof. L.Valkunas).
- Institute of Material Science and Applied Research, Vilnius University, Vilnius, Lithuania (Prof. S.Juršenas).

#### Germany:

- Lehrstuhl Physik kondensierter Materie, Universität Potsdam, Potsdam (Prof. L.Brehmer, B.Stiller).

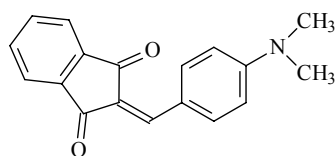
#### France:

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

## Main results

### Design of thin solid films of organic molecules and polymers

- Preparation of spin-coated or blade-casted polymer films of sPMMA incorporated with DMABI and its derivatives. The glass transition temperature is determined by Differential Scanning Calorimetry method.
- Investigated conditions of preparation and corona poling in dependence on concentration of DMABI derivative molecules between 0.1 and 25 wt%. The qualities of films are investigated by second harmonic generation, Kelvin probe and optical microscopy methods. In PBMA polymer (glass transition temperature is about 30°C) films with concentration higher than 9wt% aggregates with regular size  $1 \times 10 \mu\text{m}$  are observed.
- Bilayer structure of vacuum deposited nickel phthalocyanine and its fluorinated derivative is prepared. Al and PEDOT polymer is applied as top electrode to realize Ohmic contact for charge carrier injection.



DMABI

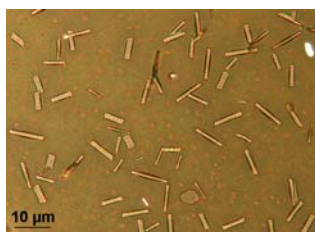
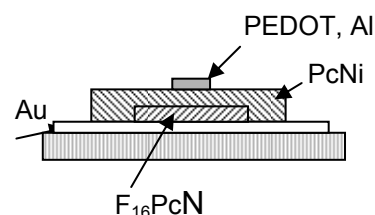


Image of 9 wt% DMABI/PBMA



Scheme of bi-layer structure

### Optically induced switching of optical and electrical properties.

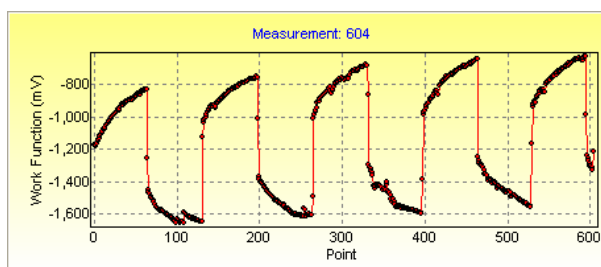
- Reversible switching of the surface potential of DMABI/sPMMA polymer films at 470 nm was observed, where intramolecular charge transfer (PIET) in molecule takes place. The main advantage from the point of view of photoinduced switching effect is the fact that in the excited state molecule does not change its geometry and, to the contrary of azobenzene molecule, photoinduced change of dipole moment of betaine molecule does not need free volume in thin films. At least two processes influence the response of surface potential to irradiation in PIET spectral region. In this

spectral region the main role in photoinduced processes has changes of the dipole moment of the molecule, which is of the order of femtoseconds. In our experiments observed response times are of the order of second and some tenths of seconds. It may be caused both by limitation of Kelvin probe method and complicate structure of the material. Investigated material includes dipole-dipole interactions between polar DMABI molecules, DMABI and polar groups of host polymer. Also forming of aggregates and crystallites by increasing of the concentration is of great importance.

- 2) We have demonstrated that the optically induced mass transport is not limited to azobenzene containing polymer films. DMABI/sPMMA host-guest films show mass transport effect, which is smaller than that in azobenzene containing film. In turn, DMABI/sPMMA films demonstrate refractive index gratings with highest value of diffraction efficiency at green light. Diffractions efficiencies of red and blue lights are one order of magnitude less.
- 3) We have focused our attention to dependence of the photosensitivity of azobenzene carboxylic acids to variations of the substituents in the sulfoamide moiety. Polymer films containing azobenzene molecules with bulky cyclohexyl and phenyl groups showed larger values of the changes of absorbance and faster response time on irradiation in cis- absorption band in comparison with azobenzene molecule with butyl group. The photostationary states in polymer films were determined mainly by photoisomerization of azobenzene moieties and remain constant on irradiation cycles.



Kelvin Probe SKP



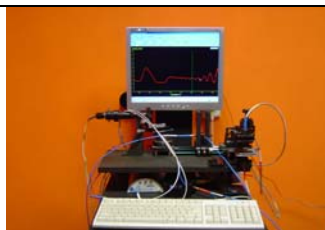
Response of the surface potential on irradiation of DMABI/sPMMA with 470nm light

### Investigations of the nonlinear optical phenomena in host-guest polymer films

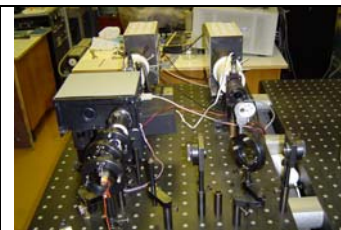
- 1) One of the major investigation tasks at the OM laboratory is search for new highly effective materials for the nonlinear optics (NLO). Magnitude of the nonlinear optical coefficients  $d_{ij}$  is basic criteria for the new material evaluation. The determination of the  $d_{ij}$  can be performed by optical second harmonic generation (SHG) effect measurements as function of incidence angle and polarization, or a Maker fringe technique. Accuracy of these  $d_{ij}$  measurements are very much dependent on accuracy of the linear optical constants ( $n_{\omega}^o, n_{2\omega}^o, n_{\omega}^e, n_{2\omega}^e, \alpha_{\omega}, \alpha_{2\omega}$  and film thickness). During the last year we have upgraded our measurement tools, methodology and software to increase reliability of measurements. The complex of available tools consist of the: a) M-line (Metricon 2010) determination of the thickness and refractive index measurements (accuracy  $\pm 0.0004$ ) at 3 wavelength (1064, 632.8 and 532 nm in both polarizations TM and TE); b) absorbance and reflectance spectroscopy (Ocean Optics HR4000UV-NIR with accessories) within a 200 -1100 nm range; c) computer-controlled SHG setup ( $\lambda_{\omega}=1064$  nm) allows us to measure SHG ( $\lambda_{2\omega}=532$  nm) intensity as function of the fundamental power, incidence angle, fundamental and SH light polarization as well as sample surface mapping by SHG intensity. The detection threshold of equipment ( $1 \times 10^{-6}$  pm/V) allows us to measure SHG effects from single monolayers of organic molecules



Metricon 2010

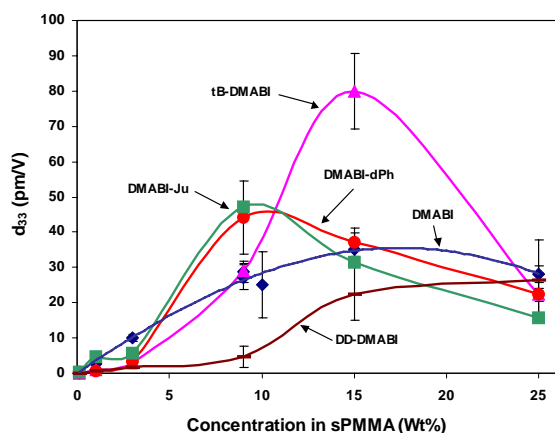


Ocean Optics HR4000UV-NIR

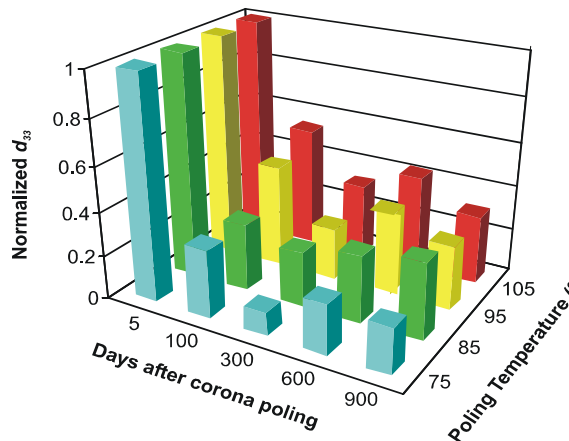


SHG setup

- 2) In order to create new highly effective NLO materials examination of eight DMABI related chromophores in host-guest systems with sPMMA have been done. Correlation chromophore concentration (0.1% - 25 wt%) influence on bulk NLO efficiency with the molecular parameters (molecular weight, molecular hyperpolarizability  $\beta_0$  and ground state dipole moment  $\mu_g$ ) confirms novel design principles of such a materials. There is some kind of contradictive impact of the ground state dipole on NLO efficiency ( $d_{33}$  value). From the one hand high  $\mu_g$  value allows to achieve higher orientation degree by external electrical field poling, from other hand, with an increase of dipole moment increases dipole – dipole interaction, especially at high chromophore loads (smaller interaction distance). This interaction causes two negative processes – aggregation of chromophores and depolarization. In the case of DMABI related chromophores in sPMMA matrix aggregation is a NLO efficiency limiting factor.
- 3) With an aim to increase NLO efficiency and polar order stability for created host-guest systems, corona poling parameter (temperature, time, current) effect on them have been studied. In the case of DMABI/sPMMA temperature (range 80 -120°C) have low impact on efficiency, at the same time increase of poling temperature significantly increasing stability of created polar order.



DMABI related chromophore concentration effect on NLO efficiency



Poling temperature impact on polar order stability

### Electro-physical properties of vacuum deposited thin organic films with heterojunction.

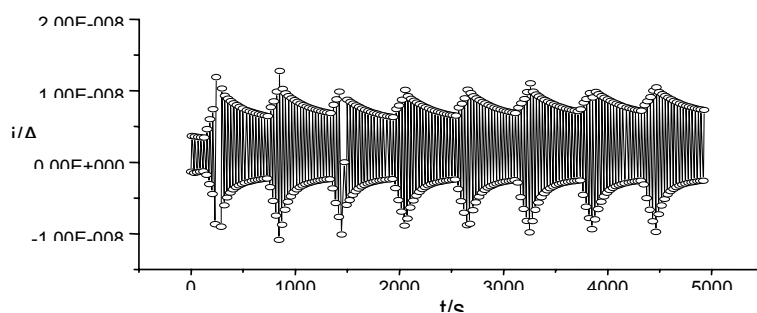
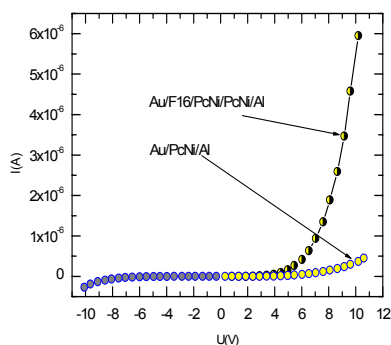
- 1) A high rectification ratio (RR) and a strong asymmetry in the current-voltage curve of Au/F16Pc|Ni/PcNi/Au device is obtained. The RR at  $\pm 10$  V bias, in an Ar atmosphere, is higher than 500, value much larger than that reported for a non-Schottky type rectification junction as Au/F8PcCu/PcNi/Au. In our case, the marked rectification effect found is assumed to be controlled by a combined effect due to the charge carrier transfer across the organic heterojunction and the presence of the PcNi/Al hole blocking junction, eventually favored by the oxygen doping at the metal/organic semiconductor interface. The energy levels (HOMO and LUMO) are

shifted to lower energies by more than 1 eV when going from non-substituted phthalocyanines to their perfluorinated derivatives. Therefore, the occurrence of an energy barrier between both molecular materials forming a heterojunction is expected.

- 2) The current voltage characteristics and dependences of activation energy on applied voltage both of monolayer structures (PcNi or F16PcNi) and bilayer structures (F16PcNi/PcNi) sandwiched between Au and Al electrodes are compared. The space-charge limited current method for bilayer structure is applied and the energy depths charge carrier traps at  $0,50 \pm 0.02 \text{ eV}$  un  $0,85 \pm 0.02 \text{ eV}$  are obtained.

### Gas sensing of thin organic films of bilayer structure with heterojunction.

- 1) The organic heterojunction formed by a *n*-type phthalocyanine as Ni(F<sub>16</sub>Pc) and a *p*-type one as NiPc, at room temperature, is very sensitive to a donor gas as NH<sub>3</sub>, as supported by the changes in RR, current and heterojunction potential. The blocking metal/organic semiconductor junction assists the performance of the device by keeping the asymmetry of the current at forward and reverses regimes (i. e. avoids the attainment of a chemiresistor behavior). Selectivity *vs.* electron acceptor gases (oxidant) would be accessible by covering the *n*-type material completely using the *p*-type layer. This novel principle of transduction offers a profitable multimodal detection for gas sensors and enlarges the field of applications of molecular material-based junctions.



Current voltage characteristics of Au/PcNi/Al and Au/F16/PcNi/PcNi/Al devices

Changes in conductivity at  $U=10\text{V}$  and  $U=-10\text{V}$  of a phthalocyanine-based heterojunction as a novel principle of transduction for ammonia sensing.

### Organizing of conferencies and workhops

1. International Workshop "Charge carrier injection and transport phenomena in organic thin films", August 20, 2006, organized in ISSP LU, 28 participants
  2. International Conference „European conference on organized films ECOF-10”, August 21-24, 2006, organized in LU, 100 participants
1. Published CD with presentations of 4 lectures of the Workshop and 11 invited lectures of ECOF-10.
  2. Special Issue of *Thin Solid Films* with papers of the participants of the ECOF-10 under preparation

### Published papers :

1. I.Muzikante, E.Fonavs, L.Brehmer, B.Stiller, Photoinduced switching of electrical properties in films of polar indandione type organic molecules, *SPIE Proceedings, Organic optoelectronics and photonics*, Vol, 6192, 6192W, 2006.
2. M.A.Rutkis, A.Vembris, V.Zauls, A.Tokmakovs, E.Fonavs, A.Jurgis, V.Kampars, Novel second-order nonlinear optical polymer materials containing indandione

derivatives as chromophores, *SPIE Proceedings, Organic optoelectronics and photonics*, Vol, 6192, 6192Q, 2006.

3. A.Sternberg, I.Muzikante, National research program of Latvia in materials science, *Latv.J.Phys, Tehn. Sci.*, No.2(I), 3-6, 2006.

#### **Submitted papers:**

1. M.Rutkis, A.Vembris, V.Zauls, A.Tokmakovs, E.Fonavs, Non-linear optical properties of polymer systems with poled indandione derivatives as chromophore, *Nonlinear optics, quantum optics*, 2006, (in print).
2. V.Parra, M.Rei Vilar, N.Battaglini, A.M.Ferraria, A.M.Botelho do Rego, S.Boufi, M.L. Rodríguez-Méndez, E.Fonavs, I.Muzikante, M.Bouvet, New Hybrid Films Based on Cellulose and Hydroxygallium Phthalocyanine. Synergetic Effects in the Structure and Properties, *Langmuir*, 2006 (in print).
3. I.Muzikante, M.Rutkis, E.Fonavs, B.Stiller, D.Neher, V.Kampars, P.Pastors, Light induced processes in thin films of indandione type organic molecules, *SPIE Proceedings*, Vol. 6470, 2007 647012 (in print).
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*, (accepted)
5. 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*, (accepted)
6. 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*, (accepted).

#### **Abstracts:**

##### **2<sup>nd</sup> Latvian conference “Functional materials and nanotechnologies FN&NT-2006”, Riga, 2006.g. 27-28 March**

1. E.Laizane, A.Vembris, A.Tokmakovs, L.Gerca, I.Muzikante, E.Markava, D.Gustiņa, Optically induced switching processes in thin films of donor and acceptor containing azobenzene derivatives, Abstract book, p.41
2. I.Muzikante, L.Gerca, D.Erts, E.Fonavs, A.Pastare, A.Tokmakovs, Formation of self assembled monolayers on gold nanoparticles inside the nanoporous domains, Abstract book, p.50
3. A.Tokmakovs Investigation of photostability of indandione derivatives in polymer matrices in dependence on glass transition temperature and stereoregularity, Abstract book, p.74.
4. M.Rutkis, V.Kampars, A.Vembris, A.Tokmakovs, Relation of the chromophore structure – second order non- linear optical properties in host – guest systems. Case of the DMABI derivatives/sPMMA, Abstract book, p.62
5. M.Rutkis, V.Zauls, Determination of second order non- linear coefficients – straightforward measurement or complex optical investigation?, Abstract book, p. 63.
6. A.Vembris, M.Rutkis, A.Tokmakov, Study of polar order stability of the poled host – guest system (s-PMMA/DMABI), Abstract book, p.76
7. I.Kaulach, I.Muzikante, L.Gerca, M.Plotniece, M.Roze, J.Kalnacs, G.Shlihta, P.Shipkovs, A.Tokmakov, E.Fonavs, V.Kampars, Photoconductivity and PV effect of fullerene and phthalocyanine doped poly(3-hexylthiophene), Abstract book, p.27

##### **International Conference, Course, Exhibition Photonics Europe (6192 – Organic Optoelectronics and Photonics II), 3-7 April, 2006, Strasbourg, France,**

8. I.Muzikante, E.Fonavs, L.Brehmer, B.Stiller, Photoinduced switching of electrical properties in films of polar indandione type organic molecules, CD
9. M.A.Rutkis, A.Vembris, V.Zauls, A.Tokmakovs, E.Fonavs, Novel second-order nonlinear optical polymer materials containing indandione derivatives as chromophores, CD

**COST Action P8, Materials and systems for optical data storage and processing, Final Workshop and MC Meeting, May 26-27, Loutraki Greece**

10. I.Muzikante, V.Kampars, P.Pastors, B.Stiller, K.Moravetz, J.Ilnytski, D.Neher, Optically induced effects in thin films of indandione type organic molecules, , Abstracts, pp.5-6.

**European Conference on Hybrid and Organic Solar Cells, ECHOS'06, June 28-30, 2006 - Paris, France**

11. I.Kaulach, I.Muzikante, L.Gerca, M.Plotniece, M.Roze, J.Kalnachs, G.Shlihta, P.Shipkovs, V.Kampars A.Tokmakov, PV and Magnetic Field Effects in Poly(3-Hexylthio-Phene)-Fullerene Cells Doped with Phthalocyanine Soluble Derivative, CD

**4<sup>th</sup> International Conference on Porphyrins and Phthalocyanines, July 2-7, 2006, Rome, Italy**

12. M.Bouvet, I.Muzikante, R.Dobulans, E.Fonavs, A.Tokmakov, V.Parra, Molecular diodes as new transducers for gas sensing, *J.Porphyrins and Phthalocyanines*, Vol. 10, Iss. 4-6, p. 431, 2006
13. M.Roze, V.Kampars, I.Kaulach, N.Kirichenko, I.Muzikante, New soluble phthalocyanines for solar cells, *J.Porphyrins and Phthalocyanines*, Vol. 10, Iss. 4-6, p. 844, 2006

**23rd European Crystallographic Meeting ECM23, August 6 -11, 2006, Leuven, Belgium**

14. A.Tokmakovs, S.Belyakov, K.Balodis, P.J.Pastors, I.Muzikante, V.Kampars, Crystal Structure of Benzylidene-1,3-indandiones, p.300

**World Renewable Energy Congress IX (WREC IX), 19-25 August, 2006, Florence, Italy,**

15. I.Kaulach, I.Muzikante, L.Gerca, M.Plotniece, M.Roze, J.Kalnachs, G.Shlihta, P.Shipkovs, A.Tokmakov, G.Kashkarova, V.Kampars, PV Effect in Cells of Fullerene and Phthalocyanine Soluble Derivatives - Doped Poly(3-Hexylthiophene), p.569.

**European Conference on Organised Films ECOF-10, Riga, 21-24 August, 2006, Riga, Latvia**

16. E.Laizane, D.Gustina, E.Markava, I.Muzikante, A.Tokmakov, A.Vembris, Photoisomerization processes of novel azobenzene derivatives in polymer host-guest films, Book of Abstracts, p. 99.
17. J.Latvels, R.Dobulans, E.Fonavs, I.Muzikante, M.Bouvet, V.Parra, Electrical properties of nickel phthalocyanine and fluorinated nickel phthalocyanine bilayer films, Book of Abstracts, p. 164
18. I.Kaulach, I.Muzikante, L.Gerca, M.Plotniece, M.Roze, J.Kalnachs, G.Shlihta, V.Kampars, A.Tokmakov, Charge Carrier Photogeneration in Poly (3-Hexylthiophene)-Fullerene Cells Doped with SnCl Phthalocyanine Soluble Derivative, Book of Abstracts, p. 160.



19. M.Rutkis, V.Kampars, A.Vembris, A.Jurgis, A. Tokmakov, Tailoring of NLO Properties of Organized Polymer Films: Achievements in Host- Guest System of the DMABI Derivatives in sPMMA, Book of Abstracts, p. 101.
20. 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, Book of Abstracts, p. 104.
21. S.Belyakov, A.Tokmakov, P.Pastors, V.Kampars, X-ray Structure Determination of DMABI Analogs, Book of Abstracts, p. 93.
22. S.W.Chan, M.Rutkis, J-M.Nunzi, SHG Investigation of Charge Transfer Induced Polarity in Organic Semiconductore Thin Films, Book of Abstracts, p. 94.
23. S.Juršėnas, 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, Book of Abstracts, p. 135.
24. M.Bouvet, V.Parra, E.Fonavs, R.Dobulans, J.Latvels, A.Tokmakov, I.Muzikante, Molecular Diodes as New Transducers for Gas Ssensing, Book of Abstracts, p. 35.
25. B.Stiller, M.Saphiannikova, K.Morawetz, J.Ilnytskyi, D.Neher, I.Muzikante, P.Pastors, V.Kampars, Optical Patterning of Azobenzene and Indandione containing Films, Book of Abstracts, p. 73.
26. VParra, M.R.Vilar, A.M.Botelho Rego, A.M.Ferraria, S.Boufi, T. del Caño, E.Fonavs, I.Muzikante, M.Bouvet, Novel Hybrid Films Based on Cellulose/Hydroxygallium Phthalocyanine: Spectroscopical and Surface Studies, Book of Abstracts, p. 66.

**International Conference on Advanced Optical Materials and Devices AOMD-5, 27-30 August, 2006, Vilnius, Lithuania**

27. E.Laizane, I.Muzikante, E.Fonavs, A.Tokmakov, A.Vembris, Optically induced switching processes in azobenzene containing polymer host-guest film, Abstracts, pp.70
28. J.Latvels, R.Dobulans, E.Fonavs, I.Muzikante, Diode properties of nickel phthalocanine and fluorinated nickel phthalocanine bilayer films, Abstracts pp.41
29. M.Rutkis, V.Kampars, A.Vembris, A.Jurgis, A.Tokmakov, Novel polymer photonic materials based on the DMABI derivatives. The chromophore structure relation to the second order non- linear optical efficiency, Abstracts, pp.69.
30. I.Muzikante, M.Rutkis, E.Fonavs, On features of organic solid state materials and technology, Abstracts pp.96
31. A.Vembris, M.Rutkis, E.Laizane, Study of polar order stability of corona poled host – guest (s-PMMA/DMABI) system, Abstracts pp.76
32. A.Tokmakov, V.Kampars, P.Pastors, I.Muzikante, Host-guest systems of indandione derivatives in PMMA matrix: influence of hromophore concentration on glass transition temperature, Abstracts pp.42

**The 21st European Photovoltaic Solar Energy Conference and Exhibition, September, 2006, Dresden, Germany**

33. I.Kaulach, I.Muzikante, L.Gerca, M.Plotniece, M.Roze, J.Kalnachs, G.Shlihta, P.Shipkovs, E.Fonavs, G.Kashkarova, V.Kampars, PV Effect in Cells of Poly(3-Hexylthiophene) Doped by Fullerene and SnCl Phthalocyanine Soluble Derivatives, Book of Abstracts, CD, No.1AV.2.63, 5pages.

***Baltic Polymer Symposium 2006, September 20-22, Birini Castle, Latvia***

34. A.Sternberg, I.Muzikante, Selected Aspects of Latvian National Research Program in Materialscience, Book of Abstracts, pp. 58.

# ELECTRONIC ENGINEERING

Head of Department *Dr. phys. A. Kristins*

## Main Problems

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

### Scientific Staff

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

### Technical Staff

1. I.Guza
2. I.Gvardina
3. J.Melderis
4. J.Tibergs
5. J.Veinbergs
6. 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

#### Estonia

1. Tallinn  
University of  
Technology
2. Competence  
Centre ELIKO

The prospects of the instruments look at appendix.



## Our Clients

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

## Lectures on Conferences

### 22<sup>th</sup> Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, March, 2006

1. A.Kristins, D.Millers, A.Zelenkovs, S.Zelenkovs, V.Zolotarjovs *Research of Opportunities of Detection and Classification buried Mine-like Objects*. Abstracts, p.42.
2. A.Grablevskis *Use BCCD-cluster for creation of the distributed systems*. Abstracts, p.43.
3. P. Annus, M.Min, E. Haldre, A. Kristins. *IO controller for modular control system*. Abstracts, p.44.
4. D.Gusevs, V.Narnicka. *Electronic procurement system*. Abstracts, p.45.

### The outlook for Latvian technology “High Tech in Latvia 2006”

1. A.Kristins. *Working Time Monitoring System*. P.34.
2. A.Kristins. *Operation with Remote Objects Based on TCP/IP Communication Protocol*. P.35.



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

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

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

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

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

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

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

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

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

Our address:

Electronic Engineering Department  
Institute of Solid State Physics  
University of Latvia  
8 Kengaraga Str., Riga  
LV-1063, Latvia  
Phones: (371) 7260856; 7260854  
Fax: (371) 7132778  
E-mail: [kristin@latnet.lv](mailto:kristin@latnet.lv)  
<http://www.cfi.lu.lv>



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

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**Apartment Security System**

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

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

Switching on and off of system security mode is implemented with the aid of the *Dallas Semiconductor Touch Memory*<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.

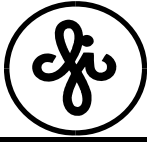
This device is very simple in using and doesn't need any special knowledge.

***Technical Specification***

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

Our address:

Electronic Engineering Department  
Institute of Solid State Physics  
University of Latvia  
8 Kengaraga Str., Riga  
LV-1063, Latvia  
Phones: (371) 7260856; 7260854  
Fax: (371) 7132778  
E-mail: kristin@latnet.lv  
<http://www.cfi.lu.lv>



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

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

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

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

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

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

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

***Technical Specification***

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

Our address:

Electronic Engineering Department  
Institute of Solid State Physics  
University of Latvia  
8 Kengaraga Str., Riga  
LV-1063, Latvia  
Phones: (371) 7260856; 7260854  
Fax: (371) 7132778  
E-mail: kristin@latnet.lv  
<http://www.cfi.lu.lv>



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

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**Car parking and access control systems**

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

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

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

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

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

Our address:

Electronic Engineering Department  
Institute of Solid State Physics  
University of Latvia  
8 Kengaraga Str., Riga  
LV-1063, Latvia  
Phones: (371) 7260856; 7260854  
Fax: (371) 7132778  
E-mail: kristin@latnet.lv  
<http://www.cfi.lu.lv>



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

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**Electronic Documentation**

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

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

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

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

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

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

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

Touch Memories can accommodate over one million data changes.

Our address:

Electronic Engineering Department  
Institute of Solid State Physics  
University of Latvia  
8 Kengaraga Str., Riga  
LV-1063, Latvia  
Phones: (371) 7260856; 7260854  
Fax: (371) 7132778  
E-mail: kristin@latnet.lv  
<http://www.cfi.lu.lv>



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

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**Digestion System**

The digestion system provides digestion of various samples in sulphuric acid, using the Kjeldahl method.

Into six deep hollows of electrical heater are placed tubes, containing samples and sulphuric acid. The temperature controller provides the thermal regime of heater. The thermal regime includes two plateaus of temperature: the first (in time) - in the temperature region of boiling water, and the second - in the temperature region of boiling acid. The temperature controller provides also three different heating rates for transition from starting temperature to the first and second plateau. The thermostation time control up to six hours is possible.

The digestion system is provided by water aspiration pump for the removal of exhaust gases, produced in digestion procedures.

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Fax: (371) 7132778  
E-mail: [kristin@latnet.lv](mailto:kristin@latnet.lv)  
<http://www.cfi.lu.lv>



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

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

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

The device controls electromagnetic keys of any construction.

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

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

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

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

This device is cheaper than most of similar ones.

***Technical Specification***

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

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Institute of Solid State Physics  
University of Latvia  
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Fax: (371) 7132778  
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<http://www.cfi.lu.lv>





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Institute of Solid State Physics  
University of Latvia**

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

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

The device controls electromagnetic keys of any construction.

Accessing in the apartment is implemented with the aid of the *Dallas Semiconductor Touch Memory*<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:	$2,8 \cdot 10^{14}$
Number of user keys (standard):	56 pcs.
Number of events registered:	500
Time of data retention in Master-key:	over 10 years

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

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**High-voltage Breaker Analyzer Device "OSKARS"**

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

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

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

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

The time resolution is 0,001 s.

Dimensions are 490 x 480 x 165 mm.

Weight is 20 kg.

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

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

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

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University of Latvia**

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

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

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

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

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

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

Practical applications:

1. The system of access, control and management is worked out for LatRosTrans company. The system consists of 24 controllers (number of technological blocks on Russia-Ventspils oil pipeline), dispatcher program (in Daugavpils) and some client applications.

2. Entrance in/out system for “Latvijas Gāze” company is worked out, which consists of three in/out gates with automatic barriers, server administrator and guard programs and some other client applications.

3. The system including checkpoint, the authorized access in cabinets and the security signal system for two buildings of the Latvian Shipping Company with a unified database.

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University of Latvia**

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**Security Drawers and Safes for the Cash Points**

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

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

	<b>SF-1</b>	<b>KT-2FA</b>	<b>KT-2FB</b>
<b>Delay times (minutes)</b>	3, 5, 10, 15	3, 5, 10, 15	3, 5, 10, 15
<b>Access times (s)</b>	5, 10, 15, 20	5, 10, 15, 20	5, 10, 15, 20
<b>Dimensions (mm)</b>	400 x 370 x 140	300 x 300 x 300	300 x 300 x 200
<b>Weight (kg)</b>	12	14	10,5

The safe is connected to the mains (50 Hz, 220 V A.C.) by a transformer or to the 9 V 300 mA D.C. source.

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University of Latvia  
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Fax: (371) 7132778  
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University of Latvia**

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**Register system on supervision of route checkpoints**

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

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

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

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

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

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

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

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

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Institute of Solid State Physics  
University of Latvia  
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LV-1063, Latvia  
Phones: (371) 7260856; 7260854  
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# **Electronic Engineering Department Institute of Solid State Physics University of Latvia**

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## **Working time monitoring system**

This system consists of a software package and a data reading block.

### ***Software package provides the following functions:***

- adding, editing and erasing of user data (name, surname, working number, key number, telephone number);
- working time calculation by four time types (ordinary working time, reserve time, evening working time + working time on days off till ten o'clock p.m., night working time) (*these parameters could be changed*);
- event searching by surname or working number, by date and time interval;
- printing of searching results;
- function "present – absent";
- text (*or different*) password system;
- calendar for setting of days off and working days and for setting of date intervals with reserve time;
- automatic archive creating in the form of text files;
- the other functions could be added by customer wishes.

### ***Data reading block with the following parameters:***

- identification device - Dallas identification button or Proxy card;
- data readers – two (entry and exit);
- real time indication / working number indication;
- user count up to 200 (*this count could be greater*);
- operational memory for 500 events (in autonomous regime) (*this count could be greater too*);
- connection with computer by RS485 port;
- powered from mains (220 V) with guarding from short voltage disappearance;
- the block is easy mounted to vertical wall.



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Institute of Solid State Physics  
University of Latvia  
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**Soft Start Devices for Electric Motors**

There are many problems with starting of high power electric devices (motors) because initial current may be some times greater as nominal current for these devices. High initial current may be dangerous for power supply devices as well as for powered devices.

In the ISSP in cooperation with “Fonons” Ltd there were worked out soft start devices for electric motors in general, but it is possible to use the soft starters also for other devices (high power heaters, for example).

The devices are based on phase drive of two thyristor pairs and are able to manage power up to 100 kVA and more.

Main features:

- digital controlled AC semiconductor soft starter
- start time from 5 to 20 seconds
- start voltage from 40 to 80%
- stop time from 1,5 to 20 seconds
- built in by-pass function.



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<http://www.cfi.lu.lv>