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

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Riga 2004

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# CONTENTS

# 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.

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 current year 5 scientists from Latvian Institute of Physical Energetics joined ISSP and established Laboratory of Organic Materials.

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;
- design and manufacturing of scientific instruments and instruments for analytical tasks and environmental monitoring;
- vision research, development of new technologies for psycho-physical testing and primary vision care.

The highest decision-making body of the Institute is the **Council** of 23 members elected by the employees of the Institute. Presently Dr. hab. M.Springis 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 8 members. In August 18, 2002 the Workshop of Supervisory Board took place at ISSP.

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

The annual report summarizes research activities of the ISSP in 2003. The staff of the Institute has succeded in 31 **national science grants** and in the **national cooperation project** (Intelligent Materials and Structures for Microelectronics and Photonics) with the total financing of 245,7 thous. lats (Ls) (exchange rate: 1 Ls ~ 1,49 EUR), see Table 1 and Fig.1., 2.

Additional funding from the **state budget** and **University of Latvia** in 2003 was 172.3 thous. Ls. The main part of this funding was used for purchasing the scientific equipment (143.2 thous. Ls) on condition, that a part of expenditures is covered by EC 5$^{th}$ Framework Programme expenses. Further, an aditional support from state budget was used for

participation in international conferences (7.8 thous. Ls) and for support to the Centre of Excellence CAMART (4.7 thous. Ls)

***Table 1***

**INCOME OF ISSP, THOUSAND Ls, FROM 1993 - 2003**

| Year | Total financing | Grants and programmes from budget | Other financing from budget | Contracts, market oriented research | Internat. funds | Rent of space |
|---|---|---|---|---|---|---|
| **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** |

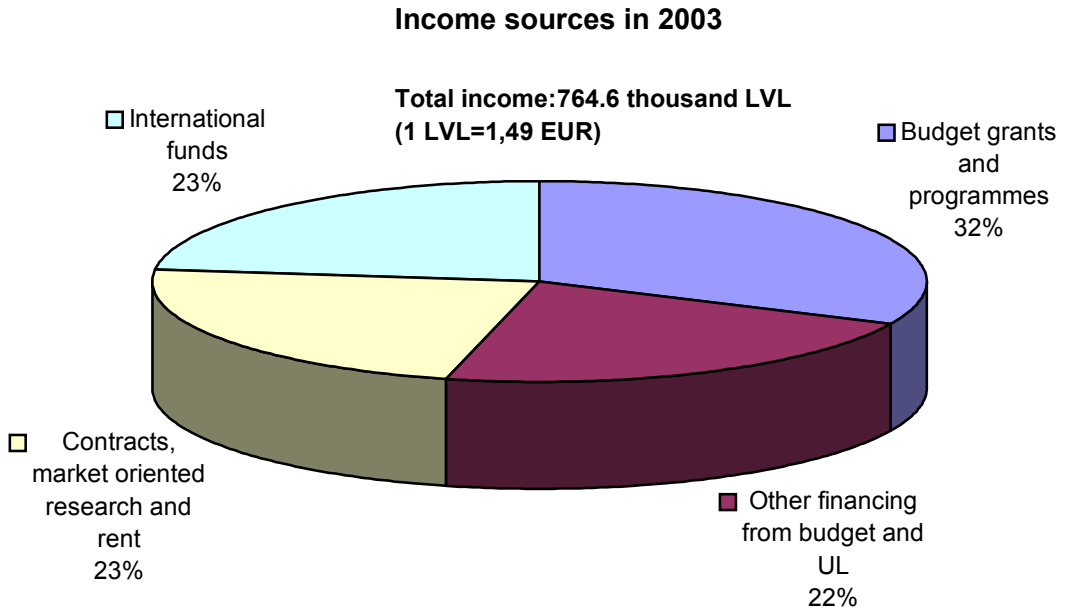



**Fig.1. Distribution of income sources during 2003**

2003 was successful for **national contracts.** The market oriented contracts reached 106.2 thous. Ls, but contracts with Latvian companies including SMEs – 52.2 thous. Ls. The descriptions of some materials and devices developed at the ISSP as a result of contracts are enclosed in the Appendix.

The ISSP income dynamics for 1993 – 2003 is given in Table 1 and Figure 2.

The **international funding** in 2003 became higher compare to 2002. The main source were the EC 5th Framework programme contracts:

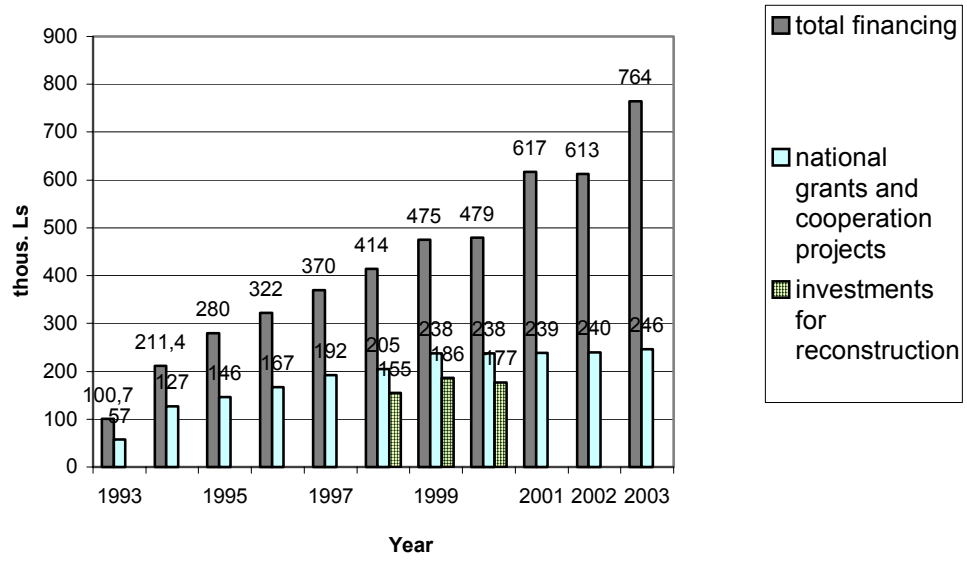
- for the Centre of Excellence CAMART – 104.6 thous. Ls;
- for four EURATOM projects – 27.1 thous. Ls.
- for POLECER project - 13.4 thous. Ls.

Additional funding was provided by Taivan - Lithuania – Latvia joint agreement – 7.7 thous. Ls and contract with the "EMBRACO" company from Brasil – 23.1 thous. Ls.

The Institute obtained 15.1 thous. Ls from **leasing part of its space.**

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 numbers of the research staff hold Dr. hab. degrees, 45 hold Dr. or PhD. At the end of 2003 there were 6 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 2003.

**Fig. 2. Grants, investments in reconstruction and total financing of the ISSP**




**Main achievments in 2003:**

1. Promotion of the research activities due to Project of Centre of Excellence CAMART (see the next chapter);
2. Essentiall increase in amount of expences spent for purchase of advanced scientific equipment (143.2 thous. Ls);
3. Dr.habil. L.Skuja was elected a member of the Latvian Academy of Sciences;
4. Dr. habil. J.Maniks received annual Science Award of Latvian Ministry of Education and Science;

5. Dr. phys. J.Kuzmin was elected as an professor of Department of Pedagogic and Psyhology University of Latvia;
6. I.Shorubalko and K.Jefimovs were acquired degree of doctor of physics at Lund University (Sweden) and Joensu University (Finland), correspondingly;
7. Succesful organization of the 10th International Symposium on Olfaction and Electronic Nose (ISOEN'2003), Riga, June 25–28, 2003 (Chairman Dr.phys. J.Kleperis);
8. The reconstruction of annex to main building of Institute was accomplished (administrades by Dr. phys. J.Klavins);
9. Two issues of International journal "Proceedings SPIE" – vol. 5122, 5123 are published in 2003 "Advanced Organic and Inorganic Optical Materials" (editors A.Krumins, D.Millers. I.Muzikante, A.Sternberg and V.Zauls) and "Advanced Optical Devices, Technologies, and Medical Applications" (editors J.Spigulis, J.Teteris, M.Ozolinsh and A.Lusis). The Proceedings contain the papers of AOMD-3 conference held in August 2002 in Riga;
10. The papers of NATO/ARW "Computational Materials Science", hold in Ciocco, Italy September 2001, have been published by Kluwer Academie Publishers in NATO Science Series III Computer and Systems Science, Vol. 187, 2003, editors: R.Catlow (UK) and E.Kotomin (Latvia).

Many thanks to everybody who contributed to this report as well as to the organizations that supported the Institute financially: Latvian Council of Science, Science Department of the Latvian Ministry of Education and Science, University of Latvia, EC 5th Framework Programme, European Community Council Program COST, NATO Scientific Affairs Division and to many foreign Universities and institutions.

Prof. Dr. A.Krumins

ACTIVITIES OF THE CENTRE OF EXCELLENCE

2003 was the third activity year of the Centre of Excellence CAMART - the Centre of Excellence for Advanced Material Research and Technologies. The project was established by the 5th framework Programme of the European Comission, **the main tasks** of the Centre being:

- to promote restructuring of the science and technology sectors;
- to promote the economic and social needs of the regions;
- to attract young researchers;
- to adopt the best experience in collaboration with the European colleagues.

The support from EC is 703 000 EUR or 400 000 Ls for three years and the **funding should be** spent on:

- extended visits (more than one month of duration) of foreign colleagues at the ISSP (31%);
- visits of the ISSP employees abroad, including attendance of conferences (35%);
- purchase of equipment and materials necessary for foreign colleagues during their visits (9%);
- overhead expenses (25%).

During the third year the following **common activities** of CAMART have been carried out:

1. Increased **activity** of the staff **in the research.** Intensification of collaboration with European universities and companies, increased participation at international conferences and collaboration with colleagues from EC Member States and Associated Countries.

2. Adoption of the best experience in **collaboration with the European colleagues**. 11 visitors from EC Member States, 7 visitors from EC Newly Associated Countries, revealed a remarkable growth of the scientific status of the Institute (Table 3).

Table 3

Long term visits to CAMART in 2003

| **From EC Member States:** | |
|---|---|
| Germany: | 1 |
| Spain: | 2 |
| Italy: | 3 |
| Finland: | 2 |
| France: | 2 |
| Portugal: | 1 |
| **Total:** | **11** |

| **From Newly Associated Countries:** | |
|---|---|
| Lithuania: | 1 |
| Czech Rep.: | 3 |
| Poland: | 3 |
| **Total:** | **7** |

3. Improvement of **scientific seminar** of the Institute, including 22 lectures being presented by highly qualitied visitors of CAMART to the staff and students of the Institute.

4. Joint **RTD projects with Latvian enterprises** for development prototypes of new multilayer solid state batteries (A/S Sidrabe), intelligent sensor instruments (RTU, A/S Alfa Pro), scintillators (Baltic Scientific Instruments), as well as development of technology of nitride thin films (A/S Alfa) and glass fibers (A/S Valmieras stikla skiedra). Presentation of these projects at international exhibition "Baltic Dynamics".

5. **Enhanced participation in other areas of 5th Framework Programme** and in other **international projects:**

- EC 5th Framework Programme:
  - MC Research Training Network "Optical Devices Using Photosensitivity for their Elaboration", supervisor Dr.hab. L.Skuja;
  - Research Network in "Growth" programme "Polar Electroceramics", supervisor Dr. V.Zauls;
  - EURATOM projects:
    - Investigation of metal ions in fusion plasmas using emmision spectroscopy, supervisor Dr.hab.I.Tale;
    - Radiation energy detectors and storage – read out materials, supervisor Dr.hab. I.Tale;
    - Irradiation effects in ceramics for heating and current drive and diagostics systems, supervisor Dr.hab. A.Sternberg;
    - Study of the dynamics of ELMs in the ASDEX Upgrade tokamak, supervisor Dr. hab. V.Kuzovkovs
- COST projects:
  - D 18 "Lanthanide chemistry for diagnosis and therapy", supervisor Dr.hab. J.Purans;
  - P8 "Materials and systems for optical data storage and proceedings", supervisor Dr.J.Teteris;
  - 525 "Advanced electronic ceramics: grain boundary engineering", supervisor Dr.hab.A.Sternbreg;
- Project of bilateral Latvian – German Cooperation in Science and Technology "Acumulating Luminiscence Dosimetrs", supervisor Dr.hab. U.Rogulis;
- Program of Mutual Funds for Scientific Cooperation of Republic of Lithuania and Republic of Latvia with Republic of China (Taiwan) "Materials Research on Wide Gape Group III Nitride Compounds for Advanced Light Emitters", supervisor Prof. I.Tale;
- Research contract "Electrocaloric materials development" with "EMBRACO" company Brasil, supervisor Dr.E.Birks.

6. Three projects of **6th Framework Programme** proposed by ISSP have been **succesfully evaluated:**

- STRP "Nanoscale chemical mapping and surface structural modification by joined use of x-ray microbeams and tip assisted local detection", Dr. hab. J.Purans;
- Collective research project "Removal of hazardous substances in electronics: processes and techniques for SME's", Dr. A.Lusis;
- Marie Curie Large Conference "ICDIM'2003", Dr.hab. I.Tale.

Four additional projects of 6th FP are on the waiting list.

7. **The 10th International Symposium on Olfaction and Electronic Nose** was organized at June 25 – 28 in Riga, Latvia. The Symposium was attended by 93 participants from 22 countries. Part of papers will be published in special issue of the International Journal from "Sensors and Actuators B" , Elsevier

8. About 40 **young researchers**, mainly students from University of Latvia have been associated with the CAMART projects.

9. Due to financial support from Latvian government, on condition that a part of expenses in covered by EC through 5th Framework Programme, the following **scientific equipment was purchased** in 2003:

- IR spectrometer Bruker Equinox 55;
- AMKO spectrometer with CCD camera;
- Digital EMG system for evoked brain potentials study;
- Dual phase lock – in amplifiers;
- Extension for Supercomputer.

The new scientific equipment was already used by our guests, thus improving the network between Centres and increasing the scientific value of the joint research.

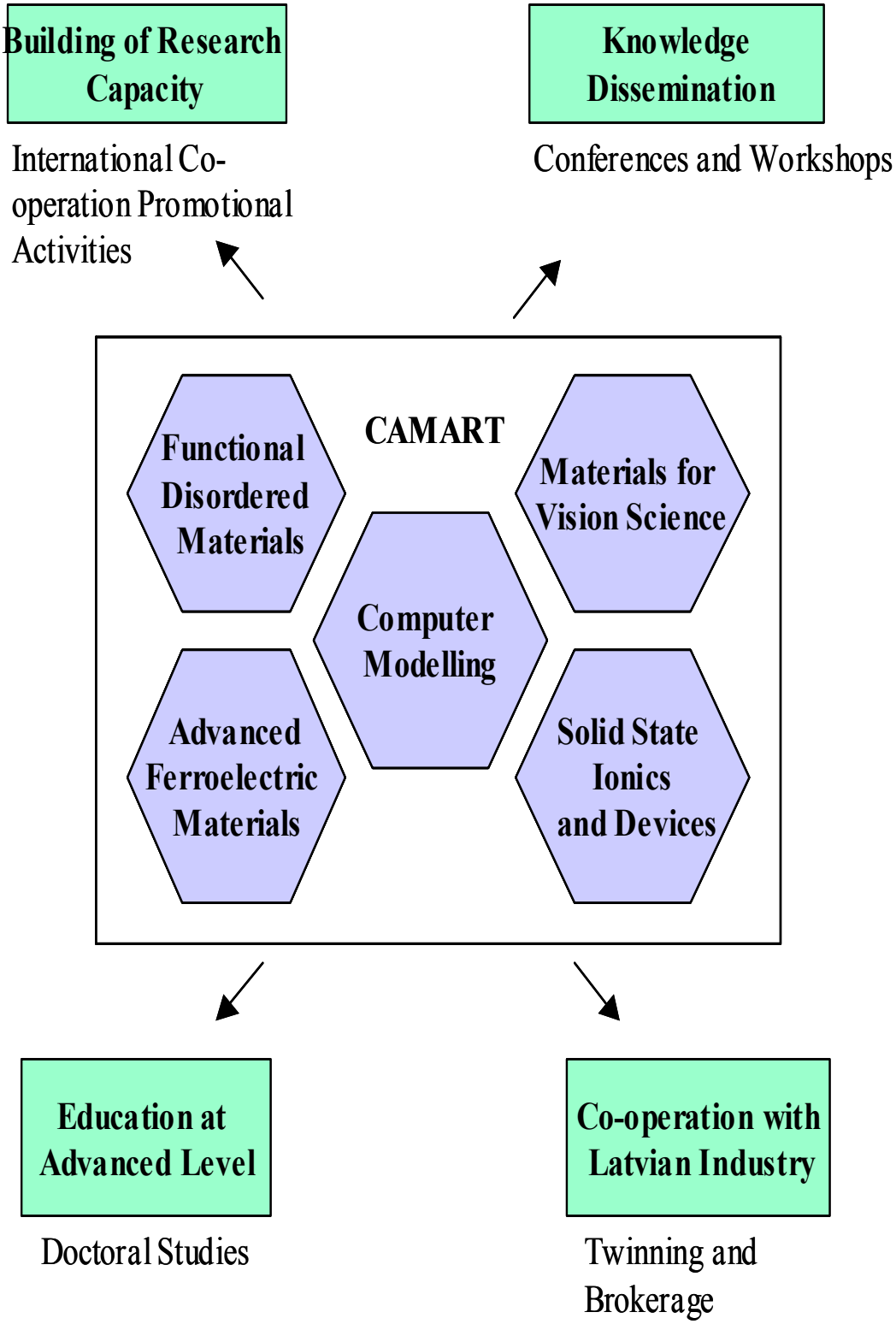
10. **Activities of Network of Centres of Excellence** "Interfacial Effects, Novel Properties and Technologies of Nanostructured Materials".
Fruitfull collaboration was developed with the following Centres of Excellence:

- HIGH PRESSURE, Poland;
- CEBIOLA, Lithuania;
- ESTOMATERIALS, Estonia;
- KFKI-CMRC, Hungary;
- AMAS, Poland.

11. The **duration** of Centre of Excellence CAMART project was extended for one year, thus project expires December 31, 2004.

Prof. Dr.A.Krumins
Scientific coordinator of CAMART

**Activities of Centre of Excellence (CAMART)**



# CRYSTALS PHYSICS

Head of Division Dr. P. Kulis

## Research Area and Main Problems

The research area of Division is concern with four main projects:

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. Technology of Al-Ga nitride semiconductor heterostructures for light-emitting and laser diodes for violet and ultraviolet spectral regions - the goal of the project is the development of light-emitting diodes and laser diodes for violet and ultraviolet spectral region. The project involves synthesis and design of corresponding new materials on the basis of the third group nitrides, elaboration of the thin film heterostructures and further development of production of multifunctional fotonic devices in joint stock company ”Alfa”.
3. 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.
4. 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 ionisation degree of metal atoms considerably depends on the plasma ion temperature. Density of metal vapours in plasma can be estimated using the spectroscopic methods.

**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. Ā. Veispals
7. Dr. hab. V. Ziraps

**Technical Staff**

1. Mg. J. Jansons
2. A. Muhins
3. E. Tale

**PhD Students**

1. L. Dmitrichenko

2. E. Elsts
3. V. Ogorodņiks

**Students**

1. Dz. Berzins
2. A. Fedotovs
3. A. Gulans
4. I. Gromuls
5. K. Paulinshs
6. M. Piesinshs
7. A. Sharakhovsky
8. A. Voitkans
9. P. Zarans

**Visitors from abroad**

Dr. J. Rosa, Institute of Physics Academy of Science of the Czech Republic, Prague, Czech Republic (60 days);
Prof. S. Jurshenas, Institute of Material Science and Applied Research, Vilnius University, Vilnius, Lithuania (30 days).

**Scientific visits abroad**

1. Dr. hab. U. Rogulis - University of Paderborn, Germany (5.5 months);
2. Dr. hab. I. Tale - University of Paderborn, Germany (1.5 week);
3. Dr. hab. I. Tale, University of Rostock, Germany (1 week);
4. Dr. hab. I. Tale, Atomic Institute of Austrian Universities, Vienna, Austria (1 week);
5. Dr. hab. I. Tale, Instituto Superior Tecnico (IST), Lisbon Portugal (1 week);
6. A. Sharakhovsky, Instituto Superior Tecnico (IST), Lisbon Portugal (30 days);
7. Dr. hab. M. Springis, Institute of Material Science and Applied Research, Vilnius University, Vilnius, Lithuania (30 days).
8. Dr. hab. M. Springis, Institute of Material Science and Applied Research, Vilnius University, Vilnius, Lithuania (1 week).
9. Dr. hab. I. Tale, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1week);
10. Dr. hab. U. Rogulis, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1week);
11. Dr. hab. M. Springis, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1 week);
12. Dr. P. Kulis, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1 week);
13. Mg. V. Ogorodniks, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1 week);
14. Mg. E. Elsts, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1 week);
15. I. Gromuls, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1 week);
16. A. Sharakhovsky, Institute of Physics Academy of Science of the Czech Republic Prague, Czech Republic (1 week).
17. A. Gulans, University of Turin, Turin, Italia (1 week)

## Cooperation

**Latvia**

Joint stock company "Alfa"

**Austria**

Atomic Institute of Austrian Universities, Vienna, Austria (Prof. H. Rauch).

**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, Prof. H. Stolz).

**Lithuania**

Institute of Material Science and Applied Research, Vilnius University, Vilnius, Lithuania (Prof. S. Jurshenas).

**Portugal**

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

**Taiwan**

Graduate Institute of Electro-Optical Engineering and Department of Electrical Engineering, National Taiwan University, Taipei, Taiwan (Prof. C.C. Yang)

## Main Results

### OPTICAL AND MAGNETIC RESONANCE SPECTROSCOPY OF STIMULATED RECOMBINATION PROCESSES IN DEFECT STUDIES

**I. Tale**

*Institute of Solid State Physics University of Latvia*

The optical and magnetic resonance spectroscopy is widely used in investigation of radiation-induced processes in wide-gap solids. Advantages of simultaneous use of optical and magnetic resonance techniques for investigation of the stimulated processes are considered.

Investigation of optically and thermally stimulated processes is a powerful tool for characterization of localized electron states in wide energy gap materials. Simultaneous use allows elucidate relation between the optical and thermal characteristics of defects. Simultaneous application of the magnetic resonance techniques serves essential knowledge about the composition and structure of point defects involved in thermally and optically stimulated processes.

The optical detection of EPR having enhanced sensitivity and the optical detection of the MCDA are of particular importance in investigation of both the nature and the optical characteristics of partners involved in stimulated reactions.

Methods of advanced thermoactivation spectroscopy – fractional glow technique FGT and glow rate technique of trap absorption bands, measured at different heating rate constants serve tools for investigation of complex trap spectra in presence of arbitrary order of reaction kinetics. The evaluated values of frequency factors reflect the reaction volume, thus giving information about the prospective process nature. Particularly, the non quasi – steady state reactions can be direct evaluated using the fractional glow.
Advantages of double optical – thermoactivation spectroscopy offered by glow rate technique of trap absorption bands can be implemented using a simultaneous study of the decay of optical absorption spectrum together with TSL or OSL.

## INVESTIGATION OF METAL IONS IN FUSION PLASMAS USING EMISSION SPECTROSCOPY

**I. Tale, M.Springis, A. Sharakovsky, I. Gromuls**
*Institute of Solid State Physics University of Latvia*

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

## METHODS AND ACTIVE MATERIALS FOR IMAGING OF THE SLOW NEUTRON FLUXES

**I.Tale, P. Kulis, M. Springis**
*Institute of Solid State Physics University of Latvia*

Neutron radiography and computed neutron tomography has been an established method for non-destructive testing with neutrons for several years. Several techniques in digital imaging including imaging plates were successfully performed. Commercially available neutron

imagine plates are composed of a fine mixture of storage phosphor ($BaFBr:Eu^{2+}$) and neutron converter ($Gd_2O_3$) powders in an organic binder coated onto a plastic support. Unfortunately, they feature a relatively high γ-sensitivity. Use of mixture of storage phosphor und neutron converter due to scattering of secondary electrons results in reduced inherent spatial resolution of imaging plates being still a factor of 2 – 3 worse than in the case of film/Gd system.
An apparent way to enhance the spatial resolution of neutron imaging plates is the development of storage phosphors using neutron sensitive Li and Gd- compounds.
Results of investigation of $libaf_3$ shows, that radiation energy storage and read out characteristics are suitable for development of imaging plates. A strong, absorption bands at 270 nm, 317 nm and 430 nm arise after x-irradiation of $LiBaF_3$ crystals. Optical bleaching at RT by selective stimulation in each of radiation created absorption bands results in their simultaneous bleaching. Stimulation in the each of absorption bands is accompanied by stimulated luminescence and results in read out almost all the accumulated information.
The main disadvantages of $LiBaF_3$ are feeding of the stored information due to the ionic processes, and considerable absorption length of slow neutrons. High spatial resolution of the imagine plates obviously requires use thin active layer, thus leading to the considerable sensitivity reduction.
Perspective use of Gd related compounds as energy storage materials are investigated.

## THERMOACTIVATION AND SPECTROSCOPY OF CHARGE LOCALIZATION STATES IN InGaN/GaN QUANTUM WELL

**M. Springis, P.Kulis, I.Tale**
*Institute of Solid State Physics, University of Latvia*

Due to the lattice constant difference and low miscibility between GaN and InN indium aggregates around InGaN quantum well (QW) layers. It can be expected that like other structure defects and impurities the QD will act as deep capture centres for charge carriers. By injection or photo-generation of free electrons and holes subsequent capture of charge carriers in QD can be important formation mechanism of excitons.
Thermostimulated depolarisation and thermostimulated recombination luminescence are utilized to investigate the relative concentration and the thermal activation energy of charge carrier release of various defects: thermal admittance spectroscopy.
The TSL curve monitored after excitation in the fundamental absorption band is represented by the temperature independent luminescence up to the main TSL peak at 255 K. The TSDC curve qualitatively coincides with the TSL curve showing peak in the 250 – 260 K region.
Temperature independent afterglow indicates that the recombination process is caused by tunnelling recombination in close donor – acceptor pairs tunnelling recombination followed by the thermoactivated recombination in the donor – acceptor pairs in the 350 – 375 nm region.

## THERMOSTIMULATED RECOMBINATION PROCESSES IN $LiBaF_3$ CRYSTALS

**P. Kulis[a], I. Tale[a], I. Gromuls[a], M. Nikl[b], N. Ichinose[c], K. Shimamura[c]**
[a] *Institute of Solid State Physics, University of Latvia,*
[b] *Institute of Physics, AS CR, Prague, Czech Republic*
[c] *Laboratory of Material Science and Technology, Waseda University, Tokyo, Japan*

Creation of radiation defects in $LiBaF_3$ crystals at 10 K and their thermostimulated recombination process are investigated. Methods of optical absorption, thermal bleaching of color centers, thermostimulated luminescence and fractional glow technique are used. The radiation defects annealed in multi stage process accompanied with thermo-luminescence at 20, 46, 105, 130, 170, 210 and 270 K. Difference of optical absorption spectra measured before and after TSL peaks are obtained and possible parameters of recombination parameters are determinate. The TSL peak at 20 K arises due to the delocalisation of H-centres. Presence of two TSL peaks of $V_K$-centres at 105 and 130 K indicates that the 60˚ and the 90˚ migration hops occur.

## THERMALLY AND OPTICALLY STIMULATED RADIATIVE PROCESSES IN $LiBaF_3$ CRYSTALS

**M. Springis, A. Sharakovsky, I. Tale**
*Institute of Solid State Physics, University of Latvia*

In $LiBaF_3$ crystals both valence-core transitions (5,4-6,5 eV) and so-called self-trapped exciton luminescence (about 4,3 eV) are important for practical application. Here we present a study of 4,3 eV luminescence under photo– and thermo-stimulation after X-irradiation of undoped $LiBaF_3$ crystals at various temperatures. Optically stimulated luminescence (OSL) as a result of electron recombination with both self-trapped holes and holes localized at some defects, was observed after X-irradiation below 130 K and that of electron recombination with defect-localized holes was observed after X-irradiation above 130 K. The spectra of thermo stimulated luminescence (TSL) contain a broad band about 4 eV related to the electron (high energy side) or hole (low energy side) recombination depending on TSL peak temperature

## MAGNETOOPTICAL STUDIES OF DEFECTS AND RECOMBINATION LUMINESCENCE IN $LiBaF_3$

**U. Rogulis[1,2], J.-M. Spaeth[1], I. Tale[2], M. Nikl[3], N. Ichinose[4], K. Shimamura[4]**
[1] *Department of Physics, University of Paderborn, Paderborn, Germany*
[2] *Institute of Solid State Physics, University of Latvia*
[3] *Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[4] *Laboratory of Material Science and Technology, Waseda University, Tokyo, Japan*

Optically detected EPR investigations have been performed on the recombination luminescence (RL-EPR) of $LiBaF_3$ crystal, X-irradiated at T = 4.2 K. RL-EPR lines of $V_K$-

centres were found, as well as further lines of a defect with $S = 1/2$ and an axial $g$- tensor with its main axis along a [100] direction of the crystal.
Measurements of the magnetic circular dichroism of the absorption (MCDA) have been performed on $LiBaF_3$ crystals X-irradiated at two temperatures (4.2 K and RT). After irradiation at T = 4.2 K, the main MCDA bands peak at 453 nm and at 500 nm, but after irradiation at T = 300 K, the main bands peak at 444 nm and at 390 nm, there is a change of the sign between the peaks in both cases. The MCDA-detected EPR (MCDA-EPR) consists of one broad EPR line in both cases and belongs to electron trap centres. Analysis of half-widths of MCDA-EPR lines showed that both defects should have $g$-tensors with their axes along the [100] direction. This symmetry has to be expected for F-type centres in $LiBaF_3$ crystals. The low temperature electron centre has a more perturbed ground state as the RT centre.

## Tl-RELATED RADIATION DEFECTS IN CsI:Tl

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Angular dependencies of the EPR spectra detected via the magnetic circular dichroism of the optical absorption (MCDA-EPR) observed in the MCDA bands at 355 nm, 411 nm, 425 nm, 442 nm, 465 nm, 536 nm, and 815 nm of □- or x-irradiated CsI:Tl crystals have been investigated. The MCDA-EPR spectrum at B || [100] consists of two quartets of intense lines. The spectrum could be satisfactorily explained taking into account *hf* interactions of unpaired electron with s = 1/2 with *three* Tl nuclei I ($^{205}$Tl, $^{203}$Tl) = ½. Therefore we propose as a model a Tl-trimmer center. Hyperfine (*hf*) interactions along a [100] direction with two equivalent Tl and one single Tl were observed. As a center model we propose $Tl^{+}_{Cs^{+}} – Tl^{0}_{I} – Tl^{+}_{Cs^{+}}$. The Tl *hf* interactions observed can be explained qualitatively in the ionic model for this trimmer center.

## EPR OF RADIATION DEFECTS IN $LiBaF_3$

**V. Ogorodnik, U. Rogulis, I. Tale, A. Veispals**
*Institute of Solid State Physics, University of Latvia*

In the present work, we investigated in more details an EPR spectrum, observed in $LiBaF_3$ after X-irradiation at room temperature, consisting of approximately 35 lines. It is unstable at RT and disappears within few hours in dark or faster in light. For an orientation of the magnetic field parallel to the <111> direction of the crystal, these EPR lines are equidistant (with a step of 0.9 mT) and their intensities follow nearly the binomial distribution. The spectrum is explained by hyperfine interaction (*hf*) of a spin S = ½ with 2 equivalent Li nuclei being in the first shell and 8 equivalent fluorine nuclei in the second shell. This model corresponds to the F centre (fluoride vacancy with electron) in the $LiBaF_3$ crystal. The strong angular dependence of the line intensities is caused by an anisotropy of the g-tensor with its main axis oriented along the [100] direction of the crystal. Angular dependencies of the *hf* lines and their intensities as well as parameters of the $g$- tensor have been discussed.

## Scientific publication

### Published in 2003

1. M. Springis, L. Brikmane, I. Tale, P. Kulis, *Electronic exitations and defects in fluorperovskite $LiBaF_3$,* – Advanced Organic and Inorganic Optical Materials, Proceedings of SPIE **5122,** 23-29, 2003.
2. M. Springis, A. Trukhin, I. Tale, *Localized exitations in fluorperovskite $LiBaF_3$ crystals,* – Advanced Organic and Inorganic Optical Materials, Proceedings of SPIE **5122,** 30-35, 2003.
3. P. Pujats, A. Veispals, *Luminescence of intrinsic defects in $LiBaF_3$,* – Advanced Organic and Inorganic Optical Materials, Proceedings of SPIE **5122,** 36-40, 2003.
4. L. Dimitrochenko, P. Pujats, *The F-type centres in $LiBaF_3$ crystals,* – Advanced Organic and Inorganic Optical Materials, Proceedings of SPIE **5122,** 41-43, 2003.
5. P. Kulis, U. Rogulis, M. Springis, I. Tale, A.Veispals, V.Ziraps, *Annealing of Radiation Defects in X-Irradiated $LiBaF_3$,* – Advanced Organic and Inorganic Optical Materials, Proceedings of SPIE **5122,** 44-49, 2003.
6. V. Ziraps, V. Graveris, *Thermostimulated electronic and ionic processes in irradiated sapphire,* – Advanced Organic and Inorganic Optical Materials, Proceedings of SPIE **5122,** 74-78, 2003.
7. P. Kulis, U. Rogulis, M. Springis, I. Tale, *Luminescent detectors of ionizing radiation*, – Nuclear Instruments and Methods in Physics Research A 509, 56-59, 2003.
8. V. Ziraps, V. Graveris, P. Kulis, I. Tale, *Ion diffusion-controled thermally stimulated processes in X-ray irradiated halide crystals*, – Radiation Effects and Defects in Solids, Vol **158**, 567-571, 2003.
9. . M. Secu, S. Schweizer, U. Rogulis, J.-M. Spaeth, *Radiation induced defects and their recombination processes in the X-ray storage phosphor $BaBr_2$*, – J. of Physics: Condensed Matter, 2003, vol. 15, p. 2061-2070,

### Accepted for publication in 2003

1. M.Springis, P.Kulis, I.Tale, *Thermoactivation and spectroscopy of charge localization states in InGaN/GaN Quantum Well,* – NATO Science Series II – Mathematics, Physics and Chemistry by Kluwer Academic Publishers (accepted for publication).
2. Tale, *Optical and magnetic resonance spectroscopy of stimulated recombination processes in defect studies*, – Radiation Measurements, 2004 (accepted for publication).
3. U. Rogulis, J.-M. Spaeth, I. Tale,M. Nikl, N. Ichinose, K. Shimamura*, Magnetooptical studies of defects and recombination luminescence in $LiBaF_3$*, – Radiation Measurements, 2004 (accepted for publication).
4. P. Kulis, I. Tale,I. Gromuls, M. Nikl, N. Ichinose, K. Shimamura, *Thermostimulated recombination processes in $LiBaF_3$ crystals*, – Radiation Measurements, 2004 (accepted for publication).
5. V. Ogorodnik, U. Rogulis, I. Tale, A. Veispals, *EPR of defects in $LiBaF_3$ crystals*, – Radiation Measurements, 2004 (accepted for publication).
6. M. Secu, U. Rogulis, S. Schweizer, J.-M. Spaeth, A. Edgar, *Radiation defects in X-ray storage phosphor fluorobromozirconate glass-ceramics activated with rare-earth ions*, – Radiation Measurements, 2004 (accepted for publication).

7. M. Springis, A, Sharakovsky, I.Tale, *Thermally and optically stimulated radiative processes in $LiBaF_3$ crystals*, – Radiation Measurements, 2004 (accepted for publication).
8. U. Rogulis, J.-M. Spaeth, E. Elsts, A. Dolgopolova, *Tl- related radiation defects in CsI:Tl*, – Radiation Measurements, 2004 (accepted for publication).

## Lectures on Conferences

**19th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 10–13, 2003.**

1. I. Tale, *Methods and active materials for imagining f the slow neutron fluxes*, – Abstracts of the 19th Scientific Conference dedicated to 25th anniversary of Institute of Solid State Physics UL, Riga, 2003, p. 23, (oral presentation).
2. I. Tale, *Investigation of metal ions in fusion plasmas using emission spectroscopy*, –- Ibid. p. 27, (oral presentation).
3. V. Ogorodnik, U. Rogulis, I. Tale, A. Veispals, *EPR of F centres in $LiBaF_3$ crystals*, – Ibid. p. 61, (oral presentation).
4. A. Fedotovs, U. Rogulis, *EPR of $Cd^+$ impurity-defects in$BaF_2$ crystals*, – Ibid. p. 62, (oral presentation).
5. U. Rogulis, J.-M. Spaeth, I. Tale, M. Nikl, N. Ichinose, K. Shimamura, *Optically detected EPR of X-irradiated $LiBaF_3$ crystals*, – Ibid. p. 63, (oral presentation).
6. E. Elsts, U. Rogulis, Hyperfine structure of EPR in CsI:Tl,– Ibid. p. 64, (oral presentation).
7. P. Kulis, I. Tale, I. Gromuls, *Thermostimulated recombination processes in $LiBaF_3$ crystals*, – Ibid. p. 69, (oral presentation).
8. I. Gromuls, P. Kulis, *Computer LABVIEW package aided fractional glow technique*, – Ibid. p. 70, (oral presentation).
9. A. Sharakhovsky, M. Springis, *Optically stimulated recombination processes in $LiBaF_3$ crystals*, – Ibid. p. 71, (oral presentation).
10. J. Jansons, *Development of the photon-counting techniques in the Institute of Solid State Physics University of Latvia*, – Ibid. p. 78, (oral presentation).
11. D. Gusevs, A. Kristins, M. Springis, J. Tibergs, J. Veinbergs, *Automation of signal measurement*, – Ibid. p. 84, (oral presentation).

**NATO Advanced Research Workshop "UV Solid-State Light Emitters and Detectors", June 17-21, 2003, Vilnius, Lithuania**

1. M. Springis, P.Kulis, I.Tale, *Thermoactivation and spectroscopy of charge localization states in InGaN/GaN Quantum Well,* – Abstracts of the NATO Advanced Research Workshop "UV Solid-State Light Emitters and Detectors", Vilnius, 2003, p.22 (poster presentation).

**5th European Conference on Luminescent Detectors and Transformers of Ionizing Radiation "LUMDETR", September 1-5,2003, Prague, Czech Republic**

1. Tale, *Optical and magnetic resonance spectroscopy of stimulated recombination processes in defect studies*, – Book of abstracts of the 5th European Conference on Luminescent Detectors and Transformers of Ionizing Radiation "LUMDETR", Prague, 2003, p. 4, (oral presentation).

2. U. Rogulis, J.-M. Spaeth, I. Tale, M. Nikl, N. Ichinose, K. Shimamura*, Magnetooptical studies of defects and recombination luminescence in $LiBaF_3$*, – Ibid p. 53, 9 (oral presentation).
3. P. Kulis, I. Tale, I. Gromuls, M. Nikl, N. Ichinose, K. Shimamura, *Thermostimulated recombination processes in $LiBaF_3$ crystals*, – Ibid. p. 99, (poster presentation).
4. V. Ogorodnik, U. Rogulis, I. Tale, A. Veispals, *EPR of defects in $LiBaF_3$ crystals*, – Ibid. p. 106, (poster presentation).
5. M. Secu, U. Rogulis, S. Schweizer, J.-M. Spaeth, A. Edgar, *Radiation defects in X-ray storage phosphor fluorobromozirconate glass-ceramics activated with rare-earth ions*, – Ibid. p. 113, (poster presentation).
6. M. Springis, A, Sharakovsky, I.Tale, *Thermally and optically stimulated radiative processes in $LiBaF_3$ crystals*, – Ibid. p. 161, (poster presentation).
7. U. Rogulis, J.-M. Spaeth, E. Elsts, A. Dolgopolova, *Tl- related radiation defects in CsI:Tl,* – Ibid. p. 191, (poster presentation).

# DISORDERED MATERIAL PHYSICS

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

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

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

## Research area and Main Problems

Optical absorption and luminescence methods including time resolved spectroscopy has been used for prospective optoelectronic materials investigations.
The optical properties of materials used for:

- nonlinear optics ($KNbO_3$, $KTaO_3$, $LiNbO_3$),
- scintillators and radiation detectors ($CaWO_4$, $ZnWO_4$, YAP, TlBr),
- fiber optics (pure and doped glassy $SiO_2$)
- luminescence of nanocrystalline powders ($ZrO_2$ and ZnO)

have been studied.

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**Students**

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2. T. Dudareva,
3. M.Shorohovs
4. T.Nestjuk
5. K.Shmits

### Scientific Visits Abroad

1. Dr.hab.phys. L.Grigorjeva,. Czech Republic, (5 days).
2. Dr.hab.phys. L.Grigorjeva, Cambridge, UK (6 days).
3. Dr.hab.phys. L.Grigorjeva, Poland, (5 days).
4. Dr.hab.phys.D.Millers, Poland (4 days).
5. Dr.phys.V.Pankratov, Germany (10 month).
6. Dr.hab.phys. S.Chernov, Kiev, Ukraine, (7 days)
7. Dr.hab.phys. L.Skuja, Italy (5 days).
8. Dr.hab.phys. L.Skuja, Brasil (5 days).
9. Dr.hab.phys. L.Skuja, Japan ( 3 months).

**Visits from Abroad**
Dr. V.Trepakov, Praha, Czech Republic (one month)
PhD student Aleksej Mironov, St.Petersburg, Russia (2 weeks)
PhD student Agniezska Opalinska, Warszaw, Poland (one month)
PhD student Tomasz Strachowski, Warszaw, Poland (2 weeks)
Dr. Simonpietro Agnello, Univ. of Palermo, Italy (one month)
Dr. Marco Cannas, University of Palermo, Italy (2 weeks)

## Cooperation

**Latvia**
University of Latvia, (Prof. J.Tiliks, Dr. D. Erts).
University of Latvia, Institute of Biology (Dr. O. Mutere).
SIA "Baltic Scientific Instruments" (Dr.V.Gostillo).

**USA**
Wake Forest University (Prof. R.T. Williams.)
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**Poland**
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Institute of Physics, University of Rzeszow (Prof.A.Matkovskii, Ph.D.Stud.P.Potera)

## Main Results

### LUMINESCENCE IN $SrTiO_3$ and $LiNbO_3$ CRYSTALS UNDER HIGH DENSITY PULSED ELECTRON BEAM EXCITATION

**L.Grigorjeva, D.Millers, V.Trepakov, S.Kapphan**

The luminescence spectra under pulsed high density excitation show a band peaking at ~2.8 eV and another band at spectral region <1.2 eV. The luminescence rise is fast and follows the 10 ns excitation pulse. The main fraction of luminescence decays during the first 50 ns after excitation pulse switching off. The 2.7 eV luminescence band with similar properties was observed in $LiNbO_3$ (stoichiometric, congruent). It is suggested that luminescence mechanism in both crystals has a similar nature. The excited electrons and holes became temporary trapped within one oxy-anion complex. Formation of the charge transfer exciton is suggested as a possible mechanism of this trapping and the exciton radiative decay is the origin of luminescence.
*In cooperation with: Institute of Physics AS CR, Prague, Czech Republic;*
*FB Physik, University of Osnabrueck, 49069, Osnabrueck, Germany*

## LUMINESCENCE SPECTRA AND DECAY KINETICS IN $ZnWO_4$ AND $CdWO_4$

**S. Chernov, L. Grigorjeva, D. Millers, A. Watterich**

The luminescence spectra and decay kinetics in $CdWO_4$, $ZnWO_4$, as well as $ZnWO_4$:Fe and $ZnWO_4$:Mo were investigated. Different kinds of luminescence excitation were used: pulsed electron beam (250 keV, 10 ns), pulsed nitrogen laser beam (337 nm, 8 ns) and steady state x-ray excitation.

Different decay kinetics were obtained in undoped $CdWO_4$, $ZnWO_4$ crystals after laser beam excitation and electron beam excitation. Along with the well-known decay component observed under photo- and electron beam excitation (~11 μs in $CdWO_4$ and ~ 22 μs in $ZnWO_4$ at RT) the additional component with shorter decay time (~2 μs in $CdWO_4$ and ~ 1.5 μs in $ZnWO_4$ at RT) was observed under electron beam excitation. A similar effect was observed in $CaWO_4$. It is suggested that two types of self-trapped excitons due to two different oxygen positions in $WO_6$ group are responsible for the two decay times observed under high energy excitation.

The luminescence spectra and decay kinetics in $ZnWO_4$:Mo ($10^{-3}$mol/mol) and $ZnWO_4$:Fe ($10^{-4}$ mol/mol) were studied. These impurity ions belong to uncontrolled impurities and are introduced into crystals in growth process. Their role on luminescence mechanism and quantum yield are under investigation. The additional slow components in luminescence decay (~175 μs in $ZnWO_4$:Mo and ~800 μs in $ZnWO_4$:Fe) were observed at RT under 3.67 eV laser excitation. In luminescence spectra only one band (~2.5 eV) was observed in $ZnWO_4$:Mo in time region 2.0-50 μs under electron beam excitation at RT. Whereas under steady state x-ray excitation along with 2.5 eV band the luminescence bands at ~1.9 eV was observed. The origin of this luminescence as well as the process, which can result to the luminescence light yield reduction in $ZnWO_4$:Mo and $ZnWO_4$;Fe was discussed.

*In cooperation with: Research Institute for Solid State Physics and Optics*
*Hungarian Academy of Sciences, Budapest*

## TlBr CRYSTALS: GROWTH, OPTICAL INVESTIGATIONS, DETECTOR PARAMETERS

**I. S. Lisitskii, M. S. Kuznetsov, V. Gostilo, S. Zataloka**
**L. Grigorjeva, D. Millers, M. Shorohov**

TlBr single crystals were grown by Bridgeman-Stockbarger method. Part of each ingots was used for ionizing radiation detector manufacturing, another – for optical studies. The content of anion impurities, specific resistance as well as some detector parameters have been controlled. The optical study included steady-state absorption and luminescence methods as well as time-resolved spectroscopy. The differences were observed in absorption in the range of fundamental absorption edge and photoluminescence as well. The initial transient absorption induced by a pulsed electron beam was twice to sample with large iodine content however two absorption bands were observed in the spectra for all samples studied. Relaxation of absorption observed and the time-resolved luminescence excited by a pulsed electron beam depend from iodine concentration. The more important were differences between luminescence kinetics at 2.3 eV spectral region. It is observed that the luminescence intensity

in the sample with iodine continues growth after the end of excitation pulse. The process, responsible for the recombination delay is suggested. A comparison of the results of optical study with the detector parameters shows some correlation. More important is that the detector from the TlBr-I ingot does not show the spectral resolution for radiation detection. It is concluded that the purification of crystal from iodine can improve the detector quality.
*In cooperation with: GIREDMET", B.Tolmachevskiy per.5, Moscow, Russia*
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## LUMINESCENCE OF ZnO and $ZrO_2$ NANOPOWDERS

**D.Millers, L.Grigorjeva, W.Lojkowski, T.Strachowski**

The development of scintillating and luminescent materials reveals two mainstreams. One - the searching for new compositions and new dopands in single crystals, other – the development of nanostructured materials. Nanostructured scintillator is foreseen in some case to be highly competitive with single crystalline devices. High transparency in the visible predicts that transparent nanostructured ceramics might be possible. The study of luminescence from nanocrystalline ZnO and $ZrO_2$ was carried out. The luminescence spectra and decay kinetics were measured for different size free-standing (not embedded in any matrices) nanocrystals. Time-resolved measurements were conducted using nitrogen laser beam and high density (up to 20 MW/cm2) pulsed electron beam excitation.

In all ZnO nanocrystals studied the main luminescence bands were located at the two regions – in the red-yellow (1.8-2.4 eV) and blue (3.0-3.4 eV). The blue emission comes from different excitonic states. This luminescence under high density excitation is observed in the nanocrystals even at room temperature. The decay of this luminescence is fast and the determination of life-time is out of time limit of equipment used (<12 ns). The luminescence in red-yellow region comes from different defects excited states. The luminescence decay is complicated – at least two decay components persist. However, all over the spectrum fast decay component was observed. The comparison of luminescence from different size nanocrystals and different sintering methods is completed.

The time-resolved luminescence from different size (from 10nm up to 50 nm) $ZrO_2$ and $ZrO_2$:Pr nanocrystals has been studied under pulsed electron beam excitation. It is suggested that the luminescence band at 2.8 eV observed in undoped $ZrO_2$ is emission from self-trapped exciton. The $Pr^{3+}$ luminescence in 1.5 – 2.5 eV was observed in $ZrO_2$:Pr nanocrystals. The luminescence intensity and decay kinetics depends on nanocrystal size, but the *quantum confinement effects* are not expected in our luminescence experiments. It is shown that nanocrystal surface play the main role of electronic excitation decay process.

*In cooperation with*: *High Pressure Research Center of the Polish Academy of Sciences, Warsaw, Poland*

## INTERCONVERSION BETWEEN NON-BRIDGING OXYGEN HOLE CENTER AND PEROXY RADICAL IN $F_2$ LASER-IRRADIATED $SiO_2$ GLASS

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

Formation processes of the peroxy radical (POR) were examined in high-purity $SiO_2$ glass exposed to $F_2$ laser light which creates mobile atomic oxygen ($O^0$) by photolyzing the interstitial oxygen molecules ($O_2$). It was proved that under these conditions POR is formed by a reaction of the non-bridging oxygen hole center (NBOHC, an oxygen dangling bond) with $O^0$ , not by a reaction between the E' center (a silicon dangling bond) and $O_2$. Subsequent exposure to KrF laser light photolyzed POR and recovered NBOHC by dissociating the O-O bond in POR. These findings corroborate the important role of $O^0$ in defect processes in $SiO_2$ glass.

*In cooperation with: Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Corporation*

## URBACH ABSORPTION EDGE OF SILICA: REDUCTION OF GLASSY DISORDER BY FLUORINE DOPING

**L. Skuja, K. Kajihara, Y.Ikuta , M. Hirano, H. Hosono**

The vacuum-ultraviolet fundamental absorption edge ("Urbach edge") of four types of synthetic silica glasses, "wet", "dry", and doped by 570 and 6010 ppm wt. fluorine, was studied in the absorption coefficient range (1 cm-1 - 500 cm-1) at room temperature. The absorption edge has exponential form in agreement with the Urbach's rule. The widely documented increase of vacuum-ultraviolet transparency upon fluorine doping is due to a steeper absorption edge (shorter "Urbach tail") as compared to undoped silicas. The increase of the edge slope in F-doped silica occurs already the lower dopant concentration (570 ppm), the slope does not increase further in the 6010 ppm doped glass. These findings show that the improved vacuum UV transparency of F-doped silicas is due to the decreased contribution of the glassy disorder and strained Si-O bonds to the width of the absorption edge.

*In cooperation with: Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Corporation*

## OPTICAL ABSORPTION OF PEROXY RADICAL IN OXYGEN-RICH GLASSY SILICON DIOXIDE

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

Synthetic silica is one of the most widely used materials for ultraviolet (UV) optics. It shows the highest radiation resistance among all glassy materials. Particle-, ionizing- or UV laser-irradiation creates a complex, poorly resolved absorption spectrum starting from ca. 4 eV and extending into deeper UV, which is still not completely understood (see [1] for review). Electron paramagnetic resonance (EPR) spectra indicate that one of the major point defects induced in oxygen-excess silica is peroxy radical (POR), ≡Si-O-O$^{\bullet}$. However, the parameters of optical absorption band of POR have remained controversial.

In the present work, POR's were selectively created in oxygen-excess silica glass by adding oxygen atoms to oxygen dangling bonds (≡Si-O$^{\bullet}$):

$\equiv Si\text{-}O^{\bullet} + O \rightarrow \equiv Si\text{-}O\text{-}O^{\bullet}$ . (1)

The oxygen dangling bonds were created by neutron irradiation ($10^{18}$n/cm$^2$). Subsequent $F_2$-laser photolysis of interstitial $O_2$ molecules produced the atomic oxygens, which reacted with the oxygen dangling bonds. This technique yielded paramagnetic centers in concentrations up to $10^{18}$ cm$^{-3}$. A subsequent UV photobleaching (≈5eV) destroyed POR's and re-created oxygen dangling bonds in a reaction reverse to reaction (1). These transformations were monitored by EPR and optical absorption. The photobleaching-induced change of optical absorption was resolved in two oppositely pointing and closely overlapping Gaussian absorption bands: positive at 4.76 eV with full-width at half-maximum (fwhm)=1.08 eV and negative at 5.05-5.2 eV with fwhm around 1.1 eV. Comparison with the EPR spectra allows assigning the latter absorption band to POR's. The ambiguity inherent for Gaussian resolution of such overlapping bands is largely removed by employing the low-energy (2 eV) absorption band of the oxygen dangling bonds to determine the intensity of the associated 4.76eV absorption band. The close overlap of optical absorption bands of the oxygen dangling bonds and POR's together with their tendency to have opposite changes of intensity explain the origin of the long-lasting controversy over the optical absorption of POR in silica.

*In cooperation with: Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Corporation*

## UV-VUV LASER INDUCED PHENOMENA IN $SiO_2$ GLASS

**K. Kajihara, Y. Ikuta, M. Oto, M. Hirano, L. Skuja, H. Hosono**

High-purity synthetic $SiO_2$ glass is widely employed in optical elements used with UV-VUV lasers, such as KrF (5.0 eV or 248 nm), ArF (6.4 eV or 193 nm), and $F_2$ (7.9 eV or 157 nm) lasers. Its main virtues are high UV-VUV transparency coupled to a good workability in forming various shapes. However, structural defects, both preexisting and induced by the UV-VUV lasers, often limit the actual transmittance and toughness of the $SiO_2$ glass. Thus reducing the structural defects is a subject of great interest. For this purpose, their configurations and formation mechanisms have been intensively studied [1,2].

In this talk we will discuss recent studies on interactions of various $SiO_2$ glasses with UV-VUV laser photons including structural defect creation, photostructural changes, photochemical reactions involving mobile interstitial species. Particular attention is paid to phenomena induced by irradiation with $F_2$ laser, which is expected to be used as a light source in the next-generation photolithography. We report on positive effects of fluorine doping in developing an $SiO_2$ glass usable with $F_2$ laser (often referred as "Modified Silica"). We discuss the significant role of the mobile interstitial hydrogenous species on laser-induced photochemical reactions. We also describe utilization of these findings to develop a deep-UV optical fiber transmitting ArF laser photons with lower radiation damage.

*In cooperation with: Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Corporation.*

**SPONTANEOUS OXYGEN LOADING INTO $SiO_2$ GLASS BY THERMAL ANNEAL**

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

The interstitial oxygen molecules ($O_2$) in $SiO_2$ glass were detected down to $10^{15}$ $cm^{-3}$ by photoluminescence of $O_2$ at 1272 nm excited at 765 nm by a continuous-wave titanium-sapphire laser. It was evidenced that $SiO_2$ glass, thermally annealed in air between 800 and 1100 C, spontaneously absorbs $10^{16}$ $cm^{-3}$ of $O_2$ from the ambient atmosphere. The time-dependent concentration change of the interstitial $O_2$ allows to determine both the diffusion coefficient and the saturation solubility of the interstitial $O_2$.
*In cooperation with: Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Corporation.*

## Scientific Publications

### Published in 2003


1. D.Millers, L.Grigorjeva, W.Łojkowski, A.Opalińska. *Luminescence of Nanosize $ZrO_2$ and $ZrO_2$:Pr powders.* Solid State Phenomena. **94**, 135-140, 2003.
2. V.Pankratov, D.Millers, L.Grigorjeva, A.O.Matkovskii, P.Potera, I.Pracka, T.Łukasiewicz. *The role of Fe and Cu dopants in electron-hole trapping and relaxation process in congruent $LiNbO_3$.* Optical Materials. **22**, 257-262, 2003.
3. P.Potera, A.Matkovskii, D.Sugak, L.Grigorjeva, D.Millers, V.Pankratov. *Transient color centers in GGG crystals.* Radiat.Effects and Defects in Solids **157**, 709-713, 2002.
4. L.Grigorjeva, N.Pankratov, D.Millers, S.Chernov, V. Nagirnyi, A.Kotlov, A.Watterich. *Time-resolved spectroscopy in $ZnWO_4$ and $ZnWO_4$Fe.* Ibid, **158**, 135-139, 2003.
5. V.Nagirnyi, S.Chernov, L.Grigorjeva, L.Jönsson, M.Kirm, A.Kotlov, A.Lushchik, D.Millers, V.A.Nefedov, V.Pankratov, B.I.Zadneprovski. *Ion-related luminescence ceters in $ZnWO_4$:Fe.* Ibid, **157**, 1123-1126, 2002.
6. D.Millers, V.Pankratov, L.Grigorjeva, S.Kapphan, V.Trepakov. *Relaxation of electronic excitations in strontium titanate.* Ibid, **157**, 589-59, 2002.
7. L.Grigorjeva, D.Millers, V.Pankratov. *Transient absorption of niobium states in photorefractive materials.* Ferroelectrics, **295**, 443-449, 2003.
8. A.Matkovskii, P.Potera, D.Sugak, Ya.Zhydachevskii, V.Pankratov, D.Millers, L.Grigorjeva, I.Pracka, T.Łukasiewicz. *Transient and stable color centers in pure and Cu-doped $LiNbO_3$.* **38**, No.3-5, 388-393, 2003.
9. L. Skuja, H. Hosono, M. Hirano, K. *Kajihara Advances in silica-based glasses for UV and vacuum-UV laser optics* Proc. SPIE vol. **5122**, "Advanced optical materials", 2003, p.1-14 (2003).
10. T. Suzuki, L. Skuja, K. Kajihara, M. Hirano, T. Kamiya, H. Hosono *Electronic Structure of Oxygen Dangling Bond in Glassy $SiO_2$ : The Role of Hyperconjugation.* Phys. Rev. Lett. v.**90**, No18, p. 186404-1 - 186404-4 (2003).

**In Press**

1. L. Grigorjeva, D. K. Milllers, V. Pankratov, R. T. Williams, R.I.Eglitis, E.A.Kotomin,G. Borstel. *Experimental and theoretical studies of optical properties of polarons and excitons in $KNbO_3$.* Solid State Commun., 2004.
2. D.Millers, L.Grigorjeva, W.Lojkowski, T.Strachwski. *Luminescence of ZnO nanopowders.* Radiat.Measur.,2004.
3. P.Potera, L.Grigorjeva, A.Matkovskii, D.Millers, T.Lukasiewicz, Z.Galazka, T.Wojciechowski. *Time-resolved optical zbsorption in YAP crystals*. Radiat.Measur.,2004.
4. L.Grigorjeva, D.Millers, M.Shorohov, I.S.Lisitskii, M.S.Kuznecov, S.Zatoloka, V.Gostilo. *Optical investigations of TlBr detector crystals.* NIMA, 2004
5. L.Grigorjeva, D.Millers, V.Trepakov. *Luminescence in $SrTiO_3$ and $LiNbO_3$ crystals under high density pulsed electron beam excitation.* Ferroelectrics, 2004.
6. S.Chernov, L.Grigorjeva, D.Millers, A.Watteroch. *Luminescence spectra and decay kinetics in $ZnWO_4$ and $CdWO_4$ crystals*. Phys.Stat.Sol. (submitted)
7. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja, H. Hosono *Spontaneous Oxygen Loading Into $SiO_2$ Glass By Thermal Anneal.* J. Non-Crystalline Solids (submitted).
8. K. Kajihara, L. Skuja, M. Hirano, H. Hosono *A fundamental defect process in $SiO_2$ glass: Interconversion between non-bridging oxygen hole centers and peroxy radicals in $SiO_2$ glass*. Phys. Rev. Letters (accepted).
9. L. Skuja, K. Kajihara, Y.Ikuta, M. Hirano, H. Hosono *Urbach Absorption Edge Of Silica: Reduction Of Glassy Disorder By Fluorine Doping.* J. Non-Crystalline Solids (accepted).
10. K. Kajihara, L.Skuja, M.Hirano, H. Hosono *Interconversion between non-bridging oxygen hole center and peroxy radical in $F_2$ -laser-irradiated $SiO_2$ glass.* J.Non-Crystalline Solids (accepted).

## Lectures on Conferences

**19. Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, 10-13. February, 2003**

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1. L.Grigorjeva, D.Millers. W.Lojkowski, A.Opalinska. *Luminescence of $ZrO_2$ nanokrystals in the nanosecond region*. Abstracts, p.57.
2. I.Pļaviņa, A.Tāle. *Creation spectra of photostimulate luminescence in doped alkali haldes at room temperature*. Ibid, 72.
3. T.Dudareva, L.Grigorjeva. Absorption and luminescence in undoped and Nd-doped $LaGaO_3$ crystals. Ibid, p.67.
4. S.Chernov L.Grigorjeva, D.Millers, A.Watterich. *Luminescence of $ZnWO_4$:Fe and $ZnWO_4$:Mo crystals.* Ibid, p.68.
5. L.Skuja , H.Hosono, K. Kajihara. *Fundamental Absorption Edge in Fluorine-Doped Synthetic $SiO_2$ Glasses.* Ibid, p.76.
6. D.Erts, B.Polyakov, A.Truhins, L.Skuja, A.Patmalnieks, K.M.Ryan, J.D.Holmes *Three-Dimensional Semiconducting Nanowire Architectures: Characterization by TEM, AFM, and Optical Methods.* Ibid, p.48.

**International Scientific and Practical Conference "Spectroscopy in Special Applications" 18-21 June, 2003, Kyiv, Ukraine**

1. S.Chernov, L.Grigorjeva,D.Millers, A.Watterich. *Luminescence spectra and decay kinetics in $ZnWO_4$ and $CdWO_4$ crystals*. Abstracts, p.137.

**The 10th European Meeting on Ferroelectricity, August 3rd - August 8th 2003, Cambridge, UK**

1. L.Grigorjeva, D.Millers, V.Trepakov, S.Kapphan. *Luminescence in $SrTiO_3$ and $LiNbO_3$ under high density pulsed electron beam excitation.* Abstracts, p.143.

**The 5th European Conference on Luminescence Detectors and Transformers of Ionizing Radiation, September 1-5, 2003, Prague, Czech Republic**

1. L.Grigorjeva, D.Millers, S.Chernov, A.Watterich. *Transient absorption and luminescence comparable investigation in $ZnWO_4$, $ZnWO_4$:Fe and $ZnWO_4$:Mo*. Abstracts, p. 135.
2. D.Millers, L.Grigorjeva, W.Lojkowski, T.Strachowski. *Luminescence of ZnO nanopowders.* Ibid, p.148.
3. P.Potera, L.Grigorjeva, A.Matkovskii, D.Millers, T.Lukasiewicz, Z.Galazka, T.Wojciechowski. *Time-resolved optical absorption in YAP crystals*. Ibid, p.192.
4. A.Matkovskii, L.Grigorjeva, D.Millers, P.Potera, D.Sugak, Ya.Zhydachevskii, I.Izhin. *Stable and transient color centers in YAP and GGG crystals*. Ibid, p.197.

**The 5th International Workshop on Radiation Imaging Detectors, 7-11 September, 2003, Riga, Latvia**

1. D.Millers, L.Grigorjeva. *Radiation induced optical properties of thallium bromide*. Abstracts, p.52.
2. F.Muktupavela, I.Manika, L.Grigorjeva, V.Skvorcova. *Effect of γ-radiation on micromechanical properties of AlN thin films*. Ibid, p.85.
3. L.Grigorjeva, D.Millers, M.Shorohov, I.S.Lisitskii, M.S.Kuznecov, S.Zotoloka, V.Gostilo. *Optical investigations of detector TlBr crystals*. Ibid, p.73.

**European Material Research Society 2003 Fall Meeting, 15th –19th September, 2003, Warsaw, Poland**

1. P.Potera, A.Matkovskii, Ya.Zhydachevskii, L.Grigorjeva, D.Millers, T.Lukasiewicz, Z.Galazka. *Color centers in YAP:Pr crystals. Abstracts, p.43.*
2. L.Grigorjeva, D.Millers. *Luminescence mechanisms: from single crystals to nanocrystals.* Ibid, p.212.
3. D.Millers, L.Grigorjeva, W.Lojkowski, A.Opalinska, T.Strachowski. *Luminescence of $ZrO_2$ and ZnO nanocrystals.* Ibid, p.214.

**10th Internat.Conference on the Physics of Non-Crystalline Solids, Jul.13-Jul.17, 2003, Parma, Italy**

1. L. Skuja, K. Kajihara, Y.Ikuta, M. Hirano, H. Hosono *Urbach Absorption Edge Of Silica: Reduction Of Glassy Disorder By Fluorine Doping.* (Abstracts, p.O-78).
2. K. Kajihara, L.Skuja, M.Hirano, H. Hosono *Interconversion between non-bridging oxygen hole center and peroxy radical in $F_2$ -laser-irradiated $SiO_2$ glass.* (Abstracts, p.O-60).

**12th Internat.Conference on Radiation Effects in Insulators (REI-12), Aug.31-Sep.5, 2003, Gramado, Brazil**

1. L.Skuja, K.Kajihara, M.Hirano, H.Hosono *Optical absorption of peroxy radical in oxygen-rich glassy silicon dioxide.* (Abstracts, p.35).
2. K.Kajihara, Y.Ikuta, M.Oto, M.Hirano, L.Skuja, H.Hosono *UV-VUV laser induced phenomena in $SiO_2$ glass.* (Abstracts, p.24).

**Topical inter-university seminar "Glasss Science", University of Tokyo, Nov.20, 2003,, chair. T. Aizawa.**

1. L.Skuja *Interstitial Oxygen in $SiO_2$ Glass* (lecture, 45 min.).

**Bachelor Thesis**

1. Tatjana Dudareva. *Radiation defects and energy transfer in undoped and Nd-doped $LaGaO_3$*, Riga, 2003.
2. Krishjanis Shimts. *Design and manufacturing of computer controlled luminescent signal apparatus,* Riga, 2003.
3. Tatjana Nestjuk. *Luminescence of oxide nanopowders,* Riga, 2003.
4. Mihails Shorohovs. *Electron and hole relaxation in TlBr crystals and TlBr application for radiatiation detection.* Riga, 2003

## SOLID STATE OPTICS LABORATORY

Head of Laboratory, Professor, Dr. habil. 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 localized due to electron-phonon interaction electronic excitations are revealed in silicon dioxide, germanium dioxide and relevant aluminum and gallium orthophosphates in crystalline and glassy states. The disorder leads to large broadening of the properties of such dynamic localized state. The static localized states of short-range order, related to a material isomorphism, are revealed in wide gap optical glasses relevant to the mentioned crystals. Found essential sensitivity of localized states to history of glass preparation and treatment by light (laser, etc.).

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 stuff**

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

**Visitors from Abroad**

1. Ph.D. Marco Cannas and Simonepietro Agnello, University of Palermo, Prof. Roberto Boscaino, Inst. Naionale di Fisica della Mat.and Dipartimento di Scienze Fisiche ed Astronomiche dell ’Università,via Archirafi, 36, I-90123 Palermo,Italy

**Scientific Visits Abroad**

1. Dr. Phil., Dr. Phys. K.Truhins, USA, Postdoctoral position at University of Illinois at Chicago, Chicago, Illinois 60607 USA
2. Professor, Dr. hab. Phys. A. Trukhin, Russia (3 weeks) University of Irkutsk, Institute of Geochemstry.
3. Professor, Dr. hab. Phys. A. Trukhin, Prague, Check Republic, 5 European conference Lumdetr 2003, 2 oral talks and one poster presentation.
4. Professor, Dr. hab. Phys. A. Trukhin, Universite Paris Sud, Orsay, Lab. Labo. Physico-Chimie des Solides, France. (2.5 months), invited professor, thesis commission member,

## Cooperation

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

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

**USA**
Wake Forest University, Winston Salem , North Caroline (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)
University of Illinois at Chicago, Illinois 60607-7061 (Professor, Robert J.Gordon)

**France**
Universite Paris Sud, Orsay, Lab. Labo. Physico-Chimie des Solides UMR8648, (Prof.A.Revcolevchi, Dr.B. Poumellec)

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

## Main Results

### SELF-TRAPPED EXCITON LUMINESCENCE IN CRYSTALLINE α-QUARTZ UNDER TWO-PHOTON LASER EXCITATION

**Anatoly N. Trukhin, Margarita F. Kink*, Yuri A. Maksimov*, Rein A. Kink***

The luminescence of pure crystalline α-quartz is studied under pulsed ArF laser excitation. The obtained luminescence parameters well correspond to that of self-trapped exciton in α-quartz, therefore the excitation process is two-photon. The efficiency of two-photon excitation is of the same order of magnitude as compared to one-photon excitation of sodium salicilate. The STE luminescence decay kinetics and their temperature dependence under photoexcitation were recorded with higher accuracy than previously. Decay kinetics changes with temperature are explained by splitting of the

STE triplet state in zero magnetic field and are analyzed with assumption of Orbach process of spin-lattice relaxation. No trace of another luminescence was detected in pure sample.

**In cooperation with: Institute of Physics, University of Tartu, Estonia*

## CATHODOLUMINESCENCE DECAY KINETICS IN $Ge^+$, $Si^+$, $O^+$ IMPLANTED $SiO_2$ LAYERS

**A. N. Trukhin, J.Jansons, H.-J. Fitting*, T. Barfels*, B. Schmidt***

Cathodoluminescence spectra shapes and respective band decay times show no similarity between luminescence centers in different crystal and amorphous modifications of $SiO_2$ and $GeO_2$. On the other hand, the additionally produced red luminescence centers (650 nm) by oxygen implantation into $SiO_2$ layers are of the same nature as in stoichiometric $SiO_2$ and are attributed to the non-bridging oxygen hole center (NBOHC). Moreover, the elevated blue (460 nm) and UV (290 nm) luminescence in Si implanted $SiO_2$ belongs to the silicon related oxygen deficient center (SiODC) as in stoichiometric layers too. Ge implantation into $SiO_2$ and thermal post annealing leads to a huge violet luminescence (400 nm) with a first rapid decay of $\tau \approx 24$ ns followed by a slow hyperbolic decay with $t^{-0.15}$ ... $t^{-0.54}$. The last 10% show again an exponential decay with a mean life time $\tau \approx 125$ μs. This complex luminescent center is related to the GeODC center formed during the thermal treatment by Ge cluster formation.

**in cooperation with: Physics department, University of Rostock, Universitätsplatz 3, d-18051 Rostock, Germany and research center Rossendorf, ion beam physics, pob 510119, d-01314 Dresden, Germany*

## LUMINESCENCE OF DIFFERENT MODIFICATIONS CRYSTALLINE SILICON DIOXIDE. STISHOVITE AND COESITE

**Anatoly N.Trukhin, Janis L.Jansons, Tatyana I.Dyuzheva [*], Ludmila M.Lityagina *, Nikolai A.Bendeliani [*]**

Luminescence of very small samples of single crystals of coesite and stishovite has been studied. The spectra were detected under ionizing radiation (x-ray and electron beam) and the decay kinetics of cathodoluminescence in the range of time from 10 ns to 3 ms was measured. The coesite luminescence possesses a broad band at 3 eV with exponential decay about 680 μs at 80 K. The nature of this luminescence was explained as a self-trapped exciton creation in tetrahedron framework. The stishovite luminescence possesses two bands – blue (2.8 eV) and UV (4.7 eV). The UV band intensity grows more than 20 times with irradiation dose from initial level. That shows the corresponding luminescence centers could be induced by the radiation. The decay of UV band possesses fast and slow decay. The fast decay parameters determination is beyond the capabilities of our apparatus (less than 10 ns), whereas the slow decay of the UV is non-exponential and takes place in the range of hundreds microsecond. The blue band decay kinetics could be well approximated by power law $\sim t^{-2}$, which may correspond to recombination of defects, created by radiation. The stishovite single crystal luminescence is very similar with that of germanium dioxide single crystal of rutile structure. The nature of stishovite luminescence was explained as recombination of defects created by irradiation in octahedron-structured lattice.

**In cooperation with: L.F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia*

## STUDY OF THE GERMANIUM LUMINESCENCE IN SILICA: FROM NON-CONTROLLED IMPURITY TO GERMANO-SILICATE CORE OF TELECOMMUNICATION FIBERS PREFORM

**Anatoly Trukhin, Bertrand Poumellec*, Jérôme Garapon***

We have studed luminescence properties of doped silica with different concentration of germanium. The basic luminescence parameters such as spectral dependencies, decay kinetics and polarization at different temperatures were measured. Three spectral ranges 3.5 – 5.5 eV (I), 5.5 – 7 eV(II), 7 – 8 eV(III) in the optical transparency range of silica could be chosen from these data. The range I possess a weak variation of basic parameters of luminescence of the germanium related oxygen deficient center (GeODC) with the change of luminescence center concentration from extremely low in pure silica to germano-silica core of optical telecommunication fibers' preforms. The temperature dependence of luminescence intensity and spectral content including excitation band are more affected by change of concentration. The deviation of those parameters could be explained mainly within framework of inhomogeneous broadening and center interaction with varying environment. The multi-typicalness of the centers' structure also takes place in the range I. The changes of decay kinetics and polarization excited in the ranges II and III are also insensitive to the change of concentration but the spectral content is more sensitive to the history of sample preparation, providing bigger changes in spectral bands relation. That could be explained as multi typicalness of similar centers due to different surrounding leading to inhomogeneous broadening of the basic parameters. The range III is more affected by host defect (ODC(I), manifesting itself through absorption band at 7.6 eV, by providing recombination mechanisms of luminescence excitation.

**In cooperation with: Physico-Chimie de l'Etat Solide, Université Paris Sud, Orsay 91405 France*

## LUMINESCENCE OF FLUORINE DOPED SILICA GLASS

**A. N. Trukhin*, J.Jansons*, T.A.Ermolenko *, I.I.Cheremisin***

The role of fluorine doping on silica properties was studied by luminescence methods. Non-doped sample of the same preparation technology possess absorption band at 7.6 eV on the level of the 2 $cm^{-1}$. A trace of this band in the fluorine-doped sample is on the level of 0.1 $cm^{-1}$. In both samples 7.6 eV photons as well as ionizing irradiation (x-ray, electron beam) excite photoluminescence of so call oxygen deficient centers with blue (2.7 eV) and UV band (4.4 eV). The luminescence of fluorine doped sample increases with dose many times from initial small level for used excitation. Also, thermally stimulated luminescence appears after irradiation. The energetic yield under ionizing irradiation of induced luminescence is the same level of reference samples. The decay kinetics of cathodoluminescence shows that blue bands' decay is faster and UV band decay is slower than use to be for known oxygen deficient center. It is concluded that structural imperfections, responsible for the absorption band at 7.6 eV, remain similar in silica glasses during preparation, however fluorine changes electronic transition nature and, therefore, the absorption band is of low intensity. Such imperfections, passivated with fluorine, interact with electronic excitation, produced by radiation. Transient changes of imperfections geometric and electronic configurations take place with probable remove of fluorine, and that provides growth of luminescence centers even at low temperature and changed decay relatively to intra-center luminescence. Therefore

fluorine-doped sample is similar to non-doped samples through corresponding recombination luminescence of oxygen deficient centers.
**In cooperation with: Institute of Silicate Chemistry, RAS, St-Petersburg*

## PHOTOLUMINESCENCE IN γ-IRRADIATED α-QUARTZ INVESTIGATED BY SYNCHROTRON RADIATION

**M. Cannas[*], S. Agnello[*], R. Boscaino*, F.M. Gelardi[*], A. Trukhin**

Investigation and comparison of the optical properties in different forms of $SiO_2$, crystalline quartz and amorphous silica, is a crucial aspect in understanding the structure of intrinsic defects. In this frame, an optical absorption (OA) band centered at 7.6 eV has been observed both in irradiated silica and quartz and associated with a oxygen deficient center, called ODC(I), common in glass and crystal matrix. Experimental and theoretical works evidenced that in silica the OA at 7.6 eV is able to excite a photoluminescence (PL) band at 4.4 eV through a conversion process of ODC(I) towards a different variant of oxygen deficient center, named ODC(II). A corresponding emission process under excitation within the OA at 7.6 eV in quartz has not been clarified.
Here we report the investigation of PL in γ-irradiated (dose 1 Grad) α-quartz under vacuum-ultraviolet (UV) excitation by synchrotron radiation within the OA band at 7.6 eV, induced by irradiation. Two emissions centered at 4.9 eV (UV band) and 2.7 eV (blue band) are observed, both excitable within the OA band at 7.6 eV. The overall photoluminescence activity is detected only at low temperature, the UV band decreases above 40 K, whereas the blue band exhibits an initial slight increase and its quenching is effective above 100 K. Furthermore, the decay kinetics of both emissions occurs in a time scale of ns, at T=17 K we measured a lifetime $\tau$=1.0 ns for the PL at 4.9 eV and $\tau$=3.6 ns for the PL at 2.7 eV.

These results give new insight on the optical properties associated with defects peculiar of crystalline matrix, also on the basis of their comparison with previous studies on neutron irradiated quartz .
**In cooperation with: INFM&Dipartimento di Scienze Fisiche ad Astronomiche dell' Università di Palermo, Via Archirafi 36, 90123 Palermo, Italy*

## LUMINESCENCE OF a-QUARTZ

**Anatoly Trukhin, Kaspars Truhins**

A short review of α-quartz crystal's luminescence properties is presented. The luminescence of the self-trapped exciton (STE), which band is situated at 2.6-2.7 eV, could be observed mainly under ionising radiation with energetic yield about 20 %. The STE does not participate in pure recombination processes and could not be used in dosimetry. However it could be used in momentary detection of radiation at temperatures lower than 180 K.
Another host material luminescence at 5 eV appears in α-quartz after heavy irradiation. It is constituted of permanent defect after neutron irradiation and transient defect after dens electron beam irradiation. This luminescence could be observed well at temperatures below 60 K. All another reviewed luminescence bands are of impurity nature. The Ge impurity luminescence in α-quartz explained as STE near Ge. The aluminium and alkali complexes in α-quartz provides at least three types of luminescence centers. One of them is with UV band at 6 eV, appears at low temperatures and could be excited only in tunnelling recombination process between pairs [$AlO_4$ - $Me^o$], where $Me^o$ is an alkali ion captured an electron and a hole remains on aluminium tetrahedron. Another luminescence with band at 3.4 eV is also luminescence of complexes [$AlO_4/Me^+$], which behaviour is similar to the luminescence

of alkali alumo-silicate glass. The third luminescence with band at 3 eV could be observed mainly in natural α-quartz, bright at temperatures below 200 K and is interpreted as STE-like luminescence at alumo-silicate clasters. The exchange of alkali ions to noble ions of copper of silver reduces original luminescence of alumo – alkali complexes and luminescence of noble ions appears. The main band of copper related luminescence is at 3.4 eV and that of silver is at 4.75 eV, both could be observed up to 500 K. their nature could be well described in terms of intra-ions transition. Exchange of noble ions back to alkali ions renews initial luminescence of the samples. All impurities luminescence could be active in dosimetry in corresponding conditions.

## PHOTOSENSITIVITY OF SILICA GLASS WITH GERMANIUM STUDIED BY PHOTOINDUCED OF THERMALLY STIMULATED LUMINESCENCE WITH VACUUM ULTRAVIOLET RADIATION

**Anatoly Trukhin , Bertrand Poumellec***

Photosensitivity of the germanium-doped silica was studied through kinetics of recombination of the created defectsin isothermal and thermally stimulated luminescence (TSL) regimes. The main observed luminescence contains bands mainly due to Ge oxygen deficient center. The maximum of photosensitivity corresponds to the high-energy part of the 7.6 eV band. The growth of TSL intensity is almost linear for the case of excitation through monochromatic light and growth with saturation in the case of excitation with white light. The efficiency of formation of TSL peaks increases with an increase of the temperature. The result was explained as multi-step process of photochemical dissociation and product separation by thermally stimulated diffusion.
**In cooperation with: Physico-Chimie de l 'Etat Solide,University Paris Sud, Orsay 91405, France*

## ENERGY TRANSPORT IN SILICA TO OXYGEN-DEFICIENT LUMINESCENCE CENTERS. COMPARISON WITH OTHER LUMINESCENCE CENTERS IN SILICA AND α-QUARTZ

**Anatoly Trukhin, Bertrand Poumellec*,**

The transport of energy absorbed by host material to oxygen-deficient luminescence centers in silica glass was studied in the range of intrinsic absorption from 8.2 eV up to 35 eV. Pure silica with excess silicon and germanium-doped samples were studied. The obtained results show very low efficiency of those luminescence centers excitation by transport of energy and that could not be ascribed only to bad transport of elementary electronic excitation in disordered network of glass. Others center ($Cu^+$, for example,) could be excited in such process with sufficiently high efficiency, however lower than in crystal. The effect of bad interaction of oxygen deficient centers with elementary electronic excitation was explained as isolation of clusters with that centers from host network of glass so that the elementary electronic excitations annihilate non-radiatively on the boundary of clusters and main network of glass.
**In cooperation with: Physico-Chimie de l 'Etat Solide,University Paris Sud, Orsay 91405, France*

## Scientific publications

1. A.N.Truhins, B. Poumellec, *Photosensitivity of silica glass with germanium studied by photo induced of thermally stimulated luminescence with vacuum ultraviolet radiation,* Journal of Non-Crystalline Solids, (2003) Vol 324/1-2, pp 21-28
2. A.N.Truhins, J.L.Jansons, T. I.Dyuzheva , L. M.Lityagina , N A.Bendeliani, *Luminescence of different modifications crystalline silicon dioxide. stishovite and coesite,* Solid State Communications, 127 (2003) 415-418.
3. A.N.Truhins, M.Kink, J.Maksimov, R.Kink, *Self-trapped exciton luminescene in crystalline alpha-quartz under two-photon laser excitation,* Solid State Communications, 127 (2003) 655-659.
4. A. N. Trukhin, J. Jansons, H. -J. Fitting, T. Barfels and B. Schmidt, *Cathodoluminescence decay kinetics in $Ge^+$, $Si^+$, $O^+$ implanted $SiO_2$ layers,* Journal of Non-Crystalline Solids, 331 (2003) 91-99.
5. Anatoly Trukhin, Bertrand Poumellec and Jérôme Garapon, *Study of the germanium luminescence in silica: from non-controlled impurity to germano-silicate core of telecommunication fiber preforms,* Journal of Non-Crystalline Solids, 332, (2003) 153-165.
6. A. N. Trukhin, J. Jansons, T. A. Ermolenko and I. I. Cheremisin, *Luminescence of fluorine doped silica glass,* Journal of Non-Crystalline Solids, V 332 (2003) 219-228.
7. A. Trukhin, B.Poumellec, *Energy transport in silica to oxygen-deficient luminescence centers. Comparison with other luminescence centers in silica and alpha-quartz,* Solid State Communications, 129 (2004) 285-289.

## Lectures in Conferences

**Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, 10-13. February, 2003**

8. A.N.Truhins, M.Kink, J.Maksimov, R.Kink, *Self-trapped exciton luminescence in crystalline α-quartz under two-photons laser excitation*, 18. CFI LU Zinātniskās konferences referātu tēzes, Rīga, Latvija, 11.-13. Februāris 2003, 75.lpp.
9. D. Erts, B.Polyakov, A.N.Truhins, L.Skuja, A.Patmalnieks, K.Mryan, J.D.Holmes, *Three dimensional semiconducting nanowire archtictures: characherisation by TEM, AFM, and optical methods.* 18. CFI LU Zinātniskās konferences referātu tēzes, Rīga, Latvija, 11.-13. Februāris 2003, 48.lpp.

**The 5th European Conference on Luminescence Detectors and Transformers of Ionizing Radiation, September 1-5, 2003, Prague, Czech Republic.**

10. M.Cannas, S.Agnello, R.Boscaino, F.M.Gelardi, A.Trukhin, *Photoluminescence in γ-irradiated α-quartz investigated by synchrotron radiation.* Book of Abstracts , p. 34.
11. A.Trukhin, K.Truhins, *Luminescence of α-quartz,* Book of Abstracts, p. 56
12. A.Truhins and B.Poumellec, *Luminescence of Ge-doped silica,* Book of Abstracts, p. 116.

### Lectures at Universities, Institutes, Companies

1. Trukhin A., *Investigation of the point defects in silica in Institute of Solid State Physics of the Uneversity of Latvia.* ODUPE meeting 22 September 2003, Lille, France, University Lille-1.
2. Trukhin A., Poumellec B., *Defects in optical Glasses,* Annual meeting of GDR of Glassy Materials. Bordeaux, France , 28/29 October 2003, Institute of Condensed Matter Chemistry of Bordeaux.

# PHYSICS OF FERROELECTRICS

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

## Research Area and Main Problems

The research issues of the Division of Ferroelectric Physics includes technology - synthesis and structure determination, theoretical modelling, study and application of functional ferroelectric materials. Chemical coprecipitation and hot pressing technologies have been used for ceramic production, and pulsed laser deposition and sol-gel processing for obtaining of ferroelectric thin films. 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, optoelectronics and microelectromechanical systems are considered.

The main areas of progress during 2003 are desribed under the following:

- theory and modeling of polarization finite size ferroelectric objects;
- relaxation dynamics of metastable systems;
- X-ray diffractometry studies of polar and centrosymmetric single crystals, ceramics and thin films;
- preparation and study of properties in doped lead scandoniobate ceramics;
- nature of dielectric dispersion in PLZT ceramics at the diffused phase transition;
- investigation of relaxor and ferroelectric epitaxial thin films by dielectric Fourier spectroscopy;
- study of dielectric and optical properties of multidimentional polar materials for microelectromechanical systems and application in photonics: new compositions of ferroelectric thin films and new non-linear optically active organic molecular layers;
- general applications of Atomic Force Microscopy for surface analysis of functional thin films; detection of local piezodeformation and polarization in ferroelectrics using Scanning Probe Microscopy
- ellipsometry and reflectometry studies and optical second harmonic investigation of properties of thin films;
- antiferroelectric $PbZrO_3$ pulsed laser deposited and sol-gel thin films: neutron and electron irradiation effects;
- application of PLZT passive and active optical elements in infrared laser systems for bio-optical experiments and medicine;
- use of PLZT ceramics controllable light scattering elements in design of "artificial eye" for vision research experiments.

**Scientific staff**

1. Dr. Eriks Birks
2. Dr. Karlis Bormanis
3. Dr. Maruta Dambekalne
4. Dr. habil. Vilnis Dimza
5. Dr. Eriks Klotins

**Technical staff**

1. Mg. Marite Kalnberga
2. Mg. Anna Kalvane
3. Modris Logins
4. Alberts Tupulis

6. Dr. habil. Andris Krumins
7. Dr. habil. Maris Ozolins
8. Dr. habil. Andris Sternberg
9. Dr. Vismants Zauls
10. Dr. Jevgeņijs Kaupužs
11. Dr. Anatolijs Mišņovs
10. Mg. Maija Antonova
11. Mg. Laila Chakare
12. Mg. Maris Kundzins
13. Mg. Maris Livins
14. Mg. Astrida Spule
15. Mg. Inta Brante
16 Mg. Karlis Kundzins

**Mag. science**

1. Ilze Aulika (grad. in 2004)

**Bachelor science**

1. A. Janovs (grad. 2003)

**Students**

1. P. Spels (2nd year B.Sc. studies)
2. Reinis Arājs

**Visitors from Abroad**

Dr. phys. **Barbara Garbarz – Glos,** Institute of Physics, Krakow Pedagogical University, Poland (1 month).

Mg. **Wlodimierz Smiga**, Institute of Physics, Krakow Pedagogical University, Poland (2 week).

Mg. **Margorzata Plonska**, Institute of Physics, University of Silesia, Sosnowice, Poland (2 week).

Dr. **Marina Tyunina**, Microelectronics and Materials Physics Laboratories, University of Oulu, Finland (2 months).

Prof. **Andrei Kholkine**, Departmet of Ceramic and Glass Engineering,Research Unit on Ceramic Materials, University of Aveiro, Aveiro, Portugal (1 month).

Dr. **Markys G. Cain,** Functional Materials Group, National Physical Laboratories, Teddington, United Kingdom (3days).

Dr. **Jirka Hlinka**, Institute of Physics ASCR, Praha, Czech Republik (1 month).

**Scientific Visits Abroad**

Mg. **Maija Antonova**

1. International Conference: Processing of Electroceramics, Bled, Slovenia (1 week).

B. sc. **Ilze Aulika**

1. Atomic Institute of Austrian Universities, Vienna University of Technology (1 month + 1 month).
2. Institute of Experimental Physics, University of Vienna (1 month).

Dr. phys. **Karlis Bormanis**

1. 7th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors, Rio de Janeiro, Brazil (1 week).
2. Company EMBRACO, Joinwille, Brzil (2 weeks).
3. The 10th European Meeting on Ferroelectrics, EMF-10, Cambridge, UK (1 week).
4. 6th International Conference “Crystals: growth, properties, real structure, applications”, Aleksandrov, Russia (3 days).
5. The Fourth International Seminar on Ferroelastics Physics, Voronezh, Russia (1 week).

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

1. 8th European Ceramic Society Meeting, Istanbul, Turkey (1 week).
2. International Conference: Processing of Electroceramics, Bled, Slovenia, (1 week).

Dr. phys**. Eriks Klotins**

1. The 10th European Meeting on Ferroelectrics, EMF-10, Cambridge, UK (1 week).
2. Institute of Physics, Academy of Sciences, Prague, Czech Republic.
3. University of Aveiro, Portugal.
4. Cagliari, Sardiny, Italy.

Dr. habil. phys. **Andris Krumins**

1. 3rd Meeting of Centres of Excellence in Cyprus (1 week).

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

1. Praha Technical University, Czech Republic. (1 week).
2. Berlin Technical University, Germany (1 week).
3. Vilnius University, Lithuania (1 week).
4. Tartu University (1 week).
5. Chalmers TH, Lund University, Sweden (2 weeks).
6. The 10th European Meeting on Ferroelectrics, EMF-10, Cambridge, UK (1 week).

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

1. 8th European Ceramic Society Meeting, Istanbul, Turkey (1 week).
2. The 10th European Meeting on Ferroelectrics, EMF-10, Cambridge, UK (1 week).
3. A symposium "55 Years of Ferroelectrics", Leeds, UK (3 days).
4. COST 525 Meeting, Prague, Czech Republic (3 days).
5. EPFL, Lousanne, Switzerland (2 days).
6. University di Napoli, Italy (2 days).
7. National Physics Laboratory, Teddington, UK (2 days).
8. International Summer School-Conference "Advanced Materials and Technologies", Palanga, Lithuania (5 days).
9. NATO Advanced Research Workshop on the Disordered Ferroelectrics, Kiev, Ukraine (5 days).
10. Atomic Institute of Austrian Universities, Vienna, Austria (4 days).
11. Institute for Experimental Physics, University Vienna, Austria (4 days).

Dr. phys. **Vismants Zauls**

1. Microelectronics and Materials Physics Laboratories, University of Oulu, Oulu, Finland (3weeks).
2. Functional materials Group, National Physical Laboratories, Teddington, United Kingdom (3days).
3. The 10th European Meeting on Ferroelectrics, EMF-10, Cambridge, UK (1 week).

# Cooperation

**Latvia**

1. Daugavpils University (Dr. habil. 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. University of Latvia, Institute of Mathematics and Computer Science (Dr. J. Kaupuzs).
5. University of Latvia, Institute of Solid State Physics
   Laboratory of Optical Recording (Dr. J.Teteris),
   Laboratory of Organic Materials (Prof. I. Muzikante),
   EXAFS Spectroscopy Laboratory (Dr.Hab. A. Purans).

**Austria**

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

**Belarussia**

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

**Czech Republic**

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

**Denmark**

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

**Finland**

1. University of Oulu (Prof. S.Leppävuori).

**Germany**

1. Institute for Solid State and Materials Research, Dresden (Dr. W.Häßler).
2. University of Saarland, Saarbrucken (Dr. H.Schmitt).
3. Institute of Optics, Berlin Technical University (Prof. H.J.Eichler).
4. Institute for Lasertechnology in Medicine, Ulm University (Prof. R.Steiner).
5. Group of Condensed Matter Physics, Institute of Physics, Potsdam University (Dr. S. Schrader).

**Japan**

1. Shonan Institute of Technology (Prof. S.Sugihara).

**Lithuania**

1. Vilnius University, Vilnius (Prof. J.Grigas, Dr. J. Banys).
2. Vilnius University Laser Research Centre (Prof. Roaldas Gadonas).

**Norway**

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

**Poland**

1. Polish Academy of Sciences, Poznan (Prof. B.Hilczer).
2. Institute of Physics, Krakow Pedagogical University, Krakow (Prof. Cz. Kus, Dr. B. Garbarz – Glos).
3. Institute of Physics, University of Silesia, Sosnowiec (Prof. Z. Surowiak, Mg. M. Plonska).

**Portugal**

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

**Russia**

1. Ural State University, Ekaterinburg (Prof. V.Shur).
2. Volgograd State Architectural and Engineering Academy, Volgograd (Prof. A.Shilnikov).
3. Russian Academy of Science, Moscow (Prof. A.Medovoi).
4. Joint Institute for Nuclear Research, Dubna (Dr. S.Tiutiunnikov).
5. Moscow State University, Moscow (Prof. B.A.Strukov).
6. Research Institute for Complex Testing of Optoelectronic Devices and Systems, (Dr. V. N. Alekseev).
7. Tver State University (Dr O.V.Malyshkina).
8. Institute of Chemistry and Technology of Rare Elements and Minerals, Apatity, (Prof. N.V.Sidorov).

**Slovenia**

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

**Spain**

1. Laboratorio de Óptica, Dpt. de Física, Universidad de Murcia (Prof. P. Artal).

**Sweden**

1. Liquid crystal group, Chalmers TH, Gotheborg, (Prof. L. Komitov).
2. Medical Laser centre Lund University (Prof. S.Svanberg).
3. Umeå university, Umeå (Dr. B.Eliasson).

**Ukraina**

1. Institute for Problems of Materials Science, National Academy of Science (Prof. M.D.Glinchuk, Prof. V. Pokropivny).

**United Kingdom**

1. Functional materials Group, National Physical Laboratories, Teddington, (Dr. M. G. Cain).

# Main Results

## RELAXATION DYNAMICS OF METASTABLE SYSTEMS: APPLICATION TO NON-EQUILIBRIUM CONDENSED MATTER

**E. Klotins**
*Institute of Solid State Physics, University of Latvia, Riga, Latvia*

Performance specifications of many ferroelectric devices are significantly influenced by a very complex intrinsic microstructure comprising regions with different orientations of spontaneous electric polarization (domains). Crucial questions related to this type of analysis address the rate of polarization switching and the role of finite size and dimensionality being a long-term challenge for theory in this field [1,2]. We precede a departure from conventional Ginzburg-Landay energy functional technique and make use of its mapping with imaginary time Schrödinger equation so addressing the problem to well-developed simulating methods of quantum electron dynamics. In the case of spatial homogeneity this imaginary time Schrödinger treatment yields thermal noise controlled dielectric relaxation, dielectric response on time periodic driving voltage, and nonlinear susceptibility [3-5]. Extension toward spatial inhomogeneity yields relaxation rate firstly found gradient specific, namely, polarization switching to the opposite direction is favored in vicinity to boundaries as manifested by the V-potential (analogue of the potential energy operator in quantum statistical calculations) plots. It gives a new perspective to the long-term problem of polarization switching that occurs at much lower field than the conventional approach suggests. However, the significance of this treatment goes far beyond of this particular solution and may benefit for a variety of problems associated with thermally activated and spatially extended metastability.

The relevant physics applications reads:

- Polarization kinetics in ferroelectric thin films.
- Performance of noise activated dynamic piezoacoustic sensors.
- Low frequency spectroscopy in non-Markovian systems (biological ion channels).

[1] J. Kaupužs. *Spatio-Temporal Correlations of Local Polarization in Ferroelectrics.* Ferroelectrics, 2003, Vol. **295**, pp. 607-616.
[2] J. Hlinka and E. Klotins. *Application of Elastostatic Green Function Tensor Technique to Electrostriction in Cubic, Hexagonal and Orthorhombic Crystals.* J. Phys.: Condens. Matter, 2003, Vol. **15**, pp. 5755-5764.
[3] E. Klotins. *Polarization Reversal in Ferroelectrics: Stochastic analysis*. Ferroelectrics, 2003, Vol. **295**, pp. 577-588.
[4] J. Aulika, E. Klotins. *Effect of thermal fluctuations on ferroelectric response: dynamic hysteresis.* Journal of Optoelectronics and Advanced Materials, 2003, Vol. **5**, No.3, pp. 747-753.
[5] E. Klotins, J. Hlinka, and J. Kaupužs. *Semiadiabatic High-Field Polarization Response in Ferroelectrics I: Hysteresis and Nonlinear Susceptibility, Ferroelectrics* (Ferroelectrics, in press).

## DIELECTRIC PROPERTIES OF PEROVSKITE RELAXOR FERROELECTRIC THIN FILMS

**M. Tyunina[1], K. Kundzins, V. Zauls, and J. Levoska[1]**
*Institute of Solid State Physics,CAMART Center of Excellence, University of Latvia, Riga, Latvia*
*[1]Microelectronics and Materials Physics Laboratories, University of Oulu, Oulu, Finland*

Epitaxial thin films of perovskite relaxors and ferroelectrics represent a special case of relaxor / ferroelectric (RFE/RE) state due to unavoidable presence of surfaces and interfaces, small thickness d < 1000 nm, crystallographic strain, specific chemical ordering, misfit dislocations and other peculiarities of microstructure. Epitaxial heterostructures of perovskite RFE thin films grown by pulsed laser deposition included samples of $(PbMg_{1/3}Nb_{2/3}O_3)_{1-x}$ - $(PbTiO_3)_x$, x = 0, 3, 32 at.% $(PbSc_{0.5}Nb_{0.5}O_3)_{1-x}$ - $(PbTiO_3)_x$, x = 0, 10, 42 at.% and $(PbLu_{0.5}Nb_{0.5}O_3)_{1-x}$ - $(PbTiO_3)_x$, x = 0, 41 at.% with thickness in 70 - 1000 nm range.
Dielectric properties of the heterostructures were studied by HP 4284A LCR-meter as a function of frequency (102-106 Hz), temperature (77-725 K), and amplitude of applied ac electric field (103-106 V/m). The true properties of the films were reconstructed and analyzed excluding effects of electrodes and passive layers. In pseudo-cubic films with the typical features of RFE were found to be essentially similar to those in single crystals *Tm = TR*, Vogel - Fulcher relationship, deviation from Curie - Weiss behavior and boardening of *G*(lnt,*T*) at low *T*. Clear dependence of *Tm* on thickness of the film and/or tetragonal strain was not detected.

## NANOSCALE PIEZORESPONSE AFM IMAGING AND PATTERNING OF FERROELECTRIC AND RELAXOR THIN FILMS

**K. Kundzins, V. Zauls, A. Janovs, and A. Kholkine[1]**
*Institute of Solid State Physics, University of Latvia, Riga, Latvia*
*[1]Departmet of Ceramic and Glass Engineering, University of Aveiro, Portugal*

The basic technologically important parameters for application of ferroelectric and relaxor thin films such as local piezoresponse and polarization state can be probed with high spatial resolution using atomic force microscopy (AFM). Moreover, various AFM operation multi-pass regimes allow us direct poling of the film in a voltage lithography mode and immediate testing local piezoresponse. In our experiments a small modulation AC voltage along with DC bias voltage has been applied to the sample local area between conductive AFM tip and the bottom electrode. Modified *"Stand Alone SMENA"* microscope (NT-MDT Co.) with versatile measurement capabilities was operating in scanning force microscopy (SFM) contact mode with external lock - in amplifier for enhanced deflection sensitivity to detect both out-of-plane and in-plane surface deformations.

Samples under investigation were pulsed laser deposited barium titanate $BaTiO_3$ (BT), lead zirconate titanate $PbZr_{0,47}Ti_{0,53}O_3$ (PZT) and lead magnesium niobate $Pb(Mn_{0,33}Nb_{0,67})O_3$ (PMN) thin films and heterostructures on $Si/SiO_2/Ti/Pt$ or MgO single crystal substrates.

Spatially resolved piezoresponse imaging of poled regions and polarization switching hysteresis loop measurements in various granular polar ferroelectric or relaxor thin films with and without top electrodes was made in comparison with results for single crystals PMN and BT used as model materials. Observed differences, electrode

edge contribution and relaxation of locally induced piezoresponse can be interpreted in terms of size effects on local polarization, presence of defects, charge accumulation and local conductivity.

## DETERMINATION OF THICKNESS AND REFRACTIVE INDEX OF THIN FILMS BY OPTICAL REFLECTOMETRY AND ELLIPSOMETRY

**I. Aulika, V. Zauls, K. Kundzins, M. Kundzins, and S. Katholy[1]**
*Institute of Solid State Physics, University of Latvia, Riga, Latvia*
*[1]Institute of Physics, University of Potsdam, Potsdam, Germany*

The reflectivity spectra under normal light incidence geometry in the range of 350 - 750 nm were made by miniature "Ocean Optics" CCD spectrometer with fibre optics input. Ellipsometric measurements were performed by variable-angle null-ellipsometer (at He-Ne laser wavelength $\lambda = 632.8$ nm, angles set from 45° to 75°, step 5°). Additional surface morphology atomic force microscopy (AFM) tests in contact mode with conventional tips were made using Stand Alone SMENA instrument from NT-MDT Co. Multilayer model numerical optimisation procedure was developed for reflectometric and ellipsometric data evaluation. The variation of refractive index and absorption coefficient has been observed for pulsed-laser deposited (PLD) $BaTiO_3$ (BT) thin films on $Si/SiO_2/Ti/Pt$ substrate with different thickness. The refractive index slightly decreases and absorption coefficient shifts to higher photon energies with thickness decrease. Estimated values of band gap energies are 2.86 eV, 3.03 eV and 3.38 eV for film thickness 320 nm, 170 nm and 130 nm respectively. The AFM surface topography analysis showed that thin film growth process depends on layer thickness resulting in various surface final roughness patterns and affecting optical properties due to band structure modifications and scattering losses.

## THICKNESS EFFECTS ON OPTICAL PROPERTIES OF $BaTiO_3$THIN FILMS

**I. Aulika, V. Zauls, K. Kundzins, and M. Kundzins**
*Institute of Solid State Physics, University of Latvia, Riga, Latvia*

The variation of refractive index and absorption coefficient has been observed for pulsed-laser deposited (PLD) $BaTiO_3$ (BT) thin films on $Si/SiO_2/Ti/Pt$ substrate with different thickness. The refractive index slightly decreases and absorption coefficient shifts to higher photon energies with thickness decrease. Estimated values of band gap energies are 2.86 eV, 3.03 eV and 3.38 eV for film thickness 320 nm, 170 nm and 130 nm respectively. The AFM surface topography analysis showed that thin film growth process depends on layer thickness resulting in various surface final roughness patterns and affecting optical properties due to band structure modifications and scattering losses.

The measurements were performed with variable-angle null-ellipsometer (at He-Ne laser wavelength $\lambda = 632.8$ nm, angles set from 45° to 75°, step 5°). A miniature "Ocean Optics" CCD spectrometer, model PC 1000, designed as a plug-in PC ISA slot with fibre optics input was used for the reflectivity measurements under normal light incidence geometry in the spectral range of 350 – 750 nm. Atomic force microscopy (AFM) measurements were performed by Stand Alone SMENA microscope from NT-MDT Co. in contact mode using conventional tips to characterize the surface morphology.

# IRRADIATION EFFECTS ON FERROELECTRIC AND ANTIFERROELECTRIC THIN FILMS

**A.Sternberg[1], K.Kundzins[1], V.Zauls[1], I.Aulika[1], L.Čakare[1,2], R.Bittner[3], H.Weber[3], K. Humer[3], D. Lesnyh[4], D. Kulikov[4], Y. Trushin[4], and E.Hodgson[5]**

[1]*Institute of Solid State Physics, University of Latvia, Riga, Latvia*

[2]*Jožef Stefan Institute, Ljubljana, Slovenia*

[3]*Atomic Institute of Austrian Universities, Vienna, Austria*

[4]*St. Petersburg State Technical University, St. Petersburg, Russia*

[5] *CIEMAT, Madrid, Spain*

Intensive neutron irradiation effects on sol - gel $PbZrO_3$ and $PbZr_{1-x}Ti_xO_3$ thin films:

In consequence of intensive neutron irradiation the changes in the dielectric properties have been observed for preferentially (100) oriented spin coated $PbZrO_3$ (PZ), $PbZr_{1-x}TI_xO_3$ (PZT, x = 0.47) sol-gel films with thickness from 200 nm until 1300 nm on $Si/SiO_2/TiO_2/Pt$ substrate. The PZ and PZT heterostructures have been exposed to high luency neutron irradiation $(0.5 \div 3)\cdot 10^{22}$ $m^{-2}$, average energy > 0.1 MeV; accompanied by gamma rays dose $7.1\cdot 10^9$ rad, energy ~ 1 MeV; $T_{irrad.} < 60\ ^0C$ in TRIGA MARK II reactor Atomic Institute of the Austrian Universities in Vienna. Decrease of dielectric permittivity $\varepsilon$, increase for PZ and decrease for PZT of spontaneous and saturation polarization has been established after irradiation. Partial recovering of dielectric properties is observed at post-irradiation isochronal annealing to elevated temperatures. The observed effects of irradiation may be related to capture of mobile charge carriers on defects (grain boundaries, interfaces) in the thin film heterostructures. Screening of depolarizing fields by charges captured in thin films may cause a decrease of dielectric permeability and polarization for ferroelectrics and increase and polarization for antiferroelectrics at irradiation.

Physical properties of ferroelectric and antiferroelectric thin films after electron irradiation:

Electron irradiation damage have been observed for preferentially (100) oriented $PbZrO_3$ (PZ) and $PbZr_{0.53}Ti_{0.47}O_3$ (PZT) sol-gel and pulse laser deposited (PLD) thin films with a thickness from 250 nm and 1000 nm, which were, deposited on $SrRuO_3/Pt/TiO_2/SiO_2/Si$ and $Pt/TiO_2/SiO_2/Si$ substrates. PZ and PZT thin films have been exposed of electron irradiation to fluency up to $\sim 10^8$ Gy (1.8 MeV) in CIEMAT Madrid, Spain.

Dielectric properties have been evaluated by measurements of capacitance and loss factor performed on a probe station and Perkin Elmer 7265 lock-in amplifier. As a rule, "zero field" measurements in the frequency range of 160 Hz – 1 MHz have been made in the temperature range of 20 °C – 400 °C. Ferroelectric properties of the films were evaluated by polarization-electric field hysteresis loops measured on a modified Sawyer-Tower circuit at frequency 15 Hz testing system. Dielectric and polarization measurements were made before and after irradiation. Post irradiation isochronic annealing to elevated temperatures was performed to study the recovery of properties. Dielectric permittivity was measured during the annealing process up to the temperature 300 °C (heating rate 2 ÷ 3 °C/min). Maximum of the dielectric permittivity $\varepsilon$ decreases, phase transition temperature $T_c$ increase and hysteresis loop becomes asymmetric for PZ thin films after electron irradiation. Decrease of $\varepsilon$ and remanent polarization have been observed for PZT after electron irradiation. Partial recovering of dielectric properties is observed at post-irradiation isochronal annealing to elevated temperatures. Internal bias field of the films relates the observed effects of irradiation.

# LIGHT SCATTERING AND DEPOLARIZATION IN PDLC OPTICAL PHANTOMS USED FOR SIMULATION OF EYE CATARACT

**M. Ozolinsh[1], D. Korenuks[1], A. Kozachenko[2], and L. Komitov[2]**
[1] *Institute of Solid State Physics, University of Latvia*
[2] *Göteborg University*

Polymer dispersed liquid crystals (PDLC) [1] besides another electrically controllable material - electrooptic PLZT ceramics [2] can be successfully used in vision science to develop eye occluders to alter continuously and relatively fast the quality and characteristics of human vision perception. In PLDC the electrical field forces optically anisotropic liquid crystal droplets, which are embedded in polymer matrix to align along the direction of the electrical field. In absence of an external influence droplets are randomly oriented causing local optical non-homogeneities and light scattering. Anisotropy created by droplets is high, and noticeable light scattering occurs passing through a PDLC layer of ten-micrometer thickness. The scattered light is polarized, and it is strongly wavelength dependent in the visible. The electrical field in the PDLC cell is applied parallel to the light beam. We use pixel values of depicted angular dependencies to extract the scattering linear polarized contribution and the polarization angle $\alpha$ according to the polarization of the incident light.

Depolarization (if assume that depolarization prevails over circular polarization for such symmetry) at small scattering angles $\theta$ increases and afterwards according to the scattering theory [3] the degree of polarization reaches its maximum. Regarding light scattering in the cataract eye the heaviest impact on the visual performance is due to scattering at smaller angles. The eye pupil size (3 - 6 mm) restricts the scattering angle inhibiting the foveal central vision at 10-15$^o$.

Scattering diffuse increases skirts of eye point spread function thus diminishing the vision quality. Scattering and depolarization are phenomena accompanying each other thus depolarization can serve as a measure to evaluate development of eye scattering segments. Using PDLC cells we have measured at different scattering levels visual acuity and contrast sensitivity of colored stimuli presenting them on computer screen. The human eye has three kinds of color discriminating photoreceptors **S** (short), **M** (medium) and **L** (long wavelength) cone in retina. However the density of the most sensitive in blue end of spectrum S cone are distributed in fovea at very low density. A scattering occluder (simulating besides a cataract eye) most effective in short wavelength region can selectively affect the processes of perception passing different channels of visual pathway. We demonstrated following stimuli: Landolt**C** black - white, high contrast blue on black background, low contrast yellow (i.e. blue subtracted out of white) - white, and low contrast gray scale at luminance similar to yellow - white. Similar color scheme was applied to contrast sensitivity measurements. Results show drastic diminishing of blue stimuli perception due to scattering. However the presence of neural signals in intensity channels, providing by **M** and **L** cones, still working at short wavelengths, ensures perception at high levels of scattering. This activity is eliminated in a yellow-white stimuli case, where **M** and **L** cones are uniformly excited within all the visual field, and only presence or absence of blue determines the stimulus. One can observe the abrupt decrease of the yellow - white contrast stimuli perception by increasing light scattering. Similar lowering of contrast sensitivity for white-yellow Gabor pattern stimuli as compared with those of grayscale and blue-black stimuli by inducing of light scattering is confirmed.

[1] S.J.Cox, T.J.Sluckin,and V.Yu.Reshetnyak, *Molecular Crystals and Liquid Crystals,* 1998, Vol. 320, p. 301.
[2] M.Ozolinsh, I.Lacis, R.Paeglis, A.Sternberg, S.Svanberg, S.Andersson-Engels, and

J.Swartling. Ferroelectrics, 2002, Vol. 273, p. 131.
[3] M. Born and E. Wolf, *Principles of Optics.* Cambridge University Press, Cambridge, 1999, p. 951.

## ELECTRICALLY CONTROLLED EYE OCCUDERS IN VISION SCIENCE

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Advanced optical materials allow to ensure efficient control of light waves entering the human eye in various ways: using of amplitude controllers – attenuators and switches based on birefringence in liquid crystals and electrooptic ceramics, and phase controllers – deformable mirrors, or spatially resolved liquid crystal phase optical phase shifters. Another type of devices to interact with visual information are electrically controllable light scattering obstacles. There exist two classes of materials where on can induce efficient the light scattering - Polymer Dispersive Liquid Crystals (PDLC) and Electrooptic Ceramics (such as PLZT ceramics).
Vision science is interested in such controllable eye occluders as tools for diagnostics and therapy and for vision research, particularly to study characteristics of monocular vision, and of binocular vision - good cooperative perception of visual information with both eyes, stereovision presence and quality (for example in cases of ambliopia, when in childhood one eye falls behind in development and it is needed to force seeing with the "bad" eye, or cataract - opaque formations in the eye lens).
Report particularly characterizes applications of liquid crystals and electrooptic ceramics ensuring switching and controllable continuous attenuation, and continuous inducing of light scattering, that affects visual information in eye diagnostic and training techniques and in modelling of eye pathologies.

## PRODUCTION TRANSPARENT PLZT CERAMICS, SYNTHESIZED BY HYDROXOPOLIMER AND SOL-GEL METHODS

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The processing of electroceramics by means of chemical solutions has become increasingly important especially in the producing transparent $Pb_{1-x}La_x(Zr_{0.65}Ti_{0.35})O_3$ (PLZT) ceramics of large size.
We have worked out original two-stage co-precipitation method from mixed solution of inorganic salts, as follows: $ZrOCl_2 \cdot 8H_2O$, $TiCl_4$, $La(NO_3)_2 \cdot 6H_2O$, $Pb(NO_3)_2$, which are commercially easy available and cheap. At the first stage hydroxopolimer of $TiO_2$-$ZrO_2$-$La_2O_3$ is obtained by co-precipitation from mixed solution of corresponding metallic salts by 10% $NH_4OH$. In result "dry" curds, snow-like deposit was obtained (without any liquid phase). After it thermal decomposition at 1000 $^oC$ for 4 h white powder of above mentioned oxides was obtained.
At the second stage PbO was introduced in powder produced at the first stage of reaction by milling in $Pb(NO_3)_2$ solution for 10 h. After co-precipitation of obtained suspension by mixture of $NH_4OH$ and $H_2O_2$ the deposit of peroxohydroxopolimer was produced. After filtration the deposit by water-pump and thermal decomposition at 600 $^oC$ for 4 h we have obtained PLZT powder of desired composition with perovskite structure. Depending on thermal regime and size of samples 1.0 ÷ 6.0 wt.% of overstoichiometric PbO was added.

Transparent PLZT ceramics of large size were produced by two-stage hot pressing sintering. The first stage was performed at 930 $^{o}$C – 980 $^{o}$C for about 1 h in forvacuum at 20 MPa pressure. The second stage was performed at 1150 $^{o}$C-1200 $^{o}$C for 1 ÷ 40 h depending on size (15 ÷ 90 mm of diameter) at pressure 20 MPa in air or rich in $O_2$ atmosphere.

The optical transmittance of ceramic plates (thickness 0.3 mm) measured at wavelength of 630 nm reached 67 - 69 %.

To study influence of different methods of synthesis on properties of ceramics PLZT ceramics were prepared from powders synthesized by sol-gel method. High purity metal alkoxide and metal carboxide salts were taken as precursors: lead (2) acetate trihydrate– $Pb(COOCH_3)_2.3H_2O$, lanthanum acetate hydrate – $La(COOCH_3)_3.1.5H_2O$, zirconium(4) propoxide – $Zr(OCH_2CH_2CH_3)_4$, titanium(4) propoxide –$Ti(OCH_2CH_2CH_3)_4$, n – propylalkohol – as a solvent, and acetyloacetate – as a stabilizing agent.

The components mixed in a proper stoichiometric ratio were solved in n-propanol. The solution was then heated for 2 h below the boiling temperature. As a result of a reaction of synthesis alkoxide complexes were formed.

The PLZT powder was calcined at 600 $^{o}$C for 2 h to remove the organic part of alkoxide complexes. Using the sol-gel method amorphes nano-powder of PLZT ceramics has been obtained. PLZT ceramics were obtained by sintering powders by hot pressing at temperatures ranging from 1100 $^{o}$C – 1200 $^{o}$C. Investigations of dielectric and ferroelectric properties of as – obtained PLZT ceramics were measured. X–ray and electron microscopy investigations revealed the nanocrystalline structure of obtained ceramics. The optical transmittance of ceramics produced from powders synthesized by peroxohydroxopolimer method is about 20% higher than that from sol–gel powder sintered ceramics. It means that we need to carry on optimising of sol-gel processing.

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## Scientific publications

### Published in 2003

1. V.N. Alekseev, and E. Klotins. *Benchtop Characteristics of PLZT Based Electrooptic Switches.* Proc. of SPIE, 2003, Vol. **5123**, Advanced Optical Devices, Technologies, and Medical Applications, pp. 18-20.
2. I. Aulika, V. Zauls, K. Kundzins, M. Kundzins, and S. Katholy. *Study of transparent ferroelectric thin films by optical reflectometry and ellipsometry.* Journal of Optoelectronics and Advanced Materials, 2003, Vol. **5**, No. 3, pp. 755 – 761.
3. I. Aulika, and E. Klotins. *Effect of thermal fluctuation on ferrolectric response: dynamic hysteresis.* Journal of Optoelectronics and Advanced Materials, 2003, Vol. **5**, No. 3, pp. 747 – 753.
4. R. Bittner, K. Humer, H. W. Weber, K. Kundzins and A. Sternberg. *Radiation-induced defects in antiferroelectric thin films.* Fusion Engineering and Design, 2003, Vol. **66-68**, C, pp. 833.
5. K. Bormanis, S.A. Satarov, A. Kalvane, A. Sternberg, A.I. Burkhanov, and A.V. Shil'nikov. *Diffuse Phase Transitions in Lead Containing Relaxor Ferroelectrics: Bias Field Effects.* Ferroelectrics, 2003, Vol. **295**, pp. 537-542.
6. K. Bormanis, M. Kalnberga, A. Patmalnieks, and M. Ozolinsh. *Microscopic Studies of the Crystalline Structure of Ferroelectric and High Temperature Superconductor Layers.* Ferroelectrics, 2003, Vol. **291**, pp. 37-47.
7. J.M. Bueno, E. Berrio, M. Ozolinsh, and P. Artal. *Degree of polarization as an objective tool to evaluate scattered light in the human eye.* In: Friesem A.A., Turunen J., eds., Uni. Joensuu Selected Papers, 2003, Vol. **8**, pp.128-129.

8. M. Dambekalne, M. Antonova, M. Kalnberga, A. Kalvane, M. Livinsh, I. Brante, L. Shebanovs, and K.Bormanis. *The Effect of Technological Factors on the Synthesis of* $PbMg_{1/3}Nb_{2/3}O_3$. Ferroelectrics, 2003, Vol. 285, pp. 259 – 264.
**9.** J. Hlinka, and E. Klotins. *Application of elastostatic Green function tensor technique to electrostriction in cubic, hexagonal and orthorhombic crystals*. J. Phys.: Condens. Matter, 2003, Vol. **15**, pp. 5755-5764.
10. E. Klotins. *Polarization Reversal in Ferroelectrics: Stochastic analysis*. Ferroelectrics, 2003, Vol. **295**, pp. 577-588.
11. M. Knite, G. Mezinskis, L. Shebanovs, I. Pedaja, and A. Sternbergs. $CO_2$ *Laser-Induced Structure Changes in Lead Zirconate Titanate* $Pb(Zr_{0.58}Ti_{0.42})O_3$ *Sol-gel Films.* Applied Surface Science, 2003, Vol. **208-209**, pp. 378-381.
12. D. A. Lesnyh, D. V. Kulikov, Yu. V. Trushin, R. Bittner, K. Humer, H. W. Weber and A. R. Sternberg. *Changes in the temperature dependence of the dielectric constant in irradiated antiferroelectric thin films.* Proc. of SPIE 2003, Vol. **5127**, pp.136.
13. J. Levoska, M. Tyunina, A. Sternberg, and S. Leppävuori. *Epitaxy and B-site ordering in thin-film heterostructures of relaxor ferroelectric perovskites.* Ferroelectrics, 2002, Vol. **271**, pp. 137-142.
14. M. Ozolinsh, D. Korenuks, A. Kozachenko and L. Komitov. *Light scattering and depolarization in PDLC optical phantoms used for simulation of eye cataract*. In: Friesem A.A., Turunen J., eds., Uni. Joensuu Selected Papers, 2003, Vol .**8**, pp.86-87.
15. M. Ozolinsh, D. Korenuks, A. Kozachenko, and L. Komitov. *Light scattering effect on colour stimuli visual response*. Perception, 2003, Vol.**32**, S178-179.
16. M. Palatnikov, N. Sidorov, I. Biryukova, K. Bormanis, and A. Sternberg. *Optical Characteristics of Doped Lithium Niobate Single Crystals.* Proc. of SPIE, 2003, Vol. **5122**, Advanced Organic and Inorganic Optical Materials, pp. 377-382.
17. G. Papelba, I. Cipane, and M. Ozolinsh. *Stereovision Studies by Disbalanced Images*. Proc. of SPIE, 2003, Vol. **5123**, Advanced Optical Devices, Technologies, and Medical Applications, pp.323-329.
18. G. Papelba, M. Ozolinsh, J. Petrova, and I. Cipane. *Stereoacuity Determination at Changing Contrast of Colored Stereostimuli.* Proc. of SPIE, 2003, Vol. **5123**, Advanced Optical Devices, Technologies, and Medical Applications, pp. 330- 338.
19. N.V. Sidorov, M.N. Palatnikov, K. Bormanis, and A. Sternberg. *Raman Spectra and Structural Defects of Lithium Niobate Crystals.* Ferroelectrics, 2003, Vol. **285,** pp. 311-320.
20. N.V. Sidorov, M.N. Palatnikov, N.A. Golubiatnik, K. Bormanis, A. Kholkin, and A. Sternberg. *Raman Studies of the FE-AFE Phase Transition in Ceramic* $Li_{0.12}Na_{0.88}Ta_{0.2}Nb_{0.8}O_3$ *Solid Solution.* Ferroelectrics, 2003, Vol. **294**, pp. 221-227.
21. A. Sternberg, L. Shebanovs, V. Zauls, K. Kundzins, M. Antonova, M. Livins, L. Cakare, M. Tyunina, J. Levoska, and I. Aulika. *Structure and Properties of* $Pb(LuNb)O_3$-$PbTiO_3$ *Ceramics and Thin Film.* Ferroelectrics, 2003, Vol. **294**, pp. 41-47.
22. Andris Sternberg. *Progress, prospects and problems in advanced ferroelectric materials for dielectric, piezoelectric and electro-optic applications: selected overwiev topics and some original issues.* International Summer School-Conference "Advanced Materials and Technologies", Palanga, Lithuania, 25-29 August 2003, CD version, PDF File.
23. A. Sternberg, A. Krumins, K. Kundzins, V. Zauls, I. Aulika, L. Cakare, R. Bittner, H. Weber, K. Humer, D. Lesnyh, D. Kulikov, and Y. Trushin. *Irradiation effects in lead zirconate thin films.* Proc. of SPIE, 2003, Vol. **5122**, Advanced Organic and Inorganic Optical Materials, pp. 341-347.

24. A. Sternberg, S.I. Tiutiunnikov, and V.V. Efimov. *Structural Changes of the PLZT Ceramics Irradiated by High-Current Pulsed Electron Beam.* Proc. of SPIE, 2003, Vol. **5122**, Advanced Organic and Inorganic Optical Materials, pp. 348-357.
25. J. Suchanicz, M. Dambekalne, L. Shebanovs, A. Sternberg, B. Garbarz – Glos, W. Smiga, and Cz. Kus. *Effect of Compressive Stress on Dielectric and Ferroelectric Properties of 0.25PSN – 0.75PluN Ceramics*. Ferroelectrics, 2003, Vol. **289**, pp.53–61.
26. M. Tyunina, K. Kundzinsh, V. Zauls, and J. Levoska. *Glass-to-Ferroelectric Phase Transition Induced by AC Electric Field in $PbMg_{1/3}Nb_{2/3}O_3$ Thin Films.* Proc. of SPIE, 2003, Vol. **5122**, Advanced Organic and Inorganic Optical Materials, pp. 334-340.
27. M. Tyunina, V. Zauls, K. Kundzinsh, and J. Levoska. *Dielectric Fourier-spectroscopy in relaxor and normal ferroelectric thin films.* Ferroelectrics, 2002, Vol. **270**, pp. 241-246.
28. M. Tyunina, J. Levoska, S. Leppävuori, V. Zauls, K. Kundzinsh, and M. Kundzinsh. *Dielectric anomalies in relaxor ferroelectric thin films.* Ferroelectrics, 2002, Vol. **270**, pp. 235-240.
29. К. Борманис, М. Дамбекалне, А. Штернберг, Л. Шебановс, М. Антонова, М. Ливиньш, А. Спуле. *Новые сегнетоэлектрические материалы на основе скандониобата свинца и редкоземельных ниобатов.* Известия Академии Наук, Серия физическая, 2003, том 67, № 8, с. 1072-1075.

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1. A.V. Alpatov, A.I. Burkhanov, A.V. Shil′nikov, K. Bormanis, A. Sternberg, A. Kalvane. *Dielectric Properties of PZN-PSN Ferroelctric Piezoceramics.* Ferroelectrics.
2. K.Bormanis, A.Sternberg, and M.Kalnberga. *Microscopic studies of the Surface Morphology of High Temperature Superconductor Thick Layers*. Submitted to Elsevier Science.
3. K. Bormanis, A.I. Burkhanov, A.V. Shil′nikov, A. Sternberg, S.A. Satarov, A. Kalvane. *Features of Polarisation Switching in the PSN-PT Ferroelectric Ceramics.* Journal of Optoelectronics and Advanced Materials.
4. M.Dambekalne, M.Kalnberga, M.Livinsh, K.Bormanis. *Production and Properties of $(1-x)PbSc_{1/2}Nb_{1/2}O_3 – xPbYb_{1/2}Nb_{1/2}O_3$ Solid Solutions.* J. of European Ceramic Society.
5. E. Klotins, J. Hlinka, J. Kaupuzs. *Semiadiabatic High-Field Polarization Response in Ferroelectrics I:Hysteresis and Nonlinear Susceptibility*. Ferroelectrics.
6. M. Ozolinsh and G. Papelba. *Eye Cataract Simulation Using Polymer Dispersed Liquid Crystal Scattering Obstacles*. Ferroelectrics.
7. A.V. Shil'nikov, S.A. Satarov, A.I. Burkhanov, K. Bormanis, A. Sternberg, A. Kalvane. *Dielectric Properties of $PbSc_{1/2}Nb_{1/2}O_3 – PbTiO_3$ Ceramics.* Ferroelectrics.
8. A. Sternberg, I. Aulika, K. Kundzins, R. Bittner, H. Weber, D. Lesnyh, Y. Trushin. *Neutron Irradiation Effects on Dielectric Properties of Sol-Gel and Pulsed Laser Deposited Ferroelectric and Antiferroelectric Thin Films.* J. of European Ceramic Society.
9. Andris Sternberg. *Impact of Structure Ordering and Defects on Properties of Complex Ferroelectric Perovskites.* Ferroelectrics.

10. J.Suchanicz, M.Dambekalne, L.Shebanovs, A.Sternberg, B.Garbarz-Glos, W.Smiga, Cz.Kus. *Effect of Compressive Stress on Dielectric and Ferroelectric Properties of 0.25PSN – 0.75PLuN Ceramic*. Ferroelectrics (accepted).
11. M. Tyunina, J. Levoska, K. Kundzinsh, V. Zauls. *Polar State in Epitaxial Films of Relaxor Ferroelectric* $PbMg_{1/3}Nb_{2/3}O_3$. Submitted to Phys. Rev. B
12. M. Tyunina, K. Kundzinsh, V. Zauls, J. Levoska. *Ferroelectric Behavior in Epitaxial Films of Relaxor* $PbMg_{1/3}Nb_{2/3}O_3$. Ferroelectrics (accepted).
13. М. Палатников, В. Калинников, К. Борманис. *Применение гранулированной шихты для выращивания монокристаллов ниобата лития*. Труды 6. Международной конференции «Кристаллы: рост, свойства, реальная структура, применение».
14. А.В. Шильников, С.А. Сатаров, А.И. Бурханов, К. Борманис, А. Штернберг, А. Калване. *Диэлектрические свойства разупорядоченной сегнетоэлектрической керамики PSN-PT.* Известия РАН.

## Lectures on Conferences

**Latvijas Universitātes Cietvielu fizikas institūta 19.zinātniskā konference, 2003.gada 10. – 13. februāris, Rīga, Latvija.**
**19th Scientific Conference, Institute of Solid State Physics, University of Latvia, February 10 –13, 2003, Riga, Latvia.**

1. M. Ozoliņš, G. Papelba, G. Anderssons. *Šķidro kristālu brilles redzes fizikas eksperimentos. Liquid Crystal Goggles for Vision Research*. Referātu tēzes, 7. lpp.
2. D. Koreņuks, M. Ozoliņš, A. Kozachenko, L. Komitovs. *Elektrovadāma izkliede polidispersajos šķidrajos kristālos. Electrically Controllable Scattering in Polydispersed Liquid Crystals.* Referātu tēzes, 8. lpp.
3. G. Papelba, M. Ozoliņš. *Stereostimulu analizēšanas metodes. The Analysing Methods of Stereo Stimuli*. Referātu tēzes, 9. lpp.
4. A. Šternbergs, I. Aulika, K. Kundziņš, V. Zauls, R. Bittners, H. Webers, D. Lesnihs, D. Kulikovs, J. Trušins. *Segnetoelektrisko un antisegnetoelektrisko plāno kārtiņu struktūras un fizikālo īpašību izmaiņas intensīva neitronu starojuma iedarbības rezultātā*. *Intensity neutron irradiation effects of the ferroelectric and antiferroelectric thin films structure and properties.* Referātu tēzes, 19. lpp.
5. J. Kaupužs, Ē. Klotiņš. *Telpiski neviendabīgi polāri materiāli: rezultāti un problēmas. Spatially Inhomogeneous Polar Materials: Results and Problems*. Referātu tēzes, 30. lpp.
6. Ē. Klotiņš, J. Kaupužs. *Segnetoelektriķi nelīdzsvara fāzē: stohastisks modelis. Modelling of the Nonequilibrium Ferroelectric Response*. Referātu tēzes, 31. lpp.
7. M. Dambekalne, M. Antonova, M. Kalnberga, M. Livins, L. Šebanovs, K. Bormanis, A. Kalvāne. $PbSc_{1/2}Nb_{1/2}O_3$ *un retzemju niobātu cieto šķīdumu sintēze un īpašības. Solid Solutions on the Bases of* $PbSc_{1/2}Nb_{1/2}O_3$ *and Rare–earth Niobates.* Referātu tēzes, 32.lpp.
8. K. Kundziņš, V. Zauls, M. Tjuņina, J. Levoska. *Mērošā maiņsprieguma lieluma ietekme uz relaksora un segnetoelektriska tipa epitaksiālo kārtiņu īpašībām. Influence of AC Drive on Relaxor or Normal Ferroelectric Behavior of Epitaxial Thin Films.* Referātu tēzes, 33. lpp.
9. I. Aulika, V. Zauls, K. Kundziņš, M. Kundziņš, S. Katoli. *Optiskā reflektometrija un elipsometrija plānu kārtiņu biezuma un laušanas koeficienta noteikšanai. Determination of Thickness and Refractive Index of Thin Films by Optical Reflectometry and Ellipsometry*. Referātu tēzes, 34. lpp.

10. V. Zauls, K. Kundziņš, K. Harnagea, B. Štilers. *Polāru dielektriķu lokālo fizikālo īpašību pētīšana ar atomspēka mikroskopu: principi, iespējas un problēmas. Investigation of Local Physical Properties of Polar Dielectrics by Atomic Force Microscopy: Principles, Prospects and Limitations*. Referātu tēzes, 51. lpp.
11. K. Kundziņš, K. Harnagea, A. Janovs, M. Kundziņš. *Lokālās pjezodeformācijas un polarizācijas detektēšana ar modificētu atomspēka mikroskopu. Detection of Local Piezodeformation and Polarization in Ferroelectrics Using Scanning Probe Microscopy*. Referātu tēzes, 52. lpp.

**7th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors, Rio de Janeiro, Brazil, May 25-30, 2003.**

1. K. Bormanis, A Sternberg, and M. Kalnberga. *Microscopic studies of the Surface Morphology of High Temperature Superconductor Thick Layers*. Book of Abstracts, p.189.

**NATO Advanced Research Workshop on the Disordered Ferroelectrics, Kiev, Ukraine, May 29 – June 2, 2003.**

1. M. Tyunina, J. Levoska. *Thin Films of Perovskite Relaxor Ferroelectrics.* Abstracts, p. 17.
2. Andris Sternberg. *Impact of Structure Ordering and Defects on Properties of Complex Ferroelectric Perovskites.* Abstracts, p. 19.

**Symposium "Polar Oxides: Properties, characterisation and Imaging", Capri, Italy, June 8-11.**

1. K. Kundzins, V.Zauls. *Nanoscale Piezoresponse AFM Imaging and Patterning of Ferroelectric Relaxor Thin Films*, Programme & Abstracts, P22, p.43.

**The 8th Conference and exhibition of the European ceramic society, Istanbul, Turkey, June 29 – July 3, 2003.**

1. M. Dambekalne, M. Kalnberga, M. Livinsh, K. Bormanis, A. Sternberg. *Production and Properties of $PbSc_{1/2}Nb_{1/2}O_3 – PbYb_{1/2}Nb_{1/2}O_3$ Solid Solutions.* Programme and Abstract Book, Turkish Ceramic Society, Ref. 976 (B2).
2. A. Sternberg, I. Aulika, K. Kundzins, R. Bittner, H. Weber, D. Lesnyh, Y. Trushin. *Neutron Irradiation Effects on Dielectric Properties of Sol-Gel and Pulsed Laser Deposited Ferroelectric and Antiferroelectric Thin Films.* Programme and Abstract Book, Turkish Ceramic Society, Ref. 977 (B2).

**ICO Topical Meeting on Polarization Optics (ICOPO) Polvijärvi, July 2003.**

1. J. M. Bueno, E. Berrio, M. Ozolinsh, and P. Artal. *Degree of polarization as an objective tool to evaluate scattered light in the human eye.*
2. M. Ozolinsh, D. Korenuks, A. Kozachenko and L. Komitov. *Light scattering and depolarization in PDLC optical phantoms used for simulation of eye cataract.*

**The 10th European Meeting on Ferroelectrics EMF-10, Cambridge, August 2003.**

1. R. Bittner, K. Humer, H. W. Weber, K. Kundzins, A. Sternberg. *Neutron Irradiation Effects in PZ and PZT Thin Films.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 77.
2. M. Dambekalne, M. Kalnberga, M. Livinsh, K. Bormanis, A. Sternberg. *Production and Dielectric Properties of PSN – PybN Binary System.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 111.

3. E. Klotins, J. Hlinka, E. Kaupuzs. *Semiadiabatic High-Field Polarization Response in Ferroelectrics II:Size Effects.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 187.
4. M. Ozolinsh. *Electrically Controlled Eye Occluders in Vision Science*. Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 250.
5. M. Palatnikov, N. Sidorov, V. Kalinnikov, K. Bormanis. *Spectroscopic Criteria of the Degree of Structural Perfection of Stoichiometric Lithium Niobate Single Crystals.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 251.
6. M. Palatnikov, N. Sidorov, V. Kalinnikov, A. Sternberg, K. Bormanis. *Anomalous Behaviour of Periodic Domain Structure in Doped $LiNbO_3$ Single Crystals at 300-400K.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 251.
7. M. Palatnikov, V. Gabrielyan, K. Bormanis, N. Sidorov, V. Kalinnikov. *Crystallization of Stochiometric Lithium Niobate in $Li_2O$-$Nb_2O_5$ and $Li_2O$-$K_2O$-$Nb_2O_5$ Systems*. Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 252.
8. M. Palatnikov, V. Kalinnikov, K. Bormanis. *Granulated Charge in Single Crystals Growth of Lithium Niobate and Tantalate.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 252.
9. A. V. Shil'nikov, S. A. Satarov, A. I. Burkhanov, K. Bormanis, A. Sternberg, A. Kalvane. *Dielectric Properties of $PbSc_{1/2}Nb_{1/2}O_3$ – $PbTiO_3$ Ceramics*. Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 302.
10. V. Shvartsman, M. Tyunina, J. Levoska, A. Kholkin. *Local Electromechanical Properties of $PbMg_{1/3}Nb_{2/3}O_3$ Thin Films Studied by Piezoelectric Force Microscopy.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 309.
11. M. Tyunina, K. Kundzinsh, V. Zauls, J. Levoska. *Ferroelectric Behavior in Epitaxial Films of Relaxor $PbMg_{1/3}Nb_{2/3}O_3$.* Journal of Conference,Vol. 8, N 1, August 2003, Abstracts, p. 339.

**International Summer School-Conference "Advanced Materials and technologies", Palanga, Lithuania, 25-29 August 2003.**

1. A. Sternberg, V. Zauls, K. Kundzins, R. Bittner, I. Aulika. *Composition-Structure-Properties Relationships in Ferroelectric Ceramics and Thin Film Heterostructures.* Book of Abstracts, p. 17.
2. J. Banys, J. Macutkevic, A. Brilingas, J. Grigas, K. Bormanis, A. Sternberg, V. Zauls. *Dielectric Dispersion and Distribution of the Relaxation Times of the Relaxor 0.4PSN-0.3PMN-0.3PZN and 0.2PSN-0.4PMN-0.4PZN Ceramics.* Book of Abstracts, p. 43.

**International Conference "Processing of Electroceramics", Bled, Slovenia, August 31 – September 3, 2003.**

1. M. Dambekalne, M. Antonova, A. Kalvane, M. Livinsh, K. Bormanis, A. Sternberg. *Producing powders of $PbB'B''O_3$ ferroelectric materials by solid phase synthesis.* Abstract Book, Jožef Stefan Institute, p.26.

**The 26th European Conference on Visual Perception (ECVP), Paris, September, 2003.**

1. M. Ozolinsh, D. Korenuks, A. Kozachenko, L. Komitov. *Light scattering effect on colour stimuli visual response.*

**The 10th Int. Conf. "Vision in Vehicles" VIV-10, Granada, September 2003.**

1. M.Ozolinsh, and J. Berzinsh. *Traffic sign recognition during night driving.*

**VI Международная конференция «Кристаллы: рост, свойства, реальная структура, применение», Александров, Россия, 8.-12. сентября 2003. года.**

1. А.В.Шильников, А.И.Бурханов, А.В.Алпатов, К.Борманис, А.Штернберг, А.Калване. *Диэлектрические свойства системы твердых растворов цинкониобата свинца – скандониобата свинца (PZN-PSN) в широкой области температур.* Материалы VI Международной конференции «Кристаллы: рост, свойства, реальная структура, применение», Александров, ВНИИСИМС, 2003, с. 274-275.

**Romanian Conference on Advanced Materials: ROCAM 2003, Constanta, Romania, September 15 – 18, 2003.**

1. I. Aulika, V. Zauls, K. Kundzins, M. Kundzins, S. Katholy. *Determination of thickness and refractive index of thin films by optical reflectometry and ellipsometry.* Abstract book, p. 139.
2. E. Klotins, I. Aulika. *Semiadiabatic high field polarization respose in ferroelectrics: dynamic hysteresis, nonlinear susceptibility and size effects.* Abstract book, p. 140.
3. K. Bormanis, A. I. Burkhanov, A. V. Shil′nikov, A. Sternberg, S. A. Satarov, A. Kalvane. *Features of Polarisation Switching in the PSN-PT Ferroelectric Ceramics.* Abstract book, p. 147.
4. N. Sidorov, M. Palatnikov, P. Chufirev, I. Biryukova, K. Bormanis. *Structure of the Cation Sublattice and Optical Damage in Lithium Niobate Crystals of Different Composition.* Abstract book, p. 67.

**The Fourth International Seminar on Ferroelastics Physics. Voronezh, Russia, September 15-18, 2003.**

1. N. Sidorov, M. Palatnikov, N. Golubjatnik, I. Birjukova, K. Bormanis, A. Sternberg. *FE-AFE Phase Transition and Morphotropic Region in Ceramic Solid Solutions* $Li_{0.12}Na_{0.88}Ta_yNb_{1-Y}O_3$. Abstracts, p. 62.
2. A.V. Shil′nikov, S.A. Satarov, A.I. Burkhanov, K. Bormanis, A. Sternberg, A. Kalvane. *Dielectric Properties of Disordered PSN-PT Ferroelctric Ceramic*. Abstracts, p. 90.

**A symposium to mark the 80th birthday of Professor Eric Cross "55 Years of Ferroelectrics", Marriott Hotel, Leeds, UK, September 21-23, 2003**

1. A. Sternberg, V. Zauls, K. Kundzins. *Effect of Structure Ordering on Properties of Some Perovskite Structure Ceramics and Thin Films: Application Prospects*. Abstracts, p. 32.

# SEMICONDUCTOR MATERIALS AND SOLID STATE IONICS

Head of Division Dr.phys. A.Lusis

## Research Area and Main Problems

*Research areas:*

- Electrophysics and electrochemistry of specific semiconductor materials, mixed conductors, ion conductors, high temperature superconductors (transition metal oxides, bronzes, metal hydrates, solid electrolytes, etc.);
- Material preparation methods: thin and thick film technologies, sol-gel process;
- Material characterisation by spectroscopic methods (Raman scattering, optical and X-ray absorption, electrical and electrochemical impedance, magnetic susceptibility, ESR, etc);
- Solid state ionics and optics:
  - 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,
  - solid state reactions in bulk of electrode and solid electrolyte materials,
  - two and three phases electrode reactions,
  - gases and ions sensing phenomena and detection technologies;
- Functional coatings and multi layer electrochemical systems;
- Hydrogen adsorption/absorption phenomena on 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:
  - physical and chemical sensors and actuators for microsystems,
  - variable optical coatings for micro optics
- 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. Inter-grain activity of solid electrolyte layers based on polymer composites.
4. Ion ($H^+$, $OH^-$, $Li^+$) insertion (extraction) in solid electrolytes and electrodes.
5. Metal hydride electrode for Ni / MH battery.
6. Hydrogen absorption in composite materials: catalytic activation of molecular hydrogen adsorption and spill-over of hydrogen atoms onto solid surface.
7. Microwave absorption of high temperature superconductors.
8. Research and development of an electronic nose
   - 8.1. Software Environment for Electronic Nose and Electronic Nose Module;
   - 8.2. Preparation of sensor elements and testing their sensitivity and selectivity;
   - 8.3. Application technologies of electronic nose for food quality, aging determination of soaps, oils, etc.
9. Odour pollution monitoring methods and instrumentation.

**Scientific staff**

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

**Technical staff**

1. A.Kursitis
2. J.Pinnis
3. M.Purane
4. U.Klavins
5. E. Zavickis
6. A. Patmalnieks

**Postgraduate students**

1. Ģ.Vēveris
2. J.Zubkāns
3. L.Grīnberga
4. K.Paegle
5. J. Hodakovska
6. V.Vorohobovs

**Students**

1. L.Jēkabsone
2. J. Gaidelene
3. I. Graudinsh
4. V. Mikelsons
5. G. Mikelsons

**Visitors from abroad**

1. Prof. A. Czervinskis, Faculty of Chemistry, Warsaw University, Poland (1 month)
2. PhD Nikos Papamichail, Chemical Institute, Tuebingen University, Germany (1 month)
3. Dr. F. Rocca – IFN-CNR, Institute for Photonics and Nanotechnologies, Section "ITC-Cefsa" of Trento, Italy (1 month).
4. Dr. hab. Fabio Comin – ESRF, European Synchrotron Radiation Facility, Grenoble, EU (6 days).
5. Prof. D. Tonneau - Université de la Méditerranée, UMR 6631 CNRS, Marseille, France (1 month).
6. Eng. D. Pailharey – GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (10 days).
7. Eng. F. Jandard – GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (10 days).
8. Dr. E. Avendaño - The Angstrom Laboratory, Uppsala University, Uppsala, Sweden (1 month).

**Scientific visits abroad**

1. BS J. Hodakovska 1) France, August, September, 2003 (5 days),

2. MS L. Grinberga 1) France, August, September, 2003 (5 days),
   2 Reikjavik, Iseland, July 2003, (6 days),
   3) Petten, Netherland, October 2003 (6 days)
   4) Copenhagen, Denmark, December 2003 (4 days)

3. Dr. J.Kleperis 1) St.Petersburg, Russia, April 2003 (6 days),
   2) Prague, Czech, March 2003 (7 days),
   3) Helsinki, Finland, May 2003 (5 days),
   4) London, England, November 2003 (4 days),
   5) Copenhagen, Denmark, December 2003 (4 days)

4. Dr. A.Kuzmin: 1) IFN-CNR, Cefsa, Trento, Italy (3 months).
   2) 12 International Conference on (XAFS), Malmo, Sweden (7 days).

| | |
|---|---|
| | 3) 5 International Conference on f-Elements, Geneve, Switzerland (7 days). |
| 5. Dr. A.Lusis | 1) Hanover Messe, Germany (3 days)<br>2) 203rd Meeting of The Electrochemical Society, Paris, France (6 days)<br>3) 2nd Workshop on eNOSE, Linkoping, Sweden (3 days)<br>4) Project "SoC-SME" Steering Committee Meeting, Kista, Sweden<br>5) Project "SoC-SME" Steering Committee Meeting, Oslo, Norway<br>6) Project "GreenRoSE" Steering Committee Meeting, Munich, Germany |
| 6. Dr.hab. J.Purans: | 1) University of Trento, Trento, Italy (3 months)<br>2) 12 International Conference on X-ray Absorption Fine Structure, Malmo, Sweden (7 days).<br>3) 5 International Conference on f-Elements, Geneve, Switzerland (4 days).<br>4) Satellite Meeting on Micro X-Ray Beam Analysis, Osaka, Japan (7 days). |
| 7. Dr. G.Vaivars: | 1) Cape Town University, Cape Town, South Africa (10 month). |
| 8. Dr. G.Vitins: | 1) Southampton University, Southampton, UK (10 month) |

## Cooperation

**Latvia**

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

**Denmark**

Technical university of Denmark (Dr. K.West )
RISO National Research Center of Denmark (A.S. Pedersen, F.W. Poulsen)

**Estonia**

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

**France**

1. LURE, Lab. of Synchrotron Radiation (Orsay, France) – Prof. S. Benazeth, Prof. J.-P. Itie.
2. GPEC, Universite de la Mediterranee (Aix-Marseille II) (Marseille, France) - Prof. Y.Mathey, Eng. D. Pailharey, Prof. D. Tonneau.

**Germany**
1. Tuebingen University – U. Weimar, N. Papamichail

**Great Britain**
2. Southampton University - Department of Chemistry (Prof. Owen)

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

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

**Poland**
1. Poznan Central Laboratory of Batteries and Power Sources (Dr. M.Kopczyk, Dr. G.Wojcik)
2. University of Warsaw , Department of Chemistry (Prof. A.Czerwinski)

**Russia**
1. Moscow State University: Faculty of Physics ( Prof. A.Tihonov), Chemistry division (Prof. E.V. Antipov).
2. Joint Instute for Nuclear Research, Dubna (Dr. S.I. Tjutjunnikov)
3. Moscow State Engineering Physics Institute, Moscow (Prof. A.Menushenkov)

**Sweden**
1. Linkoping University – Laboratory of Applied Physics (Prof. I.Lundstrom)
2. Stockholm University, Arrhenius laboratory (Dr. J.Greens)
3. Uppsala University, Angstrom Laboratory, Uppsala, – Dr. E. Avendaño, Prof. C.G. Granqvist, Dr. A. Azens.

**South Africa**
West Cape University - Porous Media Laboratory (Cape Town, Dr. Linkov).

**Switzerland**
1. ICMB, Universite de Lausanne (Lausanne, Switzerland) - Prof. A.E. Merbach.

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

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

**Research Projects:**
1. Nordic Industry Fund project No. 02050 "Provisions of System-On-Chip technology for Small and Medium sized Enterprises" Acronym: „SoC-SME" (Dr. A.Lusis)
2. Nordic Energy Research Project NERP No. 46-02 "Integration of advanced H storage materials and systems into the hydrogen society" (Dr. J. Kleperis, PhD L. Grinberga).
3. "Lanthanide Chemistry for Diagnosis and Therapy", European COST Action D18, 1999-2004 (Head: Dr.hab. J. Purans).

**Organisation of International Conference in Latvia:**

**The 10th International Symposium on Olfaction and Electronic Nose (ISOEN`2003), organized in Riga (Latvia), June 25-28, 2003**

93 participants altogether from 22 countries come together to discuss the main results in sensor and sensor array technologies, e-nose miniaturisation, odour description in electronic files and unified description language formation, e-nose application in different fields, making emphasis on product adulteration and environment pollution problems. Latest developments and new results were reported in 49 oral and 28 poster presentations, as well as in many discussions through out the symposium.

The Symposium Extended Abstracts were published before the meeting in special book on 281 pages (A4 format). Manuscripts of the prepared reports were edited during 12 months after meeting and will be published in 2004 in special issue of the International Journal from Elsevier "Sensors & Actuators, B: Chemical Sensors"; editors J. Kleperis and A. D`Amico.

The Symposium was supported by EU project CAMART.

**Didactic work at the University of Latvia**

1. Master degree course "Solid State Ionics" (A.Lusis)
2. Master degree course "e-nose" (J.Kleperis)
3. Master degree course "Structural Methods in Solid State Analysis" (J.Purans, A.Kuzmin).
4. J. Kleperis - Supervisor of MS thesis of L. Grinberga "Practical applications of physical devices based on olfactometric sensitivity", Riga, 2003; Supervisor of MS thesis of S. Skrastina "Research of correlation between air pollution, meteorological parameters and social activity behaviour of society", Riga, 2003; Supervisor of MS thesis of J. Svinskis "Air pollution with particles and benzene in Riga"; Supervisor of BS thesis of J. Hodokovska "Sensor selectivity properties based on registration of the form of molecule".
5. A.Lūsis - Supervisor of BS thesis of A.Slišāns "Cycling capacity of lithium ion batteries"
6. L. Grinberga, J. Kleperis – popular about science – lectures and demonstrations for visitors of ISSP, students and pupils.

# Main results

## ION – ELECTRON PROCESSES IN NANO STRUCTURED OR AMOURPHOUSS FILMS AND SYSTEMS BASED ON TUNGSTEN OXIDE

**J.Gabrusenoks, A.Lusis, J.Kleperis, E.Pentjuss**

The cycling capacity is actual problem for ionic devices or electrochemical cells (ECC) with intercalation electrodes. The main group of materials for such electrodes is micro or nano structured porous transitional metals oxides. The electrochromic devices based on amorphous $WO_3$ films and protons conducting electrolytes are good objects for investigation of cycling capacity. For investigation cycling capacity can be used simultaneously both electrochemical and optical spectroscopy. There are direct

correlation between charging level and optical absorption of intercalation electrode. The cycling capacity is limited by reversibility of ion insertion-extraction reactions, which causes degradation of cell electrodes.

For the Electrochromic Cells based on multi layer system on glass substrates: ITO / $WO_3$ // AAH // $IrO_2$ / ITO, where $WO_3$ and $IrO_2$ are represented hydrated oxide films, AAH – electrolyte as paste or gel based on hydrate of antimony acid, we are using model of electrochromic phenomena in tungsten oxide thin films based on assumption that the constitution of such films is heterogeneous and built up of nano size particles, pores and adsorbed substances (mainly water). From electrochemistry point of view the internal three phase interfaces in such films are distributed multiphase electrodes. The migration of water in the cell and hydration together with ion insertion-extraction reactions of the $WO_3$ film have main role in formation of new phases, which determine the value of cycling capacity. The more probable transformation of phases in hydrated $WO_3$ films during cycling, which can be related to loss of active tungsten ion sites, is transformation of octahedral structural units [$WO_6$] to tetrahedral [$WO_4$]. The cycling capacity of Electrochromic Cells at constant coloration intensity is limited by initial total number of active tungsten ion sites for induced color centers at inner surface of porous $WO_3$ film.

The developed model was base for drawing up ionic device performance - degradation scheme. During cycling for any characteristic have to be distinguish three regions of degradation intensity. The full cycling region is cycling capacity, which depends on reversibility of electrode reactions (ion insertion) and phase stability of electrode and electrolyte materials. The shift of the EC cell volt-ampere graphs during cycling is direct evidence for changes of electrodes composition. The degradation processes are related to the changes of physical and chemical state of electrode material and interface electrode-electrolyte. During cycle electrode resistance changes many times and same time changes redox potentials of electrodes.

Infrared reflection and Raman spectroscopy have been applied to study the vibrational modes of tungsten trioxide ($WO_3$) and oxy-chloride ($WOCl_4$). The software for simulation of infrared reflection spectra had been worked out in frame of the dipole oscillation model. The symmetry of vibration spectra hav been caculated for $WOCl_4$. The model parameters – oscillator strength, resonance frequency and decay coefficient – were obtained for $WO_3$. Kramers-Kronig relations are employed to yield the refractive index as vell as TO and LO functions of these materials at frequencies from 50 to 1200 cm-1. The tungsten trioxide $WO_3$ has several polymorphous phases. These $WO_3$ phases have more or less distorted $ReO_3$ - type crystal structures.

## X-RAY ABSORPTION SPECTROSCOPY USING SYNCHROTRON RADIATION

**J. Purans, A. Kuzmin, R. Kalendarev, J. Gaidelene**

EXAFS Spectroscopy Laboratory is specialised in the investigations of the local electronic and atomic structure of compounds by X-ray Absorption Spectroscopy (XAS) at synchrotron radiation facilities as ESRF in Grenoble (France). High quality experimental data and innovative theoretical analysis allow us to obtain structural and dynamic information with picometer (10-12 m) accuracy.
Main topics and results of our studies in 2003 are described briefly below.

- Research and development of advanced materials for electrochromic applications.

A number of mixed oxide thin films as tungsten oxide co-doped with Ru, nickel oxide co-doped with V, molybdenum oxide co-doped with Ni and tantalum oxide co-doped with Re were studied as promising materials for electrochromic applications.

XAS results suggest that the average local structure around both W and Ru ions in $WO_3$:Ru thin films remains unchanged up to 28 at.% of ruthenium. The films consist of tungsten trioxide grains with the structure of pure $WO_3$, which are surrounded by ruthenium oxide phase. The presence of Ru ions affects both electrochemical and optical properties of the films

Hydrated thin films of nickel vanadium oxide ($Ni_{1-x}V_xO_y$), made by reactive dc magnetron sputtering, exhibit a nanocrystalline NiO-type structure with homogeneous distribution of V ions substituting Ni ions. Exposure of the films to ozone resulted in dark brown coloration associated with an appearance of $Ni^{3+}$ ions and accompanied by a modification of the local electronic and atomic structures of the V and Ni ions. The largest changes occurred in the environment of the V ions, which presumably change their valence state from $V^{4+}$ to $V^{5+}$ and displace into off-centre positions by ~0.4 Å.

Mixed nickel molybdenum oxide thin films were produced by dc magnetron co-sputtering technique with the nickel content up to 25 at.%. The analysis of the Ni and Mo K-edges EXAFS signals suggests that (i) the films are amorphous, except for the highest nickel content (25 at.%), at which a segregation of NiO phase was observed; (ii) nickel and molybdenum atoms are octahedrally coordinated by oxygen atoms. Opposite to the $NiO_6$ octahedra, the $MoO_6$ octahedra are strongly distorted, that results in an existence of two groups of oxygen atoms – four nearest at ~1.76 Å and two distant at ~2.2 Å. It was also found that the $MoO_6$ octahedra are joined by edges, with the Mo-Mo distance about 3.26-3.31 Å.

In mixed Ta-Re oxide thin films, synthesised by dc magnetron co-sputtering, we found that rhenium atoms are four-fold coordinated by oxygen atoms with R(Re-O)=1.74 Å, whereas tantalum ions are coordinated by six oxygen atoms at R(Ta-O)=1.95 Å. The addition of rhenium ions shortens the average Ta-O distance and distorts $TaO_6$ octahedra, making the Ta-O distances distribution slightly broader.

- Investigation of the rare-earth ions structure in water, bio-inorganic molecules and oxide glasses.

The local structure of rare-earth aqua ions and bio-inorganic molecules was studied within the framework of the European COST D18 program.

The microscopic mechanisms of water exchange reaction between the hydration shells of $Ln^{3+}$ aqua ions play an important role in the development of novel diagnostic agents in Magnetic Resonance Imaging (MRI) in medicine. Here we present a temperature dependent XAFS analysis of $Eu^{3+}$ and $Lu^{3+}$ ions coordinated by water molecules in solids with *picometer accuracy*, as the dynamic properties of the analogous complexes in solutions should be closely related to the structure of the first coordination sphere. The ligand exchange rate constant, $k_{ex}$, is closely related to the Debye-Waller (DW) factor value and anharmonicity of the potential between metal ions and water molecules. Miyanaga et al. suggested a simple correlation between the DW factor ($\sigma^2$) and the exchange rate constant for water exchange for $Me^{2+}$ aqua-ions when plotting ($R^4/\sigma^4$) against $\log(k_{ex})$. Nevertheless, the previous XAFS results ($R^4/\sigma^4$) on $Ln^{3+}$ aqua-ions in solutions are an example of the controversy.

New high accuracy EXAFS measurements have also been done on $Ln^{3+}$ aqua-ions in solutions to check the ultimate limits of the cumulant analysis. For the first time the *local structure have been established* in the first shell of $Ln^{3+}$ aqua ions with *picometer*

*accuracy* ($3 \cdot 10^{-3}$ Å). The measurements have been carried out at the Ln $L_3$-edges with an energy reproducibility of 0.1 eV. The remarkable improvement of experimental data quality and analysis procedures has allowed to measure the local Ln-O expansion. For the first time, the asymmetry of the Ln-O distances distribution, probed by the third cumulant ($C_3$), has been experimentally observed.

The theoretical calculations within *ab initio* full multiple scattering formalism were first performed for the reference material – crystalline EuO. Our results show good agreement with experimental data. The main features, observed in the experimental Eu $L_3$ and O K edges signals, are reproduced taking into account a cluster of 3-4 coordination shells. An addition of more distant shells makes features just more resolved. The main peak, located just above the absorption edge, is related to the Eu 5*d*-states as follows from the *d*-projected density of states and its high intensity indicates a localized character of 5*d*-states.

Investigation of the O K-edge in lanthanides (Ln) complexes provides complementary information to that gained from the Ln absorption edge. In particularly, the O K-edge is strongly sensitive to the type of bonding and can be used in many cases as a fingerprint of the ionicity degree of Ln-O bonds. In this work we provide an interpretation of x-ray absorption near edge structure (XANES) at the O K-edge in crystalline $Ln(H_2O)_9(CF_3SO_3)_3$ (Ln=Eu, Gd, Lu) and Gd(DOTA) within *ab initio* full multiple scattering formalism. The main difference between triflates and Gd(DOTA) experimental signals appears in the intensity of the first peak, located just above the edge. The peak is attributed to the transition from O(1s) state to mixed Ln(5d)-O(2p) state and, thus, its higher intensity in Gd(DOTA) indicates more covalent bonding between gadolinium and oxygen atoms. Our theoretical results allow to discriminate contributions from non-equivalent oxygen atoms and suggest that high intensity of the first peak in Gd(DOTA) is due to strong bonding between Gd ion and nearest water molecule, located at $R$(Gd-O)=2.46 Å.

- Development of new experimental techniques for nano-materials investigation via combination of Scanning Probe Microscopy and XAS.

Development of new experimental techniques for nano-materials investigation via combination of Scanning Probe Microscopies (SPM) such as Atomic Force Microscopy (AFM), Scanning Tunneling Microscopy (STM) and Scanning Near-field Optical Microscopy (SNOM) with XAS were started in strong collaboration with scientists from other EU countries. The method will provide chemical-specific contrast at unprecedented lateral resolution of up to 10-100 nanometers, thus overcoming existing limitations of the two (SPM and XAS) methods and opening a wide range of research opportunities and challenges. This project will be supported by the STRP grant within the EC 6 Framework Program.

- Development and evaluation of novel *ab initio* theoretical methods for the local structure reconstruction from x-ray absorption spectra.

Further development of methods for the analysis of x-ray absorption spectra was performed within the framework of the "EDA" project. A universal EDACA code was created to perform *ab initio* calculations of XANES/EXAFS experimental spectra based on Molecular Dynamics simulations. This is one of the most promising approaches capable to accurate account for both thermal and static disorder and thus to overcome many existing problems.

## HIGHEST-$T_c$ MERCURY CUPRATES SUPERCONDUCTORS MICROWAVE MAGNETOABSORPTION: SELFINTERSECTION, REPTATION AND RESONANT PEAKS

**V.A. Alyoshin[1)], E.V. Antipov[1)], M.I. Shirokov[2)], A.A. Timoshin[3)]**
*[1)]Moscow State University, Inorganic Chemistry department, Moscow, 119899, Russia*
*[2)]Latvian University, Institute of Solid State Physics, Kengaraga 8, Riga, LV-1063, Latvia*
*[3)]Cardiology Centre, Institute of Experimental Cardiology, Moscow, 121552, Russia*

High-$T_c$ superconductors (HTSC) are characterized by irreversibility in magnetic fields up to H~5 T providing high critical current $j_c(H)$. It is shown that highest-$T_c$ mercury cuprates HTSC microwave magnetoapsorption signal is rather sensible to magnetic hysteresis already at H≤0.5 T due to shielding current weak links contours weak superconductivity steep $j_c(H)$ dependence. The current-induced high field hysteresis disappears at h=5÷16 Oe modulation field amplitude alternating by found in Hg-1201 samples hysteresis branches intersection leading to low field hysteresis increase. The reversible signal ~h stands out and gives ΔH-driven forward-back scans intersection effect at steep enough incline ~ $(j_c(H))^2$ low field region. The intersection field $H_i(j)$ increase is explained by critical modulated current state $I+j=j_c$ extension through distributed contours. The inner origin of ΔH is confirmed by the loop self intersection effect maintenance at maximal scan field diminution. No highly nonlinear in modulation behavior and self intersection effect are observed in Hg-1212 compound. It gives possibility to suppose that different type Josephson junction constitute weak links system in Hg-1201 and Hg-1212 HTSC. It is first observation of principal difference between single conduction plane (Hg-1201) and double conduction plane (Hg-1212) members of mercury cuprares HTSC. Coherence degradation in under doped state leads to τ distribution increase, which promotes current interactions and magnetic energy pumping to long contours containing weak sites, failing superconductivity and leading to the absorption oscillations. Their contents ~ $10^{-4}$÷$10^{-3}$ per Cu atom is estimated on the ground of universal critical current state extension tendency. It coincides with ~ $10^{-3}$ steady concentration of ESR data for paramagnetic centres (PC) found in Hg-1201, Hg-1212 samples. Substitution $Hg^{2+}\rightarrow Cu^{2+}$, dependent on synthesis conditions, is proposed for PC origin. In conclusion, it is shown that magnetic irreversibility, trapped magnetic flux relaxation, deviation from optimal nonstoichiometry and coherence influence on the superconducting state in the highest-$T_c$ mercury cuprates HTSC can be successfully investigated by microwave magnetoabsorption in moderate magnetic fields.

## SPECTROSCOPIC APPEARANCE OF SODIUM ALUMOSILICATE FIBER LEACHING

**G.Veveris, V. Eglitis, A. Lusis**
*Institute of Solid State Physics, University of Latvia*

Alkali metals alumosilicates leaching process leads to the following spectroscopical changes. First, the absorption edge shift in violet region of the spectra depends on alkali metal oxide concentration in the material. Second, Raman spectra changes give possibility to analyse the leaching different ethapes in comparison to vitreous quartz. Some broad lines and their fine structure indicate $SiO_4$ tetrahedron clusters oscillations. Despite to absence of tendency of full vitreous quartz identity, they reflect the structure

sceleton ordering degree guite well. Third, infrared reflection spectra ≈1090 $cm^{-1}$ pronounced maximum can be related to Si-O bonds oscillations superposition (Si-O-Si, 1030-1070 $cm^{-1}$ , Si-O-Al, 990-1020 $cm^{-1}$ , Si-O-Me, 940-980 $cm^{-1}$ ). Their intensity diminution is observed in the course of the leaching. The ≈ 910 $cm^{-1}$ maximum is related to Si-O none-bridge valence bond oscillations. Their intensity grows in this process. Fourth, infrared transmission spectra comparatively intense ≈1600, 5200 $cm^{-1}$ bands are observed supposed to relate to $H_2$ O molecules presence, but ≈4500$cm^{-1}$ one - to Si-OH group bonds oscillations.

## ELECTRODES WITH HIGH ENERGY CAPACITY AND ELECTROLYTES FOR POWER SOURCES

**J. Kleperis, G. Vaivars, G. Vitins, A. Vitins, A. Lusis**
**Solid State Physics Institute of University of Latvia**
**A. Czerwinski,** *Chemical Department of Warsaw University, Poland*
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It is necessary to improve the cycling properties and energy capacity for metal hydride and lithium power sources which are broadly used in mobile electronic equipment. The electrochemical characteristics (charge transfer resistance, exchange current, equilibrium potential) and impedance measured in large frequency region allow interpreting electrode/electrolyte interfaces in sealed battery and determining main blocking layers.

The some research work of development and applications of templated metal coatings using electro-deposition from liquid crystal electrolytes have been done. Such coatings allow for high electroactive surface, which can be utilised in high rate electrochemical systems e.g. capacitors.

Development of the method of combinatorial screening for battery electrode materials. The method is based on simultaneous preparation and electrochemical testing of ca. 63 electrodes arranged in an array, which can be placed in a single cell vs. single Li electrode as a reference and counter electrode. The precursor of the electrode material is deposited using an automated liquid handle, which dispenses precursor on electrode substrata, while the composition of the material on each electrode can be varied.

Development of a new method in preparation of LiFePO4/C composite using fully liquid mixing of precursor from solutions. The method gives a material having good redox capacity in range 110-130 mAh/g in lithium cells. The method allows easy and fast preparation of LiFePO4 and can be used in combinatorial studies of LiFe1-xMxPO4 (M = Co, Mn, Ni) solid solutions.

Some experimental samples were prepared by using lithium thin film electrodes from J/S company “Sidrabe”. First prototypes was compiled and investigated in Southampton University (G. Vitins). Small cycling capacity (3-6 cycles) is connected with limited thickness of Li thin film (6 mkm), and will be improved by using thicker Li coatings onto polymer substrate.

ITO (indium tin oxide) is an optically transparent semiconductor that finds extensive use in liquid crystal displays, photovoltaic cells, LCD, touch screen displays, smart windows etc. In these applications, the ITO is used as a transparent electrode. Another application of this material is humidity sensor and material for sensing another gases. In this application it is necessary to use nano-crystalline films with thin catalytically active metal coatings. We compared optical, electrical and gas sensing properties of different

ITO films onto polymer substrates, obtained from Company "SIDRABE Inc." (Riga, Latvia) and ITO films onto glass substrate obtained by us.

Development of the proton conducting materials for low temperature fuel cells were main work on 2003. Inorganic particles (zirconium phosphate, antimonic acid etc.) are suspended in a polymer or fiber matrix. The material was studied by X-ray powder diffraction, SEM analysis, differential scanning calorimetry, impedance spectroscopy, and spectrophotometry. The structure of zirconium phosphate (ZP) component and of the gel is discussed in terms of water removal from interplanar spaces by heating or exfoliation. It is suggested that an exfoliation of the layered structure of zirconium phosphate by intercalation produces a dispersion of ZP nanoparticles in the polymer matrix. The BET method was used to characterize the surface area of zirconium phosphate particles and composite membranes. Zirconium phosphate is typical surface conductor and in this case the forming of highly developed crystalline surface is crucial to provide high conductivity. The proton conductivity of composite membranes containing nanoparticles might reach values 0.01-0.05 S/cm, which makes them suitable for fuel cell applications.

## AGING OF SOAPS DETECTED BY ODOUR CHANGES

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The application of electronic nose for the detection of off-flavours of special soaps, designed for use in bathtubs was performed during 2003 by collective research work in Riga (Latvia) and Tuebingen (Germany). These soaps are extremely flavoured, intended for deodorant use rather than for cleaning and so the foaming and the smelling is the most important characteristic. In some cases the strong smell of the soaps changes in a way that the respective flavour gets mixed with another, new note, which is a little mouldy, or at least less pleasant than the intended smell. The alteration usually takes place two weeks after production and it represents a severe loss of quality. The time lag complicates the problem as the soaps usually are delivered to the retailers or sold to the end customer within this period. Therefore, besides the efforts to find and eliminate the reason for the production failure, the final objective of the investigations is to detect the spoiled soaps as soon as possible in order to be able to deliver soaps with a stable flavour. The measurements were performed with two different sensor systems: Nordic E-nose (NST), equipped with semiconducting metal oxide gas sensors (MOX) and metal oxide field effect transistors (MOSFET) was used for the measurements in Riga, and MOdular SEensor System MOSES II (Lennartz Elektronik), equipped with MOX sensors and Quartz Micro Balances (QMB) was used for subsequent measurements in Tuebingen, performed in order to have a broader statistical basis. The clustering is a little better, independently from the original flavour, good and spoiled samples are systematically discriminated. This is in contrary to the evaluation of (selected) QMB responses, which also enables discrimination, whereas it is based on a completely different pattern, concerning the scoresplot. This clearly shows that the discriminations of MOX and QMB sensors are based different analytes. A combined evaluation performs worse than both, indicating that the different information content is even diverging.

Conventional bomb detectors are designed to respond to only energetic materials, e.g. nitrates, and not to detect other background chemicals in odours.

Conversely electronic noses are designed to respond to all chemicals within an odor. Based upon this distinction, electronic noses might not be considered good bomb detectors where there are strong background odours. On the other hand bomb detectors might not be very good electronic noses because they are blind to many important environmental and olfactory chemicals. However, the diversity of today's terrorist threats (explosive, chemical, and biological) makes it increasingly apparent that there is a role for electronic noses with the ability to quickly learn and recognize threat vapours of any kind. Research in this area was started in collaboration with scientists from Vilnius University (Lithuania, prof. A. Orliukas) and REI institute in Moscow (Dr. A. Medvedev).

## INSTRUMENTAL METHOD FOR MEASURING ODOURS FROM INDUSTRIAL AND AGRICULTURAL PLANTS USING THE ARTIFICIAL NOSE

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Odours from different production facilities as well in Industry, as well as in Agriculture and also in Oil transport enterprises are causing problems throughout the world. During last 3 years complaints on odours in Latvia grew exponentially. Latvia is going toward recognition of odour problems and is preparing Guideline for odour elimination (will be finished in December, 2003; accepted in Cabinet of Ministries till June, 2004). Although odours have always been associated with specific types of production, no single factor is responsible for the drastic increase in odour related conflicts. Whatever the reason, it is clear that odours from oil transition and industrial/agricultural production must be significantly reduced or eliminated in the near future. It is also clear that the need to control odours does not exclude any species or size of operation. Researchers, farmers, and industries throughout the world are attempting to reduce odour production through various technologies.

European Standard EN 13725 "Air Quality – Determination of Odour Concentration by Dynamic Olfactometry" was accepted on April, 2003. Latvia will implement that Standard too. Nevertheless, Latvia can be first country between European countries (and in the entire World too), where instruments with artificial intellect could be adopted for odour measurements. We present our experiences with measurement of odours from different matters by use of Nordic Odour Sensor System (e-Nose) and zNose (quick chromatograph).

The main objectives is find Industrial partnet in Latvia and develop gas sensor system (collectively called electronic nose) for industrial applications, specifically a system for on-line process control. The sensors should provide real-time measurement assessment of odours at the source and possibly at the receptor location.

## SENSOR SELECTIVITY EXPLORATION BASED OF DIFFERENCE IN CHEMICAL PROPERTIES OF GAS MOLECULES

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Elaboration of mechanical organs and spare-part surgery in human society will stay marketable action field for researchers and practicists and will attract public attention.

Investigations in the area of artificial senses and spare-parts for human body allows worming out ourselves, much more percept environment thoroughly, protect ourselves from undesirable influences. The new science which originates in this special area, locates on the border between physics, chemistry, biology and medicine. *Electronic olfactometry* is separate chapter of this new science and is devoted to research of artificial olfactory instruments – electronic nose and electronic tongue. There are some special fundamental tasks which are common for most of all new science areas connected with electronics: reduction of dimensions, increasing of selectivity and sensitivity, extension of life etc.

Our research work was directed to investigation of the basics of olfaction – the main principles of aroma sensitivity of human nose and to mark out some parallels in the science of material technology. Basic assumption putted in the basement of this work was that human nose detects different aroma after the characteristic shape of molecules which forms it. The structure of a chemical compound can be described by its complete shape (Turin and Yoshii - form, volume, profile) of stereochemical configuration and its electron charge distribution over the whole molecule – it was calculated also by Isaak Bersuker. Olfaction is a particular case of bioactivity which was predicted very well by their method based on molecular structure, and they got very good results in predicting musk and other odorant activities. In our work the hypothesis about odour perception and the shape of molecules in percept odour was realised as:

- The test of some commercial gas sensors for their possibility to differ molecules by shape;
- Elaboration of hypothesis about the special material technology being able to produce selective gas sensors based on key-lock principle.

## INTEGRATION OF ELECTROLYTIC HYDROGEN INTO THE HYDROGEN STORAGE DEVICES

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In order for hydrogen to become fully integrated in the society, the production of hydrogen must become feasible in competition with the fossil fuels that dominate the energy economy today. Nowadays fuel cell technologies require hydrogen in a gaseous form to produce energy. Hydrogen is one of the most abundant elements on the Earth, but almost all of it is combined with other elements, mostly carbon and oxygen (water, fossil fuels, etc.). Currently hydrogen can be produced through electrolysis of water, various chemical processes involving fossil fuels and natural gas, and biological processes of plants and animals. Fossil fuels are the most frequent primary source of hydrogen.

Only water electrolysis has the potential for being a renewable option in hydrogen production provided the electricity is produced from renewable sources. The Project objective is a detailed study of the electrode processes during electrolysis of water; kinetics of hydrogen evolution on new materials, including metal hydrides; determination of the mechanisms of hydrogen evolution and absorption, formation and decomposition of the hydride phases during electrolysis. Studies of catalytic properties of hydrogen injection phenomena in tungsten trioxide (hydrogen storage media) were mmade with aim:

1) To test the experiments on hydrogen spillover effect by using glass substrate, thin films of Pd and WO3 – using thin film coating facilities at institute, and optical-electrical registration methods.

2) To search for another metal and-or alloy with catalytic properties similar to Pd metal – able to split H2 molecule and facilitate spillover of atomic hydrogen onto non-metallic surfaces.

## TRITIUM RELEASE EXPERIMENTS AND QUANTITATIVE IMAGE ANALYSIS OF SCANNING ELECTRON MICROGRAPHS

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The X-ray diffraction and quantitative image analysis of scanning electron micrographs of various samples of the $Li_4SiO_4$ and $Li_2TiO_3$ breeder ceramics, determination of the average grain size and the distribution of the grain size, the statistical analysis of the grain size by means of the computer software "Microsoft Excel 97 for Windows 98" had been done some onclusions:

1. X-ray diffraction showed the basic phase of $Li_4SiO_4$ and admixture phases of $Li_6Si_2O_7$ and $SiO_2$ in the thermally unconditioned $Li_4SiO_4$ ceramic samples (41/93).
2. Scanning electron microscopy of the $Li_4SiO_4$ ceramic samples (41/93) showed the dendritic microstructure and the presence of microcracks.
3. X-ray diffraction of the $Li_2TiO_3$ and $Li_{1.9}Ti_{0.9}Nb_{0.1}O_3$ ceramic samples investigated showed only the structure corresponding to the $Li_2TiO_3$ phase.
4. Scanning electron microscopy of the $Li_2TiO_3$ ceramic samples (CTJ13, CTI 4C2) showed the lamellar structure of crystallites and pores in grain boundaries. Quantitative image analysis of the micrograph of the $Li_2TiO_3$ ceramic sample (CTI 4C2) gave the average grain size 1.7 μm. Quantitative image analysis of the micrographs of the $Li_2TiO_3$ ceramic samples (CTJ13) showed the increase of the average grain size from 3.2 to 7.0 μm as a result of the electron irradiation to the dose 1200 MGy at 1050 °C for 12 h.
5. Scanning electron microscopy of the $Li_2TiO_3$ ceramic sample (S. 1673K) showed coarse grain structure having the grain size 40-100 μm.
6. Scanning electron microscopy of the $Li_2TiO_3$ and $Li_{1.9}Ti_{0.9}Nb_{0.1}O_3$ ceramic samples synthesized in the Laboratory of Solid State Radiation Chemistry of the University of Latvia showed grained microstructure and presence of large pores in grain boundaries. Quantitative image analysis of the micrographs of the $Li_2TiO_3$ and $Li_{1.9}Ti_{0.9}Nb_{0.1}O_3$ ceramic samples gave the average grain size 1.3 and 2.6 μm, respectively. Scanning electron microscopy revealed grain boundaries of the $Li_{1.9}Ti_{0.9}Nb_{0.1}O_3$ ceramic sample to a lesser extent than that of the undoped $Li_2TiO_3$ ceramic sample.

## AIR QUALITY IN RIGA: SITUATION TODAY AND FORECAST FOR 2010

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Riga, the capital of Latvia is centre of industry, business, entertainment and tourism and is most polluted area in respect to air quality. An air quality management system AIRVIRO is used for an inventory of air pollution sources in Riga. DOAS equipment is

used for air quality monitoring in city (6 stations). Inventory of emission sources in Riga shows that traffic on the streets of Riga is responsible for 65-80% of all NOx, CO and VOC emissions. Calculated dispersion concentrations coincide quit well with directly measured values on main streets with intense traffic. Latvia is going to associate with European Union and is adopting air quality guidelines accordingly EU legislation. For year 2010 it will be necessary to ensure the annual concentrations of NO2 and benzene no more as 40 and 5 μg/m3 accordingly, but for Riga it will be problems. Suggestions are given how to improve the situation.

## IMPROVEMENT OF STUDENT ACADEMIC ACHIEVEMENTS BY USING VIRTUAL STUDY ENVIRONMENT ELEMENTS

**U.Kanders, J.Kļaviņš**

The newly developed learning support system contains electronic study materials which differ in their user possibilities of those used earlier and known as printed materials, textbooks etc. Compared to old style study materials, students will have much greater flexibility in where and when they attend class or stay at home in order to fulfill their self-dependent tasks and reports. Electronic study materials are asynchronous, which means you can use them at any time-24 hours a day, 7 days a week, from any Internet connection anywhere in the world. There are no required class times for self-dependent work. Asynchronous courses allow you to maximize your time spent learning, not going to and from a classroom. Guided by teacher, students will participate in every classroom discussion; work with teams of fellow learners, and network with peers from other universities. Students will also enjoy one-to-one interaction with teacher. Faculty teachers provide individualized direction, advice and support throughout the course or program.

## E – LEARNING AND RESEARCH IN THE INSTITUTE OF SOLID STATE PHYSICS

**J.Kļaviņš**

In the year 2002 University of Latvia begun the immersion of the E-University (www.liis.lv/e-lu/) in the studies (e-learning), administration (e-administration) and research work (e-research). It means that novel information technologies must be used in the all activities of the University. The Institute of Solid State Physics already have all required facilities for to take part in these activities – really integrated research work with the studding process, developed computer network to the *Internet*, realized project *Latvian Superclaster* (www.cfi.lu.lv.lasc) – large power computer for all research users in Latvia.

With the e-research we understand *GEANT* computer network, computer *GRID* technologies, *REAL* servers and videoconferences, virtual laboratories, *Digital Library*, *Learningware*, *tele-immersion*, 622Mbps network, e-learning and research lecture-hall in the Institute of Solid State Physics.

# Scientific publications

## Published in 2003


1. A.Lusis, J. Kleperis, E. Pentjuss. *Performance problems of electrochromic coatings*. Proc. SPIE (2003), vol. 5123, p.196-201.
2. J Kleperis, A. Lusis. *Properties of ITO transparent electrode thin films onto different substrates*. Proc. SPIE (2003), vol. 5123, p. 215-220.
3. J.Kleperis, L.Grinberga, A. Lusis, P.Misans, *Quick authenticity testing of food and goods. Is it real with e/z – nose?* In book: Proceedings of ISOEN 2002, Ed. A.D`Amico, C. Di Natale, Rome, 2003, p. 89-94.
4. G. Vaivars, M. Furlani, B.-E. Mellander and C.-G. Granqvist. *Thermal Analysis of a Proton Conducting Poly(vinyl acetate)/Glycerine Gel Composite with Zirconium Phosphate*// Journal of Solid State Electrochemistry 7, 10 (2003) 724-728.
5. Janis Kleperis, Jelena Smeisa and Kristine Karklina, *"Air quality in Riga: situation today and forecast for 2010*". Proceedings of 4th Internationa Conference on Urban Air Quality: Measurement, Modelling and Management", Prague (Czech Republic), March 25-28, 2003, p. 135-142.
6. G.Moreau, L. Helm, J. Purans and A.E. Merbach, *Structural XAFS Investigation on $Eu^{2+}$ and $Sr^{2+}$ Poly (amino carboxylates): Consequences for Water Exchange Rates on MRI Relevant Complexes*, J. Phys. Chem. A 107 (2003) 758-769.
7. S. a Beccara, G. Dalba, P. Fornasini, R. Grisenti, A. Sanson, F. Rocca, J. Purans and D. Diop, *EXAFS studies of local thermal expansion*, AIP Conf. Proc. 652 (2003) 349 - 354.
8. J. Purans, S. Benazeth and C. Souleau, *Recent achievement and perspectives in synchrotron radiation x-ray absorption spectroscopy*, Molecular and Structural Archaeology: Cosmetic and Therapeutic Chemicals (2003) 231 - 234.
9. A.Kuzmin, R. Kalendarev, J. Purans and D. Pailharey, *Iridium $L_3$-edge and oxygen K-edge x-ray absorption spectroscopy of nanocrystalline iridium oxide thin films*, Proc. SPIE 5123 (2003) 210-214.
10. D.Pailharey, D. Tonneau, A. Houel, A. Kuzmin, R. Kalendarev and J. Purans, *Scanning probe microscopy of nanocrystalline iridium oxide thin films,* Proc. SPIE 5123 (2003) 259-265.
11. A Kuzmin, R. Kalendarev and J. Purans, *Local structure of Ta-Re mixed oxide thin films studied by x-ray absorption spectroscopy*, Proc. SPIE 5122 (2003) 79-85.
12. G.Dalba, P. Fornasini, R. Grisenti, S. a Beccara, N. Daldosso, A. Sanson, F. Rocca, F. Monti and A. Kuzmin, *Studies of the temperature dependence of the short range structure and local dynamics in silver borate glasses,* Phys. Chem. Glasses 44 (2003) 75-78.
13. E.Cazzanelli, M. Castriota, R. Kalendarev, A.Kuzmin and J. Purans, *Sputtering deposition and characterization of Ru-doped $WO_3$ thin films for electrochromic applications,* Ionics 9 (2003) 95-102.
14. Spong, G. Vitins, S. Guerin, B.E. Hayden, A.E. Russel, J.R. Owen. Combinatorial arrays and parallel screening for positive electrode discovery. A.D. *J. Power Sources* 119-121 (2003) 778-783.

15. G.Vitins, E.A. Raekelboom, M.T. Weller, J.R. Owen.$Li_2CuO_2$ as an additive for capacity enhancement of lithium ion cells. *J. Power Sources* 119-121 (2003) 938-942.

16. J. Tiliks, G. Kizane, A. Vitins, G. Vitins, J. Meistars. Physiochemical processes in blanket ceramic materials. *Fusion Ingenierirng and Design* 69 (2003) 519-522.

**Published Conference Thesis**

1. A.Lusis, *Cycling Capacity of Electrochromic Cells*. Abstract book of 203rd Meeting of The Electrochemical Society, vol. 2003-1, p. 1339, Pennington, USA, 2003.

2. A.Lusis, J.Kleperis, E.Pentjušs. *Cycling capacity of intercalation electrodes*. 19th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2003.

3. G.Veveris, V. Eglitis, A. Lusis. *Spectroscopic appearance of sodium alumosilicate fiber leaching.* 19th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2003.

4. P.Misans, V.Eglitis, J.Kleperis, A.Lusis, J.Zukans. *Development of Signal Processing and Identification HW/SW for E-nose Mini Modules* Abstracts of 10th International Symposium on olfaction and electronic nose ISOEN`03; June 25-28, 2003, Riga, University of Latvia, p.180-181.

5. L. Grinberga, J. Kleperis. *Fast method to determine benzene in air and fuels*. 19th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2003, p. 87.

6. G. Mikelsons, L. Grinberga, J. Kleperis, *Odour dilution system in olfactometric measurements*. 19th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2003, p. 88.

7. Hodakovska, J. Kleperis, *Relationship betwee shape of molecule and its sensoric and physical reception*. 19th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2003, p. 86.

8. L. Grinberga and J. Kleperis, *Fast Gas Chromatograph for determination of alcohols and benzene in the air and fuel;* International conference EcoBalt '2003, Riga, 2003, pp 44-45.

9. J. Blahins, G. Mikelsons, J. Kleperis *Odour problems in Latvian Environmental Protection Area.*. Abstracts of 10th International Symposium on olfaction and electronic nose ISOEN`03; June 25-28, 2003, Riga, University of Latvia, p. 35-38.

10. J. Hodakovska, L. Grinberga and J. Kleperis, *Sensor selectivity exploration based of difference in chemical properties of gas molecules*. Abstracts of 10th International Symposium on olfaction and electronic nose ISOEN`03; June 25-28, 2003, Riga, University of Latvia, p. 171-174.

11. E. Smalins, K. Zommere, J. Kleperis and S. S. Jensen. *Gaisa kvalitātes novērtējums Rīgā izmantojot modelēšanas rezultātus* (*Preliminary assessment of air quality in Riga based on aq modelling).* Abstracts of International Conference "EcoBalt `2003", Riga (Latvia), May 21-22, 2003, p. 20-21.

12. G. Miķelsons, L. Grīnberga, J. Kleperis, A. Lūsis. *Smaku elektroniska reģistrācija*. *(Electronic registration of odours).* Abstracts of International Conference "EcoBalt `2003", Riga (Latvia), May 21-22, 2003, p. 23-24.

13. L. Grinberga, J. Kleperis. *Ātrs gāzu hromatogrāfs spirtu un benzola noteikšanai gaisā un degvielā. (Fast gas chromatograph for determination of alcohols and benzene in the air and fuel).* Abstracts of International Conference "EcoBalt `2003", Riga (Latvia), May 21-22, 2003, p. 41-42.

14. K. Kārkliņa, A. Spricis, J. Kleperis. *Gaisa piesārņotājvielu koncentrāciju diennakts un sezonas variācijas Rīgā. (Diurnal and annual variations of measured air polluting substances in Riga)*. Abstracts of International Conference "EcoBalt `2003", Riga (Latvia), May 21-22, 2003, p. 18-19.

15. J. Švinskis, A. Viksna, L. Grīnberga, J. Kleperis. *Kvēpu un benzola piesārņojuma apzināšana Rīgā. (Exploration of soot and benzene pollution in Riga).* Abstracts of International Conference "EcoBalt `2003", Riga (Latvia), May 21-22, 2003, p. 37-38.

16. J. Tīliks, G. Ķizāne, A. Vītiņš, J. Meistars. *Effect of the magnetic field on the tritium release from the blanket ceramics.* – In book: Institute of Solid State Physics. University of Latvia. Abstracts of the 19th Scientific Conference, dedicated to 25th anniversary of the Institute of Solid State Physics UL. / Ed. by A. Krūmiņš. – Riga, February 10-13, 2003. – P. 20.

17. G. Ķizāne, J. Tīliks, A. Vītiņš, J. Tīliks, Jr. *Using of the ultradisperse lithium orthosilicate and lithium titanate in the blanket ceramics*. – In book: Institute of Solid State Physics. University of Latvia. Abstracts of the 19th Scientific Conference, dedicated to 25th anniversary of the Institute of Solid State Physics UL. / Ed. by A. Krūmiņš. – Riga, February 10-13, 2003. – P. 21.

18. Vītiņš, Ģ. Vītiņš, G. Ķizāne, J. Tīliks. *Effect of niobium ions on the electrical conductivity of lithium metatitanate.* – In book: Institute of Solid State Physics. University of Latvia. Abstracts of the 19th Scientific Conference, dedicated to 25th anniversary of the Institute of Solid State Physics UL. / Ed. by A. Krūmiņš. – Riga, February 10-13, 2003. – P. 22.

19. G. Kizane, J. Tiliks, A. Vitins, J. Rudzitis *Tritium localisation and release from ceramic pebbles of breeder.* – In book: Abstracts. 11th International Conference on Fusion Reactor Materials, December 7-12, 2003, Kyoto, Japan. P. 250.

20. G. Ķizāne, J. Tīliks, A. Vītiņš and E. Kolodinska *The effect of magnetic field and high temperature on the properties of blanket ceramics*. – In book: Abstracts. 11th International Workshop on Ceramic Breeder Blanket Interactions, December 15-17, 2003, Tokyo, Japan. P. 22.

21. N.W.Maxakato, G.Vaivars, V.Linkov and G.Gericke. *Preparation and characteristics of inorganic proton conducting membranes for application in Direct Methanol Fuel Cell (DMFC).* In: Abstr. Chemical Engineering R&D 2003. April 4, 2003, University of Stellenbosch, Chemical Engineering Department. O10.

22. N. W. Maxakato, G. Vaivars and V. M. Linkov. *Inorganic proton conducting membranes for application in DMFC: preparation and properties*. In: Abstr. Inorganic `03 National Conference. South African Chemical Institute. Pretoria (Roode Vallei Country Lodge), June 8 – 11, 2003. P33. P.91.

**Accepted for publication 2003**

1. G. Dalba, P. Fornasini, A. Kuzmin, F. Monti, A. Sanson, O. Sipr and F. Rocca, *XANES and EXAFS modelling of configurational disorder in silver borate glasses,* Physica Scripta (2004) (in press).

2. E. Avendaño, A. Kuzmin, J. Purans, A. Azens, G. A. Niklasson and C.G. Granqvist, *Changes in the local structure of nanocrystalline electrochromic films of hydrated nickel vanadium oxide upon ozone-induced coloration*, Physica Scripta (2004) (in press).

3. A. Kuzmin, R. Kalendarev, J. Purans, J.P. Itié, F. Baudelet, A. Congeduti and P. Munsch, *EXAFS study of pressure-induced phase transition in $SrWO_4$*, Physica Scripta (2004) (in press).

4. J. Purans, G. Heisbourg, N. Dacheux, Ph. Moisy and S. Hubert, XAFS study of local structure with picometer accuracy: $Th_{1-x}U_xO_2$ and $Th_{1-x}Pu_xO_2$ solid solutions, Physica Scripta (2004) (in press).

5. A. Kuzmin, J. Purans and G. Moreau, *Full multiple scattering analysis of x-ray absorption near edge structure at the Eu $L_3$-edge in EuO*, J. Alloys and Compounds (2004) (in press).

6. J. Gaidelene, R. Kalendarev, A. Kuzmin and J. Purans, *EXAFS study of mixed nickel molybdenum oxide thin films at the Ni and Mo K-edges,* Nucl. Instrum. and Methods A (2004) (in press).

7. J.Kleperis *"Izpratne par gaisa piesārņojumu: kvalitātes indikatori, indekss, koncentrācijas Rīgas piemērā",* iesniegts rakstu krājumam "Rīgas Vides problēmas 2003", izdevējs – Rīgas Vides centrs "Agenda 21"; 16 lpp.

8. J. Kleperis, B. Sloka. *"Information technologies in an environmental science: Air quality management in Riga"*. To be published in Proceedings of International Conference"Information Society and Modern Business" Ventspils (Latvia), January 31 – February 1, 2003; 8 pages.

## Lectures on Conferences

**19th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2003**

1. L.Grinberga. Fast method to determine benzene in air and fuels.
2. G.Mikelsons. Odour dilution system in olfactometric measurements.
3. Julija Hodakovska. Relationship between shape of molecule and its sensoric and physical reception.
4. A.Lusis, J. Kleperis, E.Pentjušs. Cycling capacity of intercalation electrodes
5. G.Veveris, V. Eglitis, A. Lusis. Spectroscopic appearance of sodium alumosilicate fiber leaching
6. J.Gabrusenoks Dipolu oscilatoru modelis WO3 IS atstarošanās spektru analīzei.
7. A.Kuzmin "Phase transition in $SrWO_4$ at high pressure"
8. J. Tīliks, G. Ķizāne, A. Vītiņš, J. Meistars. Effect of the magnetic field on the tritium release from the blanket ceramics. P.20.
A. Vītiņš, Ģ. Vītiņš, G. Ķizāne, J. Tīliks. Effect of niobium ions on the electrical conductivity of lithium metatitanate.
G. Ķizāne, J. Tīliks, A. Vītiņš, J. Tīliks, Jr. Using of the ultradisperse lithium orthosilicate and lithium titanate in the blanket ceramics.
9. J.Kļaviņš, E – learning and research in the Institute of Solid State Physics
10. U.Kanders, J.Kļaviņš, Improvement of student academic achievements by using virtual study environment elements

**203rd Meeting of The Electrochemical Society, April 27-May 2, 2003, Paris, France:**
A.Lusis, Cycling Capacity of Electrochromic Cells

**International Conference on X-ray Absorption Fine Structure (XAFS-12), Malmo (Sweden), June 23-27, 2003**.
1. G. Dalba, P. Fornasini, A. Kuzmin, F. Monti, A. Sanson, O. Sipr, F. Rocca, "XANES and EXAFS modelling of configurational disorder in silver borate glasses" [poster];
2. J. Gaidelene, A. Kuzmin, J. Purans, "Interpretation of the O K-edge XANES in crystalline $\alpha$-$MoO_3$" [poster];
3. E. Avendaño, A. Kuzmin, J. Purans, A. Azens, G. A. Niklasson, C. G. Granqvist, "Changes in the local structure of nanocrystalline electrochromic films of hydrated nickel vanadium oxide upon ozone-induced coloration" [poster];
4. A. Kuzmin, R. Kalendarev, J. Purans, J.P. Itié, F. Baudelet, A. Congeduti, P. Munsch, "EXAFS study of pressure-induced phase transition in $SrWO_4$" [poster];
5. J. Purans, G. Heisbourg, N. Dacheux, Ph. Moisy, S. Hubert, "XAFS study of local structure with picometer accuracy: $Th_{1-x}U_xO_2$ and $Th_{1-x}Pu_xO_2$ solid solutions" [poster].

**International Conference on f-Elements (ICFE-5), Geneva (Switzerland), August 24-29, 2003**.
1. J. Purans, G. Moreau, A. Kuzmin, L. Helm, A.E. Merbach, "Temperature dependent XAFS study of Ln(iii) aqua-ions and relaxation time of water molecules" [oral];
2. A. Kuzmin, J. Purans, G. Moreau, "Full multiple scattering analysis of x-ray absorption near edge structure at the Eu $L_3$-edge in EuO" [poster];
3. J. Purans, A. Kuzmin, G. Moreau, L. Helm, A.E. Merbach, "Full multiple scattering analysis of the O K-edge in crystalline Gd(iii) and Eu(iii) complexes" [poster].

**Satellite Meeting on Micro X-Ray Beam Analysis, Osaka (Japan), September 12-14, 2003.**
J.Purans, "X-Ray Scanning Probe Microscopy and Nano X-Ray Absorption Spectroscopy" [poster].

**Fifth International Workshop on Radiation Imaging Detectors (IWORID 2003), Riga (Latvia), September 7-11, 2003.**
1. J. Gaidelene, R. Kalendarev, A. Kuzmin, J. Purans, "EXAFS study of mixed nickel molybdenum oxide thin films at the Ni and Mo K-edges" [poster];

2. A. Kuzmin, R. Kalendarev, J. Purans, J.P. Itié, F. Baudelet, A. Congeduti, P. Munsch, "Structural studies of pressure-induced phase transition in $SrWO_4$ by x-ray diffraction and x-ray absorption spectroscopy" [poster].

**Invited talk on Lithium Battery Discussion, September 14-19, 2003, Bordeaux-Arcachon, France**
G.Vitins, A.D. Spong, S. Guerin, J.R. Owen.. "Combinatorial screening for battery electrode materials – A new better way?" (Extended Abstarcts: Abstract No Inv 8)

**Invited talk at Angstrom Laboratory of University of Upsala, October 1st 2003, Upsala, Sweden**
G. Vitins "Combinatorial screening for battery electrode materials – A new better way?"

**International Conference"Information Society and Modern Business" Ventspils (Latvia), January 31 – February 1, 2003**
Jānis Kleperis, Biruta Sloka. Information technologies in an environmental science: Air quality management in Riga.

**4th Internationa Conference on Urban Air Quality: Measurement, Modelling and Management", Prague (Czech Republic), March 25-28, 2003**
Janis Kleperis "Air quality in Riga: situation today and forecast for 2010".

**International conference EcoBalt '2003, Riga, May 21-22, 2003**
1. L. Grinberga, Fast Gas Chromatograph for determination of alcohols and benzene in the air and fuel.
2. E. Smalins, K. Zommere, J. Kleperis and S. S. Jensen. Preliminary assessment of air quality in Riga based on aq modelling
3. G. Miķelsons, L. Grīnberga, J. Kleperis, A. Lūsis. Electronic registration of odours.
4. K. Kārkliņa, A. Spricis, J. Kleperis. Diurnal and annual variations of measured air polluting substances in Riga.
5. J. Švinskis, A. Viksna, L. Grīnberga, J. Kleperis. Exploration of soot and benzene pollution in Riga.

**10th International Symposium on olfaction and electronic nose ISOEN`03; June 25-28, 2003, Riga, University of Latvia**
1.J. Blahins, G. Mikelsons, J. Kleperis. Odour problems in Latvian Environmental Protection Area

2. J. Hodakovska, L. Grinberga and J. Kleperis, Sensor selectivity exploration based of difference in chemical properties of gas molecules.
3. P.Misans, V.Eglitis, J.Kleperis, A.Lusis, J.Zukans. Development of Signal Processing and Identification HW/SW for E-nose Mini Modules.

**11th International Conference on Fusion Reactor Materials, December 7-12, 2003, Kyoto, Japan.**
1. G. Kizane, J. Tiliks, A. Vitins, J. Rudzitis Tritium localisation and release from ceramic pebbles of breeder.

**11th International Workshop on Ceramic Breeder Blanket Interactions, December 15-17, 2003, Tokyo, Japan.**
5. G. Ķizāne, J. Tīliks, A. Vītiņš and E. Kolodinska The effect of magnetic field and high temperature on the properties of blanket ceramics.

# DIDACTIC SYSTEM LABORATORY

Head of Laboratory – Prof., Dr. J.Kuzmins

## Research Area and Main Problems

Investigation of possibilities to use "client-server" and "virtual laboratory" technology to create new methods of e-education.

**Scientific Staff**

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

### Research Project

1."**Virtual Physics Laboratory"**, Latvian Government Grant, 2001-2004
(Head: Prof., Dr. J. *Kuzmin*).

### Didactic work at the University of Latvia

1. LU PPF "Internet and Intranet" – lectures, Prof. J.Kuzmin.
2. LU PPF "Operational Systems" – lectures, Prof. J.Kuzmin.
3. LU PPF "System Approach" – lectures, Prof. J.Kuzmin.
4. LU PPF "Informatics for Educators" – lectures, Prof. J.Kuzmin.
5. LU PPF "Modern Educational Environments" – lectures, Prof. J.Kuzmin.

**Visitors from abroad**

Dr. F. Rocca – IFN-CNR, Institute for Photonics and Nanotechnologies, Section "ITC-Cefsa" of Trento, Italy (1 month).

**Scientific Visits Abroad**

Dr. A.Kuzmin, IFN-CNR, Institute for Photonics and Nanotechnologies, Section "ITC-Cefsa" of Trento, Italy

## Cooperation

**Latvia**

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

**Italy**

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

# Main Results

## VIRTUAL PHYSICS LABORATORY

**J.Kuzmin, A. Kuzmin**

In year 2003 Didactic System Laboratory is specialised in the investigations of the Virtual Laboratory development methods and appropriate software elaboration. Main topics and results of our studies in 2003 are described briefly below.

- "client-server" technology in a e-education applications.

This part of investigations is devoted to frontal teaching computerization problem using recently developed didactic system "SOLO". The system was tested during study process at the Latvian University.

Elaboration of didactic system "SOLO" was based on following criteria:

- minimization of waste of educator time during lectures;
- taking into account of typical elements of didactical activities;
- supporting of educator-student feedback with hardware and software means;
- simplification of system procedures necessary to use for educator;
- supporting of 3 languages (Latvian, English and Russian) in dialog procedures.

System's "SOLO" technical structure can be various:

*1.* Educator PC with digital projector. In this case all educational material can be used as ordinary presentation. Educator can use "SOLO" scripting technique to organize teaching material.

*2.* PC classroom with Educator PC. All "SOLO" functions are available (additionally to regular oral presentation visual material can be presented directly on students PC screens, graphical and textual feedback is possible).

*3.* LAN with Educator PC. As in 2, but netphone is required for use in oral presentation. Educator can interact in real time regime with different classrooms.

*4.* WAN with Educator PC. As in 3, but there are limitations on size of graphical files. Educator can interact with remote students in real time regime.

Software's structure of "SOLO" consists of two parts: central part - intend to Educator and peripheral part for student. Both parts can be on Educator PC HDD or on CD ROM. It is possible to install student part of system on student PC, but in case of both parts are on Educator CD ROM everybody will use a newest version of system.

Educator CD ROM besides Educator's and Student's parts of "SOLO" usually contains all materials needed for teaching purposes:

- web pages samples, if they are included in e-lectures or e-tests. This eliminates time wasting on slow loading this information from Internet.
- EXEL, WORD, Acrobat and graphical files if they are necessary for teaching.
- programs for demonstrations, data preparation and analysis.
- lecture plans, questionnaire and e-tests
- students registration and examination results

Both parts of system interacts through IP protocol. Educator can dynamically enable or disable students access to central PC. It is possible to work with students in grope and/or in peer-to-peer modes.

- Latvian SuperCluster system and ab-initio simulations of x-ray absorption spectra from nanoparticles

Latvian SuperCluster (LASC) system represents a classical example of the "home-made" Beowulf-type cluster. It consists of five nodes: one front-end node plus four

computational nodes. The nodes, Compaq ProLiant ML350 G2 servers, are interconnected through Fast Ethernet switch, and the front-end node has also a connection with the rest of the world (Internet). The total resources available to the users are 10 Pentium III-1.26GHz CPUs, having a total peak power about 13 GFlops, 20 GB of physical memory (RAM) and 456 GB of storage space (easily expandable up to 3.3 TB).

The nodes are running under the Red Hat Linux operating system on the private subnetwork, protected from the Internet by a firewall. Most of installed software is of open source type and, thus, is available for free under GNU public license. The cluster security is maintained through the use of secure shell interface (SSH2) and client's authorisation by the IP address. For users convenience, all information related to the cluster is available on-line from the Web service .

The LASC system is used mainly for quantum chemistry calculations, Monte-Carlo modelling and x-ray absorption spectra simulations. Similar systems can be easily build up for other than scientific needs with possibly even lower price. As an example, standard off-the-shelf computers, equipped with much smaller memory and thus being much cheaper, can be used as nodes in a cluster for multimedia encoding applications, such as sound MPEG-3 or video MPEG-4 processing, and for images rendering to create stunning three-dimensional graphics.

The LASC system is currently used for data analysis of experimental x-ray spectra of advanced materials. Two direct structural techniques are currently available: x-ray/neutron/electron scattering and x-ray absorption spectroscopy (XAS). While the first method is well known and was widely used for many decades, XAS is relatively new and comes into the force during the last 10-15 years. Due to short-range order sensitivity, XAS can be used to study any material from molecules to single-crystals. In particular, XAS is the only direct structural tool, which can be applied to nano-sized and cluster-sized systems.

General approach to the analysis of the x-ray absorption spectra has been developed in the 1990s. It is based on ab initio self-consistent real space multiple-scattering calculations and, thus, requires an intensive use of modern computers.

In 2003 we performed ab initio simulations of x-ray absorption spectra from nanocrystalline nickel oxide thin films, produced by dc magnetron sputtering. The use of cluster technology allowed us to perform calculations for relatively large spherical-like nanoparticles, taking also into account atomic thermal vibrations by calculating configurational averages. We were able to simulate in reasonable time nanoparticles, consisting of up to 14000 atoms and having a size of up to 10 nm. The obtained results are in very good agreement with available experimental. They indicate that nickel oxide thin films are composed of very fine nanocrystals with the size of about 1 nm.

## Scientific Publications

### Published in 2003


1. Yu. Kuzmin, *Computorized Frontal Teaching System "SOLO"*, in Proc. 1st Int. Conf. "Information Technologies and Management", April 16-17, 2003, (Information System Institute, Riga, Latvia, 2003) pp. 186-191.
2. A. Kuzmin, *Cluster approach to high performance computing*, Computer Modelling & New Technologies 7 (2003) 7-15.
3. A. Kuzmin, *High-performance computing: application to ab-initio simulations of x-ray absorption spectra from nanoparticles,* in Proc. 1st Int. Conf. "Information Technologies and Management", April 16-17, 2003, (Information System Institute, Riga, Latvia, 2003) pp. 44-52.

**In press 2003**

1. J. Kuzmins Sistēmas *Solo didaktiakās iespējas*. Izglītības zinātnes un pedagoģija mūsdienu pasaulē: LU Zin.. Raksti. Rīga,
2. L.Kuzmina, J.Kuzmins. *E-lekcijas un e-ieskaites sistēmā SOLO*. Izglītības zinātnes un pedagoģija mūsdienu pasaulē: LU Zin. Raksti. Rīga,

## Participation in Conferences

1. Yu. Kuzmin, *Computorized Frontal Teaching System "SOLO"*, -1st Int. Conf. "Information Technologies and Management", April 16-17, 2003, (oral presentation).
2. A. Kuzmin, *High-performance computing: application to ab-initio simulations of x-ray absorption spectra from nanoparticles*, in Proc. 1st Int. Conf. "Information Technologies and Management", April 16-17, 2003, (oral presentation).
3. J. Kuzmins *Sistēmas Solo didaktiakās iespējas*. -LU 61. conference 2003. Riga.
4. L.Kuzmina, J.Kuzmins. *E-lekcijas un e-ieskaites sistēmā SOLO*. -LU 61. conference 2003. Riga.

# NONLINEAR PROCESSES IN SOLIDS

Head of Division Dr. habil. phys. Eugene A. Kotomin

## Research Area and Main Problems

Our theoretical research interests are focused on two main classes of problems related to the kinetics of diffusion-controlled processes with pattern formation and catalytic surface reactions, as well as atomic and electronic structure of advanced materials with emphasis on calculations of defect properties, surface properties and metal/oxide interfaces. We combine many different techniques, including analytical formalisms and large-scale computer simulations (both quantum chemical methods and Monte Carlo/cellular automata modelling).

**Scientific staff**

1. Dr. hab. E. Kotomin
2. Dr. hab. V. Kuzovkov
3. Dr. hab. J.R. Kalnin
4. Dr. Yu. Zhukovskii
5. Dr. A. Popov
6. Dr. R. Eglitis
7. Dr. G. Zvejnieks
8. Dr. S. Piskunov

**PhD students**

9. V. Kashcheyevs
10. D. Gryaznov

**Students**

11. D. Bocharov

**Visitors from abroad**

1. Prof. Dr. O. Dumbrajs, Helsinki University of Technology, Espoo, Finland (1 month).
2. Prof. F. Illas, University of Barcelona, Spain (1 month).
3. Prof. R. González, Carlos III University of Madrid, Spain (1 month).
4. Prof. Dr. R.A. Evarestov, St. Petersburg University, Russia (1 month).
5. Prof. C. Wilkinson, King's College London, UK (1 month).
6. Prof. Dr. V.A. Trepakov, Institute of Physics, Charles University, Prague, Czech Republic (1 month).

**Scientific visits abroad**

1. Dr. hab. E. Kotomin, Max Planck Institute, Stuttgart, Germany (9 months), University of Osnabrück, Germany (2 weeks), University of Barcelona, Spain (2 weeks).
2. Dr. hab. V. Kuzovkov, University of Osnabrück, Germany (1 month); Braunschweig University of Technology, Germany (3 months), Max Planck Institute, Garching, Germany (1 month).
3. Dr. Yu. Zhukovskii, University of Osnabrück, Germany (1 month), St. Petersburg University, Russia (2 weeks), Uppsala University, Sweden (6 weeks).
4. Dr. A. Popov, European Molecular Biology Laboratory, Grenoble, France (11 months).
5. Dr. R. Eglitis, University of Osnabrück, Germany (12 months).
6. Dr. G. Zvejnieks, Max Planck Institute, Garching, Germany (2 months), Helsinki University of Technology, Espoo, Finland (1 month),
7. Dr. S. Piskunov, University of Osnabrück, Germany (11 months)
8. V. Kashcheyevs, Tel Aviv University, Israel (11 months)
9. D. Gryaznov, Max Planck Institute, Stuttgart, Germany (11 months)

## Cooperation

| | |
|---|---|
| **Canada** | University of Western Ontario, London (Prof. P.W.M. Jacobs) |
| **Czech Republic** | Institute of Physics, Charles University, Prague (Prof. V. Trepakov) |
| **Estonia** | Institute of Physics, Tartu University (Prof. A. Lushchik) |
| **Finland** | Helsinki University of Technology, Espoo, Finland (Prof. O. Dumbrajs) |
| **France** | European Molecular Biology Laboratory (EMBL), Grenoble (Dr. D.A.A. Myles) |
| **Germany** | University of Osnabrück (Prof. G. Borstel)<br>Max Planck Institut (MPI) für Festkörperforschung, Stuttgart (Prof. J. Maier)<br>Max Planck Institut (MPI) für Plasmaphysik, Garching (Prof. H. Zohm)<br>Braunschweig University of Technology (Prof. W. von Niessen)<br>Gesellschaft für Schwerionenforschung, Darmstadt (Prof. K. Schwartz) |
| **Israel** | School of Physics and Astronomy, Tel Aviv University (Prof. A. Aharony)<br>Ben Gurion University of the Negev, Ber Sheeva (Prof. D. Fuks)<br>Israel Institute of Technology (Technion), Haifa (Prof. S. Dorfman) |
| **Latvia** | Institute of Solid State Physics (ISSP) (Prof. J. Purans)<br>Transport and Telecommunication Institute (TTI) (Prof. Yu.N. Shunin) |
| **The Netherlands** | Eindhoven University of Tehnology (Prof. A.P.J. Jansen) |
| **Russia** | St. Petersburg University (Prof. R.A. Evarestov) |
| **Spain** | Carlos III University of Madrid (Prof. R. González)<br>University of Barcelona (Prof. F. Illas) |
| **Sweden** | Uppsala University (Prof. K. Hermansson) |
| **UK** | King's College London (Prof. C. Wilkinson)<br>University College London (Prof. A.M. Stoneham) |
| **USA** | California Institute of Technology, Pasadena (Dr. E. Heifets) |

## Main Results

### DEFECTS AND SURFACES OF ADVANCED PEROVSKITES

**E.A. Kotomin, R.I. Eglitis, and S. Piskunov** (*ISSP*),
**G. Borstel** (*University of Osnabrück, Germany*),
**R.A. Evarestov** (*St. Petersburg University, Russia*),
**E. Heifets** (*California Institute of Technology, Pasadena, USA*),
**D. Fuks** (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
**S. Dorfman** (*Technion, Haifa, Israel*), J. Maier (*MPI, Stuttgart, Germany*)

Large-scale first principles quantum chemical calculations have been performed for a number of advanced $ABO_3$ materials, including $BaTiO_3$, $KNbO_3$, $KTaO_3$, $LaMnO_3$, $PbTiO_3$, $SrTiO_3$, and their solid solutions, widely used in technological applications.

In collaboration with *Osnabrück University, Germany*, and *California Institute of Technology, Pasadena, USA,* we performed first principles calculations, using both Hartree-Fock method (with electron correlation corrections, HF-CC) and Density Functional Theory (DFT), as well as semi-empirical INDO calculations. We have studied the atomic and electronic structure of polar surfaces of $ABO_3$ perovskites, *e.g.*

$SrTiO_3$ (110) surfaces, which serve as substrates for growth of technologically important high $T_c$ materials. We have optimized the atomic coordinates in four planes near the surface, considered surface rumpling and compression, and estimated their effective charges and surface polarization. Results are compared with LEED and RHEED experiments. We studied also the atomic and electronic nature of the polarons and excitons in perovskites and suggested an interpretation of widely observed "green" luminescence (2.2-2.3 eV) as a radiative recombination of nearest electron and hole polarons localized on Ti(Nb) ion and neighboring $O^{2-}$ ion. This theoretical study permits to make choice between many hypothetical models of the green luminescence. In collaboration with *Technion Institute in Israel*, we studied also the atomic structure of the $KNb_xTa_{1-x}O_3$ perovskite solid solution and demonstrated that Nb impurities even at very low concentrations reveal a cooperative self-ordering effect, which drives the phase transition in incipient $KTaO_3$ ferroelectric. In collaboration with *St. Petersburg University, Russia,* we studied *ab initio* Fe impurity in $SrTiO_3$ perovskite and demonstrated the single $Fe^{4+}$ ions reveal Jahn-Teller effect: 4 equatorial O ions relax towards Fe whereas two vertical O ions (along the *z* axis) go outwards. This local lattice distortion stimulates the covalent Fe-O bonding and strongly affects the electronic structure and position of defect energy levels within the gap. At the time being our prediction is checked by means of the EXAFS spectroscopy (Prof. J. Purans, *ISSP*).

Progress in solid fuel cells needs new materials for cathodes. One of promising materials is $LaMnO_3$ perovskite. Of principle interest is $O_2$ molecule adsorption on its surface, dissociation, O atom diffusion and penetration through the electrolyte to anode, where O meets with H atoms. In collaboration with *Max Planck Institute for Solid State Researches, Stuttgart, Germany*, *St. Petersburg University, Russia, and California Institute of Technology, Pasadena, USA* we performed detailed *ab initio* and shell model calculations of the (100) and (110) $LaMnO_3$ surfaces, with emphasis on the surface energies and polarization. We have demonstrated that the (110) surface needs a reconstruction through incorporation of large concentration of O vacancies. This removes an infinite dipole moment and stabilizes the surface. On the other hand, the polar (100) surface could be stabilized by the charge redistribution near the surface. Both surfaces, the (100) and (110), reveal a strong increase of the Mn-O bond covalency in the first three planes nearest to the vacuum, which should affect the defect structure and oxygen adsorption properties which is now in progress.

## ANDERSON LOCALIZATION PROBLEM AND DISTINGUISHING DETERMINISTIC&NOISE COMPONENTS IN EDGE LOCALIZED MODE TIME SERIES

**V.N. Kuzovkov and G. Zvejnieks** (*ISSP*),
**W. von Niessen** (*Braunschweig University of Technology, Germany*),
**O. Dumbrajs** (*Helsinki University of Technology, Espoo, Finland*),
**H. Zohm** (*MPI, Garching, Germany*)

In collaboration with *Braunschweig University, Germany* we studied the Anderson localization problem in one and two dimensions. The problem is solved analytically *via* the calculation of the generalized Lyapunov exponents. This is achieved by making use of signal theory. The phase diagram can be analyzed in the following way. In the one dimensional case all states are localized for arbitrarily small disorder in agreement with existing theories. In the two dimensional case for larger energies and large disorder all states are localized but for certain energies and small disorder extended and localized states coexist. The phase of delocalized states is marginally stable. We demonstrate that the metal-insulator transition should be interpreted as a first-order phase transition. Consequences for perturbation approaches, the problem of self-

averaging quantities and numerical scaling are discussed. The method proposed to deal analytically with the problem of Anderson localization *via* disorder is generalized for higher spatial dimensions D. In this way the generalized Lyapunov exponents can be calculated analytically and exactly. This permits to determine the phase diagram of the system. For all dimensions D > 2 one finds intervals in the energy and the disorder where extended and localized states coexist: the metal-insulator transition should thus be interpreted as a first-order transition. The qualitative differences permit to group the systems into two classes: low-dimensional systems (2<=D <= 3), where localized states are always exponentially localized and high-dimensional systems (D>= $D_c$=4), where states with non-exponential localization are also formed. The value of the upper critical dimension is found to be $D_0$=6 for the Anderson localization problem; this value is also characteristic of a related problem - percolation.

Frequently problems arise in science, which involve both additive and multiplicative noise. The first type is relatively easy to handle with the help of the central limit theorem. The situation changes dramatically with the appearance of multiplicative noise. Famous examples are the Anderson localization, turbulence, and the kicked quantum rotator among others. In this field results of an importance comparable to the central limit theorem are still lacking. Moreover, the approaches are in general numerical ones and analytical tools are the rare exception. One of the main problems in the preliminary data analysis is distinguishing the deterministic and noise components in the experimental signals. For example, in plasma physics the question arises when analyzing edge localized modes (ELMs): does observed ELM behavior is governed by a complicate deterministic chaos or just by random processes. In collaboration with *MPI, Garching, Germany*, and *Helsinki University of Technology, Finland* we have developed methodology based on financial engineering principles, which allows us to distinguish deterministic and noise components. We extended the linear auto-regression method (AR) by including the non-linearity (NAR method). As a starting point we have chosen the non-linearity in the polynomial form, however, the method can be extended to any other type of non-linear functions. The best polynomial model describing the experimental ELM time series was selected using Bayesian Information Criterion (BIC). With this method we have analyzed type I ELM behavior in a subset of 26 ASDEX Upgrade shots. Obtained results indicate that the ELM behavior can be described by a linear AR model. In turn, it means that type I ELM behavior is of a relaxation or random type.

## QUANTUM THEORY OF TRANSPORT PHENOMENA IN MESOSCOPIC SYSTEMS

**V. Kashcheyevs** (*ISSP*),
**A. Aharony and O. Entin-Wohlman** (*Tel Aviv University*)

Recent technological advances have made possible the study of phase coherent nanoscale electronic devices (*mesoscopic nanostructures*), such as semiconductor quantum dots. A particular effect that has attracted much recent experimental and theoretical attention, is the generation of a dc current through a mesoscopic device by a periodic modulation of the confining potential – quantum charge pumping. A possibility to control the exact number of carriers transferred per cycle leads to important metrological applications.

In collaboration with *Tel Aviv University, Israel*, we have studied the mechanism of adiabatic charge pumping within a generic non-interacting model. Previous numerical calculations have shown that the pumped charge is close to an integer number of electrons when the pumping contour surrounds a resonance, but the transmission remains small on the contour. We have developed a resonance approximation for adiabatic quantum pumping that gives a quantitative account of the detailed exchange of

electrons between the quantum dot and the leads (to the electron reservoirs) during a pumping cycle. Near isolated distinct resonances, we use approximate Breit-Wigner expressions for the dot's Green function to discuss the loading/unloading picture of the pumping: the fractional charge exchanged between the dot and each lead through a single resonance point is related to the relative couplings of the dot and the leads at this resonance. If each resonance point along the pumping contour is dominated by the coupling to a single lead (which also implies a very small transmission), then the crossing of each such resonance results in a single electron exchange between the dot and that lead, ending up with a net quantized charge. When the resonance approximation is valid, the fractional charges can also be extracted from the peaks of the transmissions between the various leads.

## FIRST PRINCIPLES MODELING AND THERMODYNAMIC STUDY OF METAL FILM GROWTH, METAL OXIDATION AND CORROSION

**Yu.F. Zhukovskii and E.A. Kotomin** (*ISSP*),
**A.M. Stoneham** (*University College London, UK*),
**P.W.M. Jacobs** (*University of Wwestern Ontario, Canada*),
**D. Fuks** (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
**S. Dorfman** (*Technion, Haifa, Israel*), K. Hermansson (*Uppsala University, Sweden*),
**G. Borstel** (*University of Osnabrück, Germany*), J. Maier (*MPI, Stuttgart, Germany*),
**Yu.N. Shunin** (*Transport and Telecommunication Institute, Latvia*)

*Ab initio* DFT calculations using CRYSTAL'98 and CRYSTAL'03 codes are performed, in order to describe both bulk and surface properties of Al, Ag and Cu metals as well as their reactivity towards molecular oxygen and MgO(001) surface, respectively. Optimization procedure realized in both CRYSTAL'03 and VASP codes is used also to understand better the nature of conductivity in the AgCl(111)/$\alpha$-$Al_2O_3$(0001) interface.

In collaboration with *Osnabrück University, Germany, University College London, UK, Uppsala University, Sweden, Ben Gurion University, Ber Sheeva, Israel,* and *Technion Institute, Haifa, Israel*, we continue large-scale *ab initio* calculations and thermodynamic study of copper and silver adhesion onto magnesia substrate. We carefully re-optimized basis sets of Ag and Cu for reliable CRYSTAL calculations and then checked both bulk and surface properties of copper and silver. Due to a 15% mismatch between the lattice constants of Cu and MgO the probability of the aggregation of adsorbed Cu atoms into clusters is noticeably higher than in the case of the Ag/MgO(001) interface where this mismatch is markedly smaller (~3%). We also continue to study various adhesive and electronic properties of both regular and defective Ag/MgO(001) and Cu/MgO(001) interfaces, which allow us to make a comparative analysis of the nature of various metals adhesion on ceramic substrate depending on the electronic structure of adsorbate and structural morphology of adsorbent.

In collaboration with the *Western Ontario University, Canada*, we completed a series of first principles DFT simulations on both regular and stepped close-packed O/Al interfaces to clarify the mechanism of oxygen interaction with single-crystal aluminium surfaces. It has been shown that the less density of atomic packing on the aluminium surface, its reactivity towards oxygen is energetically more favorable and faster. Together with earlier suggested mechanism of the initial growth of $Al_2O_3$ formula units on the Al(111) substrate this study can be considered as the first attempt to describe atomistically the most important stage of metal oxidation between adsorption of molecular oxygen and oxide film growth.

In collaboration with *Max Planck Institute for Solid State Research, Stutttgart, Germany*, we continue first principles calculations on the AgCl(111) slabs of various

thickness as well as the AgCl(111)/α-$Al_2O_3$(0001) interface using procedure of geometry optimization realized in both CRYSTAL'03 and VASP codes. For optimal adsorption configuration of silver chloride film on the corundum substrate we have shown enhanced probability of diffusion of $Ag^+$ ions, which may cause ionic conductivity, which is predicted from experimental studies of this interface.

## KINETIC MC STUDY OF REVERSIBLE PATTERN FORMATION IN INITIAL STAGES OF METAL FILM GROWTH ON CRYSTALLINE SUBSTRATE

**G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, and Yu.F. Zhukovskii** *(ISSP),*
**A.M. Stoneham** (*University College London, UK*)

The kinetics Monte Carlo (kMC) simulations of the reversible pattern formation during the adsorption of mobile metal atoms on crystalline substrates were performed for the interfaces between metals and metal oxide surfaces.

In collaboration with *Centre for Materials Science, University College London, UK,* we performed kMC simulations based on the first principles calculations of the energy parameters. Pattern formation, simulated for submonolayer metal coverage, is characterized in terms of the joint correlation functions for a spatial distribution of adsorbed atoms. A wide range of situations, ranging from the almost irreversible to strongly reversible regimes, is simulated. We demonstrate that the metallic patterns obtained are defined by a key dimensionless parameter: the ration of the mutual attraction energy between metal atoms to the substrate temperature. Our *ab initio* calculations for the nearest Ag-Ag adsorbate atom interaction on an MgO substrate give an attraction energy as large as 1.6 eV, close to that in a free molecule. This is in contrast to the small Ag adhesion and migration energies (0.23 eV and 0.05 eV, respectively) on a defect-free MgO substrate.

## STORAGE PHOSPHOR AND IMAGE PLATE DEVELOPMENT FOR NEUTRON IMAGING

**A.I. Popov** *(ISSP),*
**D.A.A. Myles and F. Dauvergne** (EMBL, Grenoble, France),
**C. Wilkinson** (*King's College London, UK*)

Storage phosphor imaging plate (IP) are widely used as two-dimensional integrating position-sensitive detector based on the effect of photo-stimulated luminescence (PSL). By admixture of $Gd_2O_3$ the storage phosphor can be sensitized to thermal neutrons utilizing the extremely high absorption cross section of gadolinium in this energy range. In collaboration with *European Molecular Biology Laboratory, Grenoblé, France,* and *King's College London, UK,* we have studied neutron sensitive image plates in combination with a suitable scanning system, which exhibit excellent characteristics. We have performed comparative measurements PSL recorded using a Molecular Dynamics 'Storm' scanner (635 nm) after neutron irradiation of a number of new combinations of converter/storage phosphors. Measurements have been made for a number of advanced materials, in order to characterize the intrinsic fading of the PSL signal with time after neutron irradiation. The X-ray sensitivity and fading of several of these compounds have also been measured.

We have prepared image plates by layering $Eu^{2+}$ doped BaSrFBr phosphor alternately with $Gd_2O_3$ converter. Prototype image plates have been constructed and tested using a spraying technique for the phosphor/converter. The method has the potential to produce large image plates with good uniformity.

Use of optical spectroscopy for the characterization of radiation defect aggregation in oxide materials.

## Scientific publications

### Published in 2003

1. *NATO Science Series III: Computer and Systems Sciences*, Vol. 187: "Computational Materials Science"; Eds. C.R.A. Catlow and E.A. Kotomin, IOS Press, Amsterdam, *etc.*, 2003 (E.A. Kotomin, R.I. Eglitis, G. Borstel, and P.W.M. Jacobs, Modelling of point defects, polarons and exitons in ferroelectric perovskites, p. 291-307).
2. R.A. Evarestov, S. Piskunov, E.A. Kotomin, and G. Borstel, Single impurities in insulators: *ab initio* study of Fe-doped $SrTiO_3$. – *Physical Review B*, 2003, **67**, 064101 (p. 1-9).
3. B. Herschend, K. Hermansson, M. Alfredsson, Yu.F. Zhukovskii, E.A. Kotomin, and P.W.M. Jacobs, Characterization of the metal-ceramic bonding in the Ag/MgO(100) interface from *ab initio* calculations. – *Journal of Physical Chemistry B*, 2003, **107**, 11893-11899.
4. Yu.F. Zhukovskii, P.W.M. Jacobs, and M. Causá, On the mechanism of the interaction between oxygen and close-packed single-crystal aluminum surfaces. – *Journal of Physics and Chemistry of Solids*, 2003, **64**, p. 1317-1331.
5. G. Borstel, R.I. Eglitis, E.A. Kotomin, and E. Heifets, Modelling of defects and surfaces in perovskite ferroelectrics. – *Physica Status Solidi (b)*, 2003, **236**, p. 253-264.
6. E.A. Kotomin, V.N. Kuzovkov, G. Zvejnieks, Yu.F. Zhukovskii, D. Fuks, S. Dorfman, and A.M. Stoneham, The kinetic MC modelling of reversible pattern formation in initial stages of thin metallic film growth on crystalline substrates. – *Solid State Communications*, 2003, **125**, p. 463-467. V
7. R.I. Eglitis, V.A. Trepakov, S.E. Kapphan, and G. Borstel, Quantum chemical modelling of "green" luminescence in self activated perovskite-type oxides. – *Solid State Communications*, 2003, **126**, p. 301-304.
8. R.A. Evarestov, E.A. Kotomin, E. Heifets, J. Maier, and G. Borstel, *Ab initio* Hartree-Fock calculations of $LaMnO_3$(110) surfaces. – *Solid State Communications*, 2003, **127**, p. 367-371.
9. E.A. Kotomin, E. Heifets, J. Maier, and W.A. Goddard III, Atomistic simulations of the $LaMnO_3$(110) polar surface. – *Physical Chemistry and Chemical Physics*, 2003, **5**, p. 4180-4184.
10. A. Gunhold, L. Beuermann, K. Gömann, G. Borchardt, V. Kempter, W. Maus-Friedrichs, S. Piskunov, E.A. Kotomin, and S. Dorfman, Study of the electronic and atomic structure of thermally treated $SrTiO_3$(110) surfaces. – *Surface and Interface Analysis*, 2003, **35**, p. 998–1003.
11. R.I. Eglitis, E.A. Kotomin, G. Borstel, S.E. Kapphan, and V.S. Vikhnin, Semi-empirical calculations of the electronic and atomic structure of polarons and excitons in $ABO_3$ perovskite crystals. – *Computational Materials Science*, 2003, **27**, p. 81-86.
12. E.A. Kotomin and Yu.F. Zhukovskii, *Ab initio* modelling of metal adhesion to ceramics. – *Defect and Diffusion Forum*, 2003, **218-220**, p. 67-78.
13. V.S. Vikhnin, S.E. Kapphan, I.L. Kislova, R.I. Eglitis, and P.A. Markovin, Manifestation of polaronic states in ferroelectric relaxor PMN. – *Ferroelectrics*, 2003, **285**, p. 291-302.
14. E.A. Kotomin, J. Maier, Yu.F. Zhukovskii, D. Fuks, and S. Dorfman, *Ab initio* modelling of silver adhesion on the corundum (0001) surface – *Materials Science and Engineering C*, 2003, **23**, p. 247-252.

15. R.I. Eglitis, E. Heifets, E.A. Kotomin, J. Maier, and G. Borstel, First-principles calculations of perovskite thin films. – *Materials Science and Semiconductor Processing*, 2003, **72**, p. 129-134.
16. R.I. Eglitis, D. Fuks, S. Dorfman, E.A. Kotomin, and G. Borstel, Large-scale modelling of the phase transitions in $KTa_{1-x}Nb_xO_3$ perovskite solid solutions. – *Materials Science and Semiconductor Processing*, 2003, **72**, p. 153-157.
17. O. Entin-Wohlman, A. Aharony, and V. Kashcheyevs, Quantized adiabatic quantum pumping due to interference. – *Journal of Physical Society of Japan*, 2003, **72A**, p. 77-82.
18. O. Entin-Wohlman, A. Aharony, and V. Kashcheyevs, Adiabatic quantum pumping of coherent electrons. – *Turkish Journal of Physics*, 2003, **27**, p. 371-381.
19. R.I. Eglitis, E.A. Kotomin, G. Borstel, and V.S. Vikhnin. Quantum chemical modeling of electron and hole polarons in $ABO_3$ perovskites. – *AIP Conference Proceedings*, Vol. 677: "Fundamental Physics of Ferroelectrics", 2003, p. 205-209.
20. E. Heifets, R.I. Eglitis, E.A. Kotomin, W.A. Goddard III, and G. Borstel, Calculations of perovskite polar surface structures. – *AIP Conference Proceedings*, Vol. 677: "Fundamental Physics of Ferroelectrics", 2003, p. 210-219.
21. R. I. Eglitis, D. Fuks, S. Dorfman, E. A. Kotomin, G. Borstel, and V.A. Trepakov, Large-scale quantum chemical modeling of the phase transitions in KNT solid solutons. – *AIP Conference Proceedings*, Vol. 677: "Fundamental Physics of Ferroelectrics", 2003, p. 231-241.
22. Yu.F. Zhukovskii, E.A. Kotomin, and P.W.M. Jacobs, Large scale computer simulations of metal-oxide interfaces with defects. – *SPIE Proceedings*, Vol. 5122: "Advanced optical materials and devices", 2003, p. 104-111.
23. G. Borstel, R.I. Eglitis, and E.A. Kotomin, Computer modelling of point defects, polarons and excitons in perovskite ferroelectrics. – *SPIE Proceedings*, Vol. 5122: "Advanced optical materials and devices", 2003, p. 258-268.
24. S. Piskunov, R.A. Evarestov, R.I. Eglitis, E.A. Kotomin, and G. Borstel, Large scale first-principles calculations of Fe-doped $SrTiO_3$. – *SPIE Proceedings*, Vol. 5122: "Advanced optical materials and devices", 2003, p. 276-284.
25. Yu.F. Zhukovskii, A. Kovalevska, P.W.M. Jacobs, and Yu.N. Shunin, DFT simulations on a regular O/Al(001) interface. – *Computer Modelling and New Technologies*, 2003, **7**(1), p. 7-17.
26. P.W.M. Jacobs, Yu.F.Zhukovskii, A. Kovalevska, and Yu.N. Shunin, DFT simulations of the interaction between oxygen and a stepped Al(111) substrate. – *Computer Modelling and New Technologies*, 2003, **7**(1), p. 18-23.
27. S. Piskunov, E. Heifets, E.A. Kotomin, and Yu.N. Shunin, B3PW and B3LYP exchange-correlation techniques in CRYSTAL computer code: the case of $ABO_3$ perovskites. – *Proceedings of 1st International Conference:* "Information Technologies and Management", Riga, 2003, p. 70-81
28. O. Sychev, G. Borstel, Yu.F. Zhukovskii, E.A. Kotomin, and Yu.N. Shunin, DFT simulations of the Cu/MgO(001) interface. – *Proceedings of 1st International Conference:* "Information Technologies and Management", Riga, 2003, p. 82-94.
29. Yu. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, and Yu.N. Shunin, Hartree-Fock simulation on the AgCl(111)/*a*-$Al_2O_3$(0001) interface – *Proceedings of 1st International Conference:* "Information Technologies and Management", Riga, 2003, p. 95-98.
30. Yu.N. Shunin, K. Budilov, Yu.F. Zhukovskii, O. Sychev, and G. Borstel, Electronic and elastic properties of Cu-interconnects. – *Proceedings of 1st International Conference:* "Information Technologies and Management", Riga, 2003, p. 99-110.

31. A. Kovalevska, Yu.F. Zhukovskii, P.W.M. Jacobs, and Yu.N. Shunin, On the mechanism of interaction between oxygen and regular Al(111) surface. – *Proceedings of 1st International Conference:* "Information Technologies and Management", Riga, 2003, p. 111-122.

**Popular Science Articles**

1. J.R. Kalnin, Knowledge acquisition in the information age. – *Proceedings of 1st International Conference:* "Information Technologies and Management", Riga, 2003, p. 59-63.

## Presentations at Conferences

**I. International Workshop "Fundamental Physics of Ferroelectrics" (Williamsburg, VA, USA, February 2003)**

1. R.I. Eglitis, E.A. Kotomin, G. Borstel, and V.S. Vikhnin, "Quantum chemical modeling of electron and hole polarons in $ABO_3$ perovskites". Abstracts: p. 32.
2. R.I. Eglitis, D. Fuks, S. Dorfman, E.A. Kotomin, G. Borstel, and V.A. Trepakov. "Large-scale quantum chemical modeling of the phase transitions in KNT solid solutions". Abstracts: p. 33.
3. E. Heifets, R.I. Eglitis, E.A. Kotomin, W.A. Goddard III, and G. Borstel, "Calculations of perovskite polar surface structures". Abstracts: p. 43.

**II. 19th ISSP Conference dedicated to 25th anniversary of the Institute of Solid State Physics (Riga, Latvia, February, 2003)**

4. G. Zvejnieks and V.N. Kuzovkov, "Analysis of ELMs dynamics". Abstracts: p. 25.
5. Yu.F. Zhukovskii, Yu. Mastrikov, and E.A. Kotomin, "*Ab initio* simulations on AgCl(111) surface and AgCl(111)/$\alpha$-$Al_2O_3$(0001) interface". Abstracts: p. 40.
6. G. Zvejnieks, V.N. Kuzovkov, and E.A. Kotomin, "Modeling of pattern formation in thin metallic film growth on crystalline substrates". Abstracts: p. 58.

**III. 1st International Conference "Information Technologies and Management", IT&M'03 (Riga, Latvia, April, 2003)**

7. S. Piskunov, E. Heifets, E.A. Kotomin, and Yu.N. Shunin, "B3PW and B3LYP exchange-correlation techniques in CRYSTAL computer code: the case of $ABO_3$ perovskites". Abstracts: p. 10-11.
8. O. Sychev, G. Borstel, Yu.F. Zhukovskii, E.A. Kotomin, and Yu.N. Shunin, "DFT simulations of the Cu/MgO(001) interface". Abstracts: p. 12-13.
9. Yu. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, and Yu.N. Shunin, "Hartree-Fock simulation on the AgCl(111)/*a*-$Al_2O_3$(0001) interface". Abstracts: p. 14-15.
10. Yu.N. Shunin, K. Budilov, Yu.F. Zhukovskii, O. Sychev, and G. Borstel, "Electronic and elastic properties of Cu-interconnects". Abstracts: p. 18-19.
11. A. Kovalevska, Yu.F. Zhukovskii, P.W.M. Jacobs, and Yu.N. Shunin, "On the mechanism of interaction between oxygen and regular Al(111) surface". Abstracts: p. 23-24.
12. J.R. Kalnin, "Knowledge acquisition in the information age". Abstracts: p. 48.

**IV. Spring European Materials Research Society (E-MRS) Meeting (Strasbourg, France, June, 2003)**

13. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, S. Dorfman, A.M. Stoneham, O. Sychev, and G. Borstel, "First principles simulations of 2D Cu supperlattices on the MgO(001) surface". Abstracts: p. F13.
14. E. Heifets, R.A. Evarestov, E.A. Kotomin, S. Dorfman, and J. Maier, "Atomistic modelling of polar $LaMnO_3$ surfaces". Abstracts: p. N20.

**V. International Scientific School "Quantum computation at the atomic scale" (Istanbul, Turkey, June, 2003)**

15. O. Entin-Wohlman, A. Aharony, and V. Kashcheyevs, "Adiabatic quantum pumping of coherent electrons". Abstracts: p. 33.
16. V. Kashcheyevs, "Single-electron transport by surface acoustic waves". Abstracts: p. 34.

**VI. 10th European Meeting on Ferroelectricity, EFM-03 (Cambridge, UK, August, 2003)**

17. R.I. Eglitis, E. Heifets, E.A. Kotomin, J. Maier, and G. Borstel, "*Ab initio* modelling of the atomic and electronic structure of $SrTiO_3$ polar (110) surface". Abstracts: p. 120.
18. R.I. Eglitis, E.A. Kotomin, G. Borstel, D. Fuks, S. Dorfman, and V.A. Trepakov, "Quantum chemical modeling of the atomic and electronic structure of $KNbO_3$, $KTaO_3$, $KNb_xTa_{1-x}O_3$, $BaTiO_3$, and $PbTiO_3$". Abstracts: p. 121.
19. R.I. Eglitis, G. Borstel, V.A. Trepakov, and S.E. Kapphan, "Computer modeling of interacting Li impurities in $KTaO_3$ and $K_{1-x}Li_xTa_{1-y}NbyO_3$ solid solutions". Abstracts: p. 121.
20. V.S. Vikhnin, S.E. Kapphan, R. Blinc, R. Pirc, R.I. Eglitis, and A.S. Sigov, "Polarons, bi-polarons, and bi-polaronic excitons in ferroelectric relaxors". Abstracts: p. 347.

**VII. International Workshop on Computational Physics dedicated to the memory of Stanislav Merkuriev (St. Petersburg, Russia, August, 2003)**

21. E.A. Kotomin, J. Maier, and E. Heifets, "Hartree-Fock calculations of the surface structure for $ABO_3$ perovskites". Abstracts: p. 20.
22. G. Borstel, R.I. Eglitis, and E.A. Kotomin, "Computer modeling of point defects in $ABO_3$ perovskites". Abstracts: p. 27.

**VIII. 9th European Conference on Solid State Chemistry, ECSSC-9 (Stuttgart, Germany, September, 2003)**

23. E.A. Kotomin, J. Maier, E. Heifets, and R.I. Eglitis. "First principles calculations of the surface structure for $ABO_3$ perovskites". Abstracts: p. P046.
24. R. Merkle, J. Maier, E.A. Kotomin, and J. Purans. "Joint theoretical and experimental studies of polycrystalline $SrTiO_3$". Abstracts: p. P047.

**IX. 22nd European Conference on Surface Science, ECOSS'22 (Prague, Czech Republic, September, 2003)**

25. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, and S. Dorfman, "First principles simulations of the regular Cu/MgO(001) interface". Abstracts: 17104 (p. 1-2).

26. E.A. Kotomin, E. Heifets, S. Dorfman, A. Gordon, and D. Fuks, "Atomistic calculations of perovskite polar surface structures". Abstracts: 17446 (p. 1-2).

**X. International Workshop on Surface Physics, IWSP'03 (Polanica Zdrój, Poland, September, 2003)**

27. Yu.F. Zhukovskii, E.A. Kotomin, and G. Borstel, "Comparative analysis of copper and silver adhesion on the MgO substrate". Abstracts: p. 64.

**XI. Fall European Materials Research Society (E-MRS) Meeting (Warsaw, Poland, September, 2003)**

28. O. Sychev, Yu.F. Zhukovskii, E.A. Kotomin, and G. Borstel, "*Ab initio* calculations of copper nanostructures on MgO substrate". Abstracts: p. 204-205.

**XII. International Meeting on Applied Physics, APHYS-2003 (Badajos, Spain, October, 2003)**

29. S. Piskunov, G. Borstel, S. Dorfman, E.A. Kotomin, and D. Fuks, "Quantum chemical calculations of $BaSrTiO_3$ solid solutions". Abstracts: p. 12.
30. E. Heifets, R.A. Evarestov, E.A. Kotomin, S. Dorfman, and J. Felsteiner, "Surface relaxation and rumpling of the (110) oxygen-terminated surface of $LaMnO_3$". Abstracts: p. 35.

**XIII. IEEE International Integrated Reliability Workshop (Stanford, CA, USA, October, 2003)**

31. Yu.N. Shunin, K. Budilov, Yu.F. Zhukovskii, O. Sychev, and G. Borstel, "Calculations of electronic and elastic properties of Cu-interconnects". Abstracts: p. P7.

**XIV. 85$^{th}$ Bunsen Colloquium "Atomic Transport in Solids: Theory and Experiments (Gießen, Germany, October, 2003)**

32. E.A. Kotomin, J.R. Kalnin, and J. Maier, "The effective diffusion coefficient for inhomogeneous media". Abstracts: p. 25.

**XV. 2$^{nd}$ International Conference on Materials for Advanced Technologies, ICMAT'03 (Singapore, December, 2003)**

33. R.I. Eglitis and G. Borstel, "Towards practical 5 V re-chargeable Li ion battery". Abstracts: p. 149.
34. R.I. Eglitis E. Heifets, E.A. Kotomin, J. Maier, and G. Borstel, "*Ab initio* calculations for $SrTiO_3$ perovskite thin films with different termination". Abstracts: p. 155.
35. R.I. Eglitis, E.A. Kotomin, D. Fuks, S. Dorfman, and G. Borstel, "Modeling of the phase transitions in $KTa_{1-x}Nb_xO_3$ perovskite solid solutions". Abstracts: p. 240.
36. R.I. Eglitis, E.A. Kotomin, and G. Borstel, "Computer modeling of point defects in $ABO_3$ perovskites and MgO". Abstracts: p. 495.
37. R.I. Eglitis, M.R. Philpott, and S.V. Izvekov, Large-scale computer modeling of corrosion". Abstracts: p. 504.
38. R.I. Eglitis and G. Borstel, Modeling of Li impurities in $KTaO_3$ and $K_{1-x}Li_xTa_{1-x}Nb_xO_3$ perovskite solid solutions". Abstracts: p. 636.
39. R.I. Eglitis and G. Borstel, "*Ab initio* calculations of Ni clustered aggregates on graphite surfaces". Abstracts: p. 636.

**Doctor Thesis**

1. S. Piskunov, "***Electronic structure of perfect and defective perovskite crystals by means of ab initio hybrid functional theory***". Defended at the University of Osnabrück, Germany, on December 16, 2003. Supervisor: Prof. Dr. G. Borstel (UOs).

# 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 and electron beam lithography have been performed. Photoinduced changes of optical properties, holographic recording and hologram self-enhancement effects, and relaxation processes in amorphous films were studied. The main task was R&D of high sensitive photoresists in the visible region for holography and electron-beam resists for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed. R&D of Bragg grating structures for optical communication DWDM systems in planar waveguides based on amorphous chalcogenide semiconductor thin films were performed. The methods for fabrication of subwavelength-gratings with nanometer scale surface-relief features were developed.

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**Scientific visits abroad**

1. Dr. K.Jefimovs, University of Joensuu, Finland (12 months).
2. Dr. P.Stradins, National Renewable Energy Laboratory, Colorado, USA (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).

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7. Institute of Optics of the Technical University Berlin (Prof. H. J. Eichler ).

# Main Results

## OPTICAL AND HOLOGRAPHIC STUDIES OF AZOBENZENE OLIGOMERS

**A.Ozols and M.Reinfelde**

Third generation of azobenzene oligomer (ABO) layers brought on the glass substrates has been experimentally investigated. The new ABO layers differ from previously studied samples in three ways: 1) azobenzene chromophore groups are modified by adding different acceptors; 2) new spacers including anyline and polydiol groups are used; 3) double –matrix approach was used when azobenzene chromophores with spacers were doped in another polymer matrix. The samples were prepared by V.Kokars at Riga Technical University.

In contrast to the first and second generation samples, the third generation ABO layers exhibit photobleaching instead of photodarkening and much stromger photoinduced anisotropy. Vector holographic gratings with the diffraction efficiency up to 0.32% and specific recording energy down to 30 J/($cm^2$%) have been recorded. The corresponding values for scalar holographic gratings were 0.80% and 0.38 J/($cm^2$%).

Mainly the refractive index increase takes place under the influence of He-Ne laser 632.8 nm light irradiation due to *trans-cis* photoisomerisation.

Nonlinear phototransistor effect has been observed for samples with double tolyle-polyvinylpirrolidone host. In this case the transmission of one light beam can be modulated in real time by changing another crossing light beam intensity.

The stability and optical erasure of holographic gratings in the third generation ABO layers is also studied.

## FABRICATION OF SURFACE RELIEF DIFFRACTIVE OPTICAL ELEMENTS AND THEIR APPLICATIONS

**K.Jefimovs**

In this work the fabrication methods of diffractive elements are discussed. The basic concepts of tehniques including electron beam lithography, lift-off, reactive ion etching, sputter etching, and electroplating through a mask are presented and specificē diffractive elements are manufactured employing these methods. Several fabrication methods are developed and their possible application for fabrication of surface relief diffractive elements are discussed. In addition, novel chalcogenide based resist are studied as a recording media for electron beam lithography.

On the basis of the presented methods a large number of diffractive elements were fabricated for different applications. Linear optical properties and second harmonic generation by metal nanoparticle arrays and the effect of their mutual orientation in the array are studied. Optical activity by quasi-planar subwavelegth-period arrays of chiral metal particles is demonstrated. Inductive grid filters, which are capable of rejecting near infrared radiation while transmitting shorter wavelength, are fabricated and

characterized. A method for identification of propagation- invariant Bessel beam′s phase rotation and the order of the Bessel mode by inclining the diffractive element, which produces the Bessel beam, is demonstrated.

## HOLOGRAPHIC RECORDING IN AMORPHOUS CHALCOGENIDE SEMICUNDUCTORS

**M.Reinfelde, J.Teteris**

The holographic recording parameters of amorphous chalcogenide semiconductor (AChS) thin films under optimization depend on hologram type. The possibility to decrease recording energy by self-enhancement effect during recording and wet etching after recording for multilevel hologram recording was studied. Such necessity arises during embossed hologram formation process. The possibility to manage the holographic parameters through the choice of film thickness and recording wavelength was studied.

## HOLOGRAPHIC RECORDING IN AMORPHOUS As-S-Se FILMS

**I.Kuzmina and J.Teteris**

Thin films of amorphous chalcogenide semiconductors (As-S-Se) have been recently studied as promising materials for optical recording. The essential photoinduced changes of optical refractive index ($\Delta n \leq 0.5$ ) enable to perform real time phase recording in these materials. Thin films of AChS can be applied both as a medium for direct phase recording and as photoresists where recording is formed by surface modulation.

The phenomenon of photo-stimulated changes of *wet* etching rate in AChS films was studied. The main functional principles and possibilities of the practical application of amorphous As-S-Se photoresists for the production of the embossed *rainbow* holograms and holographic optical elements are discussed.

The self-enhancement of holograms (an increase of diffraction efficiency after holographic recording) was studied. The changes of diffraction efficiency in amorphous AChS films have been measured as a function of ageing time, initial diffraction efficiency and recording light intensity. The possibility of light- and thermo-induced amplification of diffraction efficiency of holograms after their recording was studied.

## APPLICATION OF AMORPHOUS CHALCOGENIDE SEMICONDUCTORS IN INFORMATION TECHNOLOGY

**J.Teteris**

Thin films of amorphous chalcogenide semiconductors (As-S, As-Se, Ge-S, Ge-Se ) have been recently studied as promising media for optical recording and processing of information. The essential photoinduced changes of optical properties ($\Delta n \leq 0{,}8$ ; $\Delta E_g \leq 0{,}4$ eV) enable to perform real time phase or amplitude recording in thin films of these materials. The photoinduced changes in amorphous chalcogenide semiconductors are due to transformation of the chemical bonds. Therefore these materials possess extremely high resolution ( $\sim 10^4$ $mm^{-1}$) and they can be successfully used in holography and photolithography. The photoresists with a light sensitivity $\sim 10$ $mJ/cm^2$ for visible spectrum ($\lambda \leq 700$ nm) were produced on the base of these compounds. The main

functional principles and possibilities of the practical use of these photoresists for the production of embossed holograms and holographic optical elements are discussed. The possibility to apply the thin films of amorphous chalcogenide semiconductors as planar waveguides has been shown.

### PHOTOINDUCED PROCESSES IN a-Si:H

**P.Stradins**

In hydrogenated amorphous silicon (a-Si:H) materials we usually observe the various photoconductivity even when the films contain almost the same number of defects. It indicates that ability to capture the photocarrier by the defect is not unique. We have studied the photocarrier capture intothe light induced defects (LIDs) in a-Si:H. The ability of the LID to capture photocarriers would be influenced by microscopic enviroment around it. This microscopic enviroment is determined by several factors, such as hydrogen bonding structure and Si network order. What kind of structure is responsible for the observed photocarrier capture coefficients is the focus of this work. First we studied a-Si:H prepared at various substrate temperatures. Those films were then degraded by the exposure to the nanosecondlaser pulses. After each exposure step, the bandgap photoconductivity, subgap absorption spectra and spin density were measured. We observe a significantly stronger photocarrier capture in the film deposited at 150 $^{o}$C, which is 10 times larger than those of the films deposited at higher temperatures up to 250 $^{o}$C. This indicates that the microscopic structure around the defect, which governs the photocarrier capture ability, is different throughout those films. The film deposited at lower temperatures contains a large amount of hydrogen, whereas the higher temperature deposited films do not. The photocarrier recombination event would have much chance to release the recombination energy to Si-H bond rather than Si-Si bond due to their vibrational energy difference. Therefore, when the Si-H bond is located close to the defect, the ability to capture photocarriers is likely to become larger. We also studied the photocarrier capture coefficient in thea-Si:H films prepared under various hydrogen dilution ratio including the microcrystalline nucleation threshold regime. The a-Si:H network is modified by the change in deposition precursors due to the hydrogen dilution during the preparation, resulting in different microscopic environment around the defects. We also discuss the photocarrier capture coefficient in these films, as they approach the transition region for the nucleation of crystallites.

## Scientific Publications

### Published in 2003

1. J.Teteris and M.Reinfelde, *Holographic recording in amorphous chalcogenide semiconductor thin films*, Journ.Non-Cryst.Sol. **326&327**, pp.494-499, 2003.
2. M.Reinfelde, J.Teteris and I.Kuzmina, *Amorphous As-S-Se films for holographic recording*, Proc.SPIE **5123**, pp.125-132, 2003.
3. J.Teteris, *Holographic recording in amorphous chalcogenide thin films*, Current Opinion in Solid State and Materials Science **7,** pp.127-134, 2003.
4. J.Teteris and M.Reinfelde, *Application of amorphous chalcogenide semiconductor thin films in optical recording technologies*, Journ.Optoelectronics and Advanced Materials **5,** pp.1355-1360, 2003.

5. J.Teteris, *Holographic recording in amorphous chalcogenide semiconductor thin films*, Proc.SPIE **5123**, pp.107-116, 2003.
6. J.Teteris, *Holographic recording in amorphous chalcogenide thin films,* in book: Contributions to non-crystalline semiconductor physics and to optoelectronics, Ed. by M.Iovu, Chisinau, Moldova, 2003, pp.202-212.
7. I.Kuzmina, J.Teteris and M.Reinfelde, *Relief holographic recording in amorphous As-S-Se*, Proc.SPIE **5123**, pp.139-143, 2003.
8. T.Vallius, K.Jefimovs, J.Turunen, P.Vahimaa and Yu.Svirko, *Optical activity in subwavelength-period arrays of chiral metallic particles*, Appl.Phys Lett*.,* 83, pp.234-236, 2003.
9. A.Ozols, Ģ.Ivanovs and S.Lazarevs. *Impulse holograms in amorphous semiconductor films.* Scientific Proc. of Riga Technical University, 2003.Series 7.Telecommunications and Electronics, 2002, vol.2, pp. 63 – 67.
10. A.Ozols, V.Kampars, M.Reinfelde and V.Kokars. *Hologram recording in azobenzene oligomers,* Proc.SPIE, **5123**, pp.102 – 109, 2003.
11. A.Ozols, M.Reinfelde. *Theoretical and experimental studies of light diffraction anisotropy by holograms in a-As-S-Se films.* Proc.SPIE, **5123**, pp.136 – 141, 2003.
12. V.Kampars, V.Kokars, A.Ozols and M.Reinfelde. *Azobenzene polymer films for holographic recording in the red spectral region.* Proc. of Baltic Polymer Symp., 2003, Jurmala, September 17 – 19, pp. 264 – 268.

**In Press**

*1.* A.Ozols and M.Reinfelde, *Polarization holograms and diffraction anisotropy in amorphous chalcogenides*, Journal of Optics A: Pure and Applied Optics*.*
*2.* K.Jefimovs, T.Vallius, V. Kettunen, M.Kuittinen, J.Turunen, and P.Vahimaa, *Inductive grid filters for rejection of infrared radiation,* J. Modern Optics.
*3.* S.N. Khonina, R.V. Skidanov, V.V. Kotlyar, K. Jefimovs, and J. Turunen, *Phase diffractive filter to analyze an output step-index fiber beam,* Proc. SPIE.
4. S.N. Khonina, V.V. Kotlyar, V.A. Soifer, K. Jefimovs, and J. Turunen, *Generation and selection of laser berams represented by a superposition of two angular harmonics ,* J. Modern Optics.
5. S.N.Khonina, V.V.Kotlyar, V.A.Soifer, K.Jefimovs, P.Paakkonen and J.Turunen, *Astigmatic Bessel Laser Beams,* J. Modern Optics.
6. J. Teteris, *Recording of subwavelength-period gratings in amorphous chalcogenide thin films.* Journal of Optics A: Pure and Applied Optics*.*
7. Mara Reinfelde, Janis Teteris and Ilona Kuzmina, *Amorpohous chalcogenide thin films as a media for holographic recording.* Proc.SPIE.

## Lectures on Conferences

**19th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, February 10-13, 2003.**

8. A.Ozols, M.Reinfelde*. Angular selectivity of thin holograms.*Abstracts, p.3.
9. J.Teteris. *Application of amorphous chalcogenide semiconductors in information technology.* Abstracts, p.4.
10. M.Reinfelde, J.Teteris. *Optimization of holographic recording in amorphous chalcogenide semiconductors* . Abstracts, p.5.
11. I.Kuzmina, J.Teteris. *Holographic recording in amorphous As-S-Se films.* Abstracts, p.6.

**International Conference NORTHERN OPTICS 2003**, 16-18 June 2003, Espoo, Finland.

12. J.Teteris. *Subwavelength-period gratings in amorphous chalcogenide semiconductors.* Abstracts, p.101.
13. K. Jefimovs, T. Vallius, P. Vahimaa, J. Turunen, and Yu. Svirko, *Optical activity of chiral nanogratings.* Abstracts, p.62.

**International Conference ICO TOPICAL MEETING ON POLARIZATION OPTICS, June 30 – July 3, 2003, Polvijärvi, Finland.**

14. J. Teteris, *Recording of subwavelength-period gratings in amorphous chalcogenide thin films.* Abstracts, p.186.
15. A.Ozols and M.Reinfelde, *Polarization holograms and diffraction anisotropy in amorphous chalcogenides.* Abstracts, p.52.
16. T. Vallius, Yu. P. Svirko, P. Vahimaa, K. Jefimovs, and J. Turunen, *Polarization control by arrays of chiral metallic nanoparticles.* Abstracts, p.196.

**The 20th Nordic Semiconductor Meeting, August 25-27, 2003, Tampere, Finland.**

17. Janis Teteris and Mara Reinfelde, *Subwavelength-period gratings in amorphous chalcogenide semiconductors.* Abstracts, p.29.

**International Conference on DIFFRACTIVE OPTICS 2003, Oxford, 17-20 September 2003.**

18. J. Teteris, *Subwavelength-period gratings in amorphous chalcogenide thin films.* Abstracts, p.13.

**The 44th Scientific Conference of Riga Technical University, Riga, Latvia, October 10-14, 2003.**

19. J.Porins, A.Ozols, J.Eimuss, G.Ivanovs. *Nonlinear optical losses in telecommunication fibers.* Conf. Papers. Section for Electronics and Telecommunications, pp. 24 – 26 (poster presentation).
20. A.Ozols, M.Reinfelde. *Anisotropy of light diffraction by holographic gratings in a-As-S-Se films* (poster presentation).

**International Conference on Systems of Optical Security, 11 – 12 December 2003, Warsaw, Poland.**

21. Mara Reinfelde, Janis Teteris and Ilona Kuzmina, *Amorpohous chalcogenide thin films as a media for holographic recording.* Abstracts.

**Master Thesis**

I.Kuzmina *Holographic recording in amorphous As-S-Se thin films*, 2003.

**Dh.D. Thesis**

K.Jefimovs *Fabrication of surface relief diffractive optical elements and their applications*. 2003.

# DEFECT PHYSICS IN IONIC MATERIALS

Head of Division Dr. habil. phys., Assoc. prof. B. Berzina

## Research Area and Main Problems

During the last decades a special interest from the physicists working at different world laboratories is focused on wide band gap materials which properties are promising not only for revealing the material nature related to fundamental physics, but also for high-power, high-temperature semiconductor device development. In the same time a special interest is paid to a change of material properties when reducing the size from macro crystalline to nanoscale and for this reason the wide band gap materials are appropriate. The present research is carried out on AlN, cBN and diamonds, which belong to the wide band gap material group and could be manufactured either with macrocrystalline size or as nanomaterials. AlN ceramics and nanomaterials, cBN ceramics as well as natural and synthetic diamonds are used for investigations.

The properties of each material in a large extent depend on various defects forming their energy levels inside the bad gap. Therefore, the optical methods based on luminescence are useful for defect investigation. The experimental methods used include research of UV light induced photoluminescence, its excitation spectra, characteristics of optically stimulated luminescence and thermally stimulated luminescence using samples previously irradiated with UV light or X-rays.

The results obtained allow determine some defect groups responsible for light-induced processes occurring in the material as well as to reveal these processes ending with luminescence or energy accumulation in the material. The last is important for evaluation of the usefulness of every material for dosimetry or detection of UV light or ionising radiation.

| **Scientific Staff** | **Ph. D. Students** | **Students** |
|---|---|---|
| 1. Dr. hab., Assoc. prof. B.Berzina | 1. J.Sils | 1. R.Krutohvostov. |
| 2. Dr. L.Trinkler | | 2. I.Megnis |
| | | 3. A.Auzina |

**Visitors from abroad**

1. Dr. M.Benabdesselam. University of Nice-Sophia Antipolis, Nice, France (1 weak).

**Scientific Visits Abroad**

**1.** J.Sils. Ludvigs Maximillian University Munich, Germany (10 month).
**2.** L.Trinkler . University of Nice-Sophia Antipolis, Nice, France (2 weaks).
**3.** B.Berzina. University of Nice-Sophia Antipolis, Nice, France (1 weak).

## Cooperation

**Latvia**

Institute of Inorganic Chemistry, Riga TU (Dr. E.Palcevskis)
Baltic Scientific Instruments BSI, Riga (Dr.V.Costilo)

**Denmark**

RISO National Laboratory, Roskilde (Dr. A.Botter-Jensen)

**Germany**

Ludvigs Maximillian University, Munich (Prof. M. Reichling)

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

**Japan**
Naruto University of Education, Department of Physics (Prof. K.Atobe)

**USA**
Wake Forest University, Winston-Salem (Prof. R.Williams)

## Main Results

### SPECTRAL CHARACTERISTICS OF cBN CERAMICS

**B. Berzina, L.Trinkler, R.Krutohvostov, I.Megnis, J.Sils**

cBN ceramics, which does not contain a binder and is manufactured in Sumitomo Electric Co., Japan was investigated.

The spectral characteristics of cBN under continuous wave ultraviolet (UV) light irradiation are studied. The photoluminescence (PL) spectra, its excitation spectra, as well as optically stimulated luminescence (OSL) characteristics and thermoluminescence (TL) were investigated. PL forms a wide band peaking at 500 nm at room temperature. Besides the main green band at 500 nm, two more weak luminescence bands located in the UV-blue (~380 nm) and red (~600 nm) spectral regions can be also selected. Excitation spectra characterizing all three luminescence bands are differing. A recombination character of luminescence is shown in our previous investigations. Coexistence of three different luminescence bands allows consideration that there is at least three various types of defect pairs participating in the luminescence formation. Unfortunately, at present we could not reveal the defect structure responsible for the luminescence observed. Solely we can consider that the red PL is caused by the defect aggregation because its intensity increases after providing some procedures stimulating this process.

### SOME OPTICAL PROPERTIES OF NATURAL AND SYNTHETIC DIAMONDS

**L.Trinkler, B.Berzina, R.Krutohvostov, A.Auzina**

Two types of diamonds are used. One of them is natural diamonds from Yakutia collection in a form of ~1 mm thick plates and the other ones are synthetic CVD diamond in a form of thin layer.

In the case of natural diamond photoluminescence (PL) spectrum as well as optically stimulated luminescence (OSL) spectrum consists of well-known blue (450 nm) and green (510 nm) bands related to luminescence centres containing two differing types of nitrogen-related defects. Excitation spectra are similar for both two PL bands. They form a weak broad band at ~280 nm (240-360 nm region), but the main and more intensive excitation band is situated close to the fundamental absorption region at its long wavelength side. As a very important fact the fine structure of this excitation band is observed. We are attributed this band to the bound excitons which transfer their excitation energy to the defects responsible for typical the blue and green luminescence. From the OSL and TL measurements it follows that the UV light energy accumulation in

the material is caused mainly by a direct defect excitation within the spectral region of 240-360 nm, whereas the role of bond excitons in this case seems to be miserable. There are different defect types participating in the energy accumulation and OSL formation. Stimulation spectrum of OSL consists of several bands located in a wide spectral range from 500 nm up to 1600 nm. At the low temperature region the TL curve shows two main peaks at 65 K and 175 K. At the high temperature region the predominant is TL peak at 585 K.

In the case of the synthetic CVD diamond the PL forms one 430 nm band but OSL and TL spectra form a wide 500 nm band. The excitation spectra of PL, OSL and TL are approximately close to those observed for natural diamond.

Some dosemetric characteristics of natural and synthetic diamonds were measured and examined.

### SPECTRAL CHARACTERISTICS OF AlN NANOSTRUCTURES

**L.Trinkler, B.Berzina**

Spectral characteristics of AlN nanotipes made in Taiwan University are investigated and results obtained are compared with those from AlN ceramics. Photoluminescence (PL) of AlN nanotipes under UV light continuous wave irradiation consists of an intensive wide luminescence band at 400 nm and more intensive one at 600-620 nm. This luminescence spectrum practically coincides with those obtained for AlN ceramics investigated in our laboratory during previous years. Excitation of 400 nm PL realizes within the spectral region of 240–260 nm which coincides with the PL excitation for AlN ceramics, newertheles, in a case of AlN nanostructures well pronounced band at 200 nm appears, which can be attributed to the defect bound excitons. Optically stimulated luminescence (OSL) spectra and thermoluminescence (TL) of nanotipes previously irradiated with UV light are also investigated.

The results obtained allow us conclude that in the AlN nanotipes like in the AlN ceramic macromaterial the oxygen-related defects are presented being responsible for the luminescence processes as well as for light energy accumulation in the material which could be released either optically via OSL or thermally as TL.

## Scientific Publications

### Published in 2003

**1.** L.Trinkler, B.Berzina, M.Benabdesselam. *Use of AlN ceramics in ultraviolet radiation dosimetry.* Proc. SPIE vol. 5123, "Advanced Optical Devices", 2003, pp. 50-55.

***2.*** *L.Trinkler, B.Berzina, M.Benabdesselam, P. Iacconi, "Wide band gap materials as potential UV radiation dosemeters", to be published in Latvian Journal of Physics and Technical Sciences, N5, 2003.*

### Accepted for publication 2003

**1.** L. Trinkler, B. Berzina, M.Benabdesselam, P.Iacconi, K. Atobe, L. Bøtter-Jensen, "Radiation induced luminescence processes in c-BN" submitted to journal "Radiation measurements".

## Lectures on Conferences

**5th European Conference on Luminescent Detectors and Transformators of ionizing Radiation LUMDETR (Prague, Czech Republic, September 1-5, 2003).**
L.Trinkler, B.Berzina, R.Krutohvostov, M.Benabdesselam, K.Atobe and L.Botter-Jensen.
*Radiation-induced luminescence propertiess in cBN.* Book of Abstracts LUMDETR, pp. 165, 2003;

**14th European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, Nitrides & Silicon Carbide (Salzburg, Austria, September 7-12, 2003).**
L.Trinkler, B.Berzina, R.Krutohvostov, K.Atobe and L.Botter-Jensen. *Luminescence properties of cBN.* Abstract Book, pp.5.7.12.

**19. LU CFI Zinātniskā konference (Scientific Conference in Riga): Rīga. 10.-13. februāris, 2003.**

1. J.Sils, I.Megnis, R.Krutohvostovs, L.Trinklere, M.Reichlings un B.Bērziņa. *Skābekli saturošie defekti $CaF_2$ kristālā*. Referātu tēzes, 65. lpp.
2. R.Krutohvostovs, L.Trinklere, B.Bērziņa. *Dažu nitrīdu spektrālās īpašības.* Referātu tēzes, 66. lpp.

**Lecture (Scientific Seminar, Nice, France, December 5, 2003)**
L.Trinkler. *Luminescent and dosimetric characteristics of some wide band gap materials.*

# LABORATORY OF OPTICAL MATERIALS

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

## 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 (spatial frequency analyse, crosscorrelation of binocular visual stimuli, stereodisparity evaluation);
- 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;
- visual perception of different (conventional, luminous, retroreflective) road signs and marks at dazzling conditions during night driving.

**Scientific Staff**

1. Dr.habil.phys. I.Lacis
2. Dr.habil.phys. M.Ozolinsh
3. Dr. J.Dzenis
4. Dr. V.Grabovskis

**PhD Students**

1. M.Sc. A.Balgalve
2. M.Sc. G. Krūmiņa
3. M.Sc. J. Fridrihsons
4. M.Sc. A. Švede
5. M.Sc. D.Rācene

**Graduate Students**

1. M.Sc. I. Dilāne
2. M.Sc. G.Ikaunieks

Each year around 20 bachelor grade and up to 10 master grade students (mainly optometrists) perform their diploma work in the laboratory. Student research works have been appreciated at the national and international level (in 2003 - *M.Sc.* D.Rācene – ***Valter von Siemens*** *Excellence award,* PhD.stud. G.Krūmiņa – ***SPIE*** *education award*).

**Visitors from abroad**

Prof. S.Villani, Florence University , Italy (4 weeks)

**Scientific visits**
M. Ozolinsh – University of Murcia, Optics Laboratory 9.03.- 13.09.2003.
M.Ozolinsh – Universities of Glasgow, Bradford and Buskerud 10.07.- 20.07.2003.
G.Krumina – Utrecht University 1.11.-31.11.2003.
A.Švede – Universität Dortmund 4.12.-17.12.2003.

**Partners abroad**

| | |
|---|---|
| **Italy** | Florence University , Italy, (Prof. S. Villani)<br>Universita` di Roma "Tor Vergata" (Prof. I. Davoli) |
| **Sweden** | Lund University (Prof. S.Svanberg)<br>Department of Clinical Science of Karolinska Institute (Dr. H. Richter)<br>Chalmers TH, Sweden (Prof. L.Komitov) |
| **Norway** | Buskerud HØgskolan, Institut for optometri (Prof. J.R.Bruenich). |
| **England** | Bradford University (Prof. D.Whittaker)<br>City University (Dr. W.Thomson) |
| **Spain** | Laboratorio de Optica, Universidad de Murcia, Spain (Prof. P. Artal) |
| **Scotland** | Psychology Department, University of Glasgow, Scotland (Dr.D.Simmons) |
| **Germany** | Institut fur Arbeitsphysiologie an der Universität Dortmund |
| **The Netherlands** | Utrecht University (Prof. R. van Ee) |

## Main Results

### STEREO STIMULI CHROMATIC CONTRAST IN AMBLYOPIA

**G.Krumina, G. Ikaunieks, M.Ozolinsh**
*Institute of Solid StatePhysics andDepartment of Optometry and Vision Science, University of Latvia*

**Background:** Subject with anisometropic amblyopia sees contrast difference in blue chromatic stereostimuli. Bigger contrast sees with amblyopic eye, but stimuli are seen unclear with this eye. Subject has good color vision of both eyes.
**Case report**: To compare the visual acuity and contrast vision for the normal eye and amblyopic eye in standard conditions and under chromatic isoluminant conditions and VEP with color stimuli wishing to balance eye neural activities to teach amblyopic patient to depth sense. Experiments were done using standard and isoluminant conditions. Isoluminant tests had many steps with different tasks: visual acuity tests with color and isoluminant elements. Contrast vision patterns were simulated on the PC screen: with achromatic gray, and with the same luminance contrast for chromatic gray-blue patterns. VEP was measured for both eyes using color check board patterns reversal. Blurring conditions (similar as in amblyopia) were induced for the non-amblyopic eye and for another subject with good vision. The visual acuity measurements of thresholds were different for the non-amblyopic eye with different color stimuli, but the amblyopic eye had low acuity practically equal for all stimuli. The VEP amplitudes for the amblyopic eye were greater for the small blue objects of pattern as for green and red color pattern. There was a small unimportant difference between normal achromatic grey and chromatic blue-grey with similar isoluminant contrast tests both for each. Parallel the subject learned to acquire the steresense for different color

stimuli and blur degrees. This process was successful, eventually using blurred stimuli for both eyes demonstrated on the PC screen. Once acquired the subject managed to pass large stereodisparity.

**Conclusions:** With VEP and color visual acuity tests it is possible to reveal differences in color vision perception. The most peculiar for the studied case amblyopic patient was perception of blue stimuli, especially for the amblyopic eye. We show that taking into account peculiarities of the amblyopic patient visual response it is possible to find favorable condition facilitating the formation of their stereosense.

## LIGHT SCATTERING EFFECT ON COLOUR STIMULI VISUAL RESPONSE

**M. Ozolinsh, D. Korenuks, A. Kozachenko*, L. Komitov***

*Institute of Solid StatePhysics andDepartment of Optometry and Vision Science, University of Latvia*

**Gëteborg University, 412 96 Göteborg, Sweden*

We have modelled situation similar to scattering in a cataract eye. An obstacle of Polymer Dispersed Liquid Crystal (PLDC) was placed in front of patients' eyes. Light scattering in such obstacle can be continuously controlled applying the pulsed bipolar voltage up to 30V, thus bringing the obstacle from an opaque light scattering to transparent state.

At first, human visual response tests at distance 3m was performed simulating on the computer screen Landolt C, using quasi-monochromatic stimuli - R, G and B phosphors. Secondly, we carried out the contrast sensitivity tests of same colour Gabor patterns displaying them on the computer screen. Experiments were performed in a darkened room to avoid the influence of background light scattering. At last we determined the flicker fusion frequency as colour stimuli using blue, green and red light emitting diodes.

Light scattering induced by a PLDC cell very efficient lowers the visual acuity for blue Landolt C stimuli. Using one such cell the acuity VS decreased down to 0.6 (decimal), if two cells were used – down to VS<0.4 . The acuity of white stimuli was affected weaker, acuity of monochromatic red Landolt C stimuli practically did not changed as compared with the case of transparent obstacle. The contrast sensitivity however decreased for all R, G and B Gabor stimuli, most for short wavelength and high spatial frequency patterns. Similar experiments for patients with real cataract eyes are in progress, allowing to evaluate ability of such controllable scattering obstacles for simulation of cataract eye visual performance.

## TRAFFIC SIGN RECOGNITION DURING NIGHT DRIVING

**M.Ozolinsh and J. Berzinsh**

*Institute of Solid StatePhysics andDepartment of Optometry and Vision Science, University of Latvia*

Drivers' ability to recognize retroreflective and light emitting red, yellow, and green LED (light emitting diodes) traffic signs were studied when dazzling light luminance was changed in conditions similar to night driving. Various psychophysical and objective procedures were applied to determine the "dead time" when driver lost visual ability. Signs to recognize were illuminated either continuously during the dazzling cycles or they were demonstrated only for a short $t_s = 0.1$ s time either before the maximum intensity of the dazzling illumination or after it. To evaluate retinal illumination, restrictions of the eye pupil area were registered by an infrared CCD

camera. The dead time $t_d$ (subject losses his ability to detect visual stimuli) can reach up to t = 3 s for unfavourable dazzling illumination – corresponding to incorrect dipping of the vehicle beams, and if the driver pupil reaction is artificially or under the influence of alcohol or drugs blockaded. Visually evoked potential (VEP) measured was used as a criterion in conditions when road sign stimuli were intensity modulated in order to detect corresponding frequency in the VEP spectral response.

## CLINICAL INVESTIGATION OF STEREOACUITY FOR PATIENTS HAVING REAL OR INDUCED ANISOMETROPIA AND CATARACT

**Gunta Krumina, Maris Ozolinsh**
*Department of Optometry and Vision Science and Institute of Solid StatePhysics, University of Latvia*

**Purpose:** We investigated stereovision in induced conditions of anisometropia or cataract and compared the data of patients with anisometropic amblyopia and with cataract.
**Methods:** The induced anisometropia was simulated with ophthalmic lenses and the induced cataract was simulated on computer screen. Stereovision was detected using clinical TNO test and established random dot test. We have tested 300 patients of age 13 to 79. In experiment there were detected stereovision in the conditions of crossed and uncrossed disparity. We have simulated blurring (as in cataract) with special program and have tested the 12 subjects' stereo threshold. We have detected the stereoacuity of 135 subjects in the condition of simulated anisometropia.
**Results:** We have observed that blurring effect in one eye in both situations (induced anisometropia and cataract) decreases stereoacuity. The condition of anisometropia decreases stereoacuity more then blurring in both one together. Approximately 40 percent from patients have difference between the stereoacuity of crossed and uncrossed disparity. Stereovision threshold are bigger for younger patients and for older patients with the clear lens of human eye.
**Conclusion:** Stereoacuity depends on visual acuity in one or in both eyes. Difference between visual acuity of the eyes decreases stereoacuity. Induced anisometropic amblyopia and cataract show approximately the same data as in these real eye conditions.

## RELATION BETWEEN FIXATION DISPARITY AND VISUAL FATIGUE

**Aiga Švede, Lolita Krokša, Ilze Dilāne, Jānis Dzenis, Jurijs Daugulis**
*Department of Optometry and Vision Science, University of Latvia*

The purpose of this work is to describe the tendencies of fixation disparity to change after specific kind computer work. At near work, where the visual system is used to collect the newest information, we need quite precise eye movements – vergences to make binocular fusion possible. But during the visual processes there is still a very small amount of residual misalignment of two visual axes known as fixation disparity. Fixation disparity is so small that the image can still be fused binocularly. Normal fixation disparity should be between 6 arc minutes exo or 4 arc minutes eso, but it is quite changeable depending of different factors. If the amount of necessary information is increasing and computers are used more and more, the fatigue of the visual system is increasing. Accordingly fixation disparity can change, too. A near work-produced enlargement of fixation disparity will influence the keeping of normal and comfortable binocular vision. There are analyzed five parameters of fixation disparity curve – type of

the curve, slope, y-intercept (fixation disparity), x-intercept (associated phoria), and center of symmetry. The changes of slope or type of the fixation disparity curve or its drifting dynamics could be explained by astenopies or the fatigue of the visual system depending of the time, how long the visual system is under the stress.

### TREATMENT EFFICIENCY OF ACCOMMODATIVE ESOTROPIA USING BIFOCALS

**A.Svede, I.Kuzmova, Dr. S.Valeine, Dr. I.Valeine, Dr. A.Zorgevica**
*Department of Optometry and Vision Science, University of Latvia*
*Children's Eye Diseases clinic, Children's Clinical Hospital of Riga, Latvia*

Although biforcals are common form of accommodative esotropia treatment for a long period in other countries, they are not so widely used in Latvia. The bifocals are used in Latvia only since middle of 90-ties. The purpose of this work is to analyse the efficiency of bifocals for treatment of accommodative esotropia in Latvia.
There were taken children, who were or still are using bifocals. As the efficiency criteria were they response on this kind of treatment for accommodative esotropia. The follow up period was at least 6 months. To determine the characteristics predicting children response on bifocal correction were analysed binocular functions, deviation with and without bifocals on onset of bifocals and on a last visit, AC/A ratio, refractive error and the prescribed bifocal correction. The results of our study will be presented on a poster during the conference.

## Scientific publications

### Published in 2003

1. M. Ozolinsh, D. Korenuks, A. Kozachenko, L. Komitov "Light scattering effect on colour stimuli visual response." *Perception*, **32**, S178-179 (2003).
2. I.Supe and V.Grabovskis, "Selective filters for improvement of color discrimination." In: "Advanced Optical Materials and Devices", *Proc.SPIE* **5123**, pp.350-353 (2003).

3. A. Svede and J, Dzenis, "Additional usage possibilities for the computerized Hess In: "Advanced Optical Materials and Devices", *Proc.SPIE* **5123**, pp.354-359 (2003).

4. G. Papelba, I. Cipane, and M. Ozolinsh "Stereoacuity studies by disbalanced images" In: "Advanced Optical Materials and Devices", *Proc.SPIE* **5123**, pp.334-340 (2003).

5. G. Papelba, M. Ozolinsh, J. Petrova, and I. Cipane "Stereoacuity determination at changing contrast of colored stereostimuli". In: "Advanced Optical Materials and Devices", *Proc.SPIE* 5123, pp.341-349 (2003).

6. D. Racene, "Computerized device for critical flicker fusion frequency determination," In: "Advanced Optical Materials and Devices", *Proc.SPIE* **5123**, pp.360-365 (2003).

7. G.Krumina, M.Ozolinsh "Clinical investigation of stereoacuity for patients having real or induced anisometropia and cataract," *Optometry and Vis.Scie.,* Vol.**80** (N12s), pp.41. (2003).

### Accepted for publication in 2003

1. M. Ozolinsh and G. Papelba "Eye cataract simulation using polymer dispersed liquid crystal scattering obstacles," *Ferroelectrics* (in print).

# Reports in conferences

**18th Scientific Conference of the Institute of Solid State Physics University of Latvia, Riga, February 11-13, 2002.**

1. D. Koreņuks, M. Ozolinsh, A. Kozachenko un L. Komitov "Electrically controllable scattering in polydispersed liquid crystalls."
2. M. Ozolinsh, G. Papelba, and G. Andersson "Liquid crystal goggles for vision research."
3. L.Krokša, I.Dilāne, A.Švede, J.Dzenis "Relation between fixation disparity and visual fatique."
4. A.Līce, A.Žilēvica, and A.Balgalve "Contactlenses and eye microflora"
5. G.Papelba "The calculation and evaluation of minimal stereoangle."
6. G.Papelba and M.Ozolinsh "The analysing methods of stereo stimuli."

**The 3rd Int. Conf. "Transmission and Processing of Images", St.Petersburg, June 2003.**

V.A.Lyakhovetskii, G.Papelba "Spectral composition description of images for objects in the perception of depth."

**The 10th European Meeting on Ferroelectrics EMF-10, Cambridge, August 2003**

M. Ozolinsh "Electrically Controlled Eye Occluders in Vision Science."

**The 12th European Conference on Eye Movements, Dundy 2003**

A.Švede, L.Krokša, I.Dilāne, J.Dzenis, J.Daugulis. "Relation between fixation disparity and visual fatigue."

**The 26th European Conference on Visual Perception (ECVP), Paris, Sept. 2003**

M. Ozolinsh, D. Korenuks, A. Kozachenko, L. Komitov
"Light scattering effect on colour stimuli visual response."

**Irish-British Orthoptics Conference 2003, Dublin. August 2003**

A.Švede, I.Kuzmova, S.Valeine, I.Valeine, A.Zorgevica. "Treatment efficacy of accommodative esotropia using bifocals."

**The 10th Int. Conf. "Vision in Vehicles" VIV-10, Granada, September 2003**

M.Ozolinsh and J. Berzinsh "Traffic sign recognition during night driving."

**American Academy of Optometrists Dallas-2003, December 2003**

G.Krumina, M.Ozolinsh "Clinical investigation of stereoacuity for patients having real or induced anisometropia and cataract."

# SURFACE PHYSICS

Head of Laboratory Dr.habil.phys. J.Maniks

## Research Area and Main Problems

The basic research area includes surface modifications of novel materials by different treatments (light-, ion- and electron irradiations, air exposure), investigations of micromechanical properties of solid surfaces and thin films, strength properties, adhesion and related processes on phase boundaries and interfaces in heterogeneous and nanostructured materials.

The research during 2003 is focused on following problems:

- photo-, thermo- and atmosphere-induced effects in fullerite $C_{60}$ single crystals and polycrystalline films studied by microindentation, dislocation mobility and AFM methods,
- structural modifications and hardening of ionic crystals under irradiation by MeV-GeV heavy (Au, Pb, Bi) and light (S, Ni) ions, the ion energy loss and fluence effects in the hardening.
- interfacial effects in superplastic alloys.

**Scientific staff**

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

**Technical staff**

4.A.Petersons

**Students**

5. L.Gailīte

**Scientific Visits Abroad**

1. Dr.F.Muktepavela, Crimea, Ukraine (1 week).
2. Dr.F.Muktepavela, Chernogolovka, Russia (1 week).
3. Dr.F.Muktepavela, St.Petersburg, Russia (1 week).
4. Dr.I.Manika, Crimea, Ukraine (1 week).
5. Dr.I.Manika, St.Petersburg, Russia (1 week).
6. Dr.J.Maniks, St.Petersburg, Russia (1 week).

## Cooperation

**Latvia**

1. Institute of Physical Energetics, Latvian Academy of Sciences (Dr.J.Kalnacs).
2. Riga Technical University (Prof.V.Mironovs).

**Germany**

GSI, Darmstadt (Prof.K.Schwartz).

**Ukraine**

Institute of Metal Physics, Ukrainian Academy of Sciences, Kiev (Prof. M.Vasylyev).

**Israel**

Technion, Haifa (Dr.S.Stolyarova).

# Main Results

## PHOTOINDUCED MODIFICATIONS OF STRUCTURE AND MICROHARDNESS OF FULLERITE $C_{60}$

**I.Manika, J.Maniks**

The polymerization of pristine and oxygen-contaminated fullerite $C_{60}$ single crystals (99.9 % $C_{60}$) under light irradiation has been investigated by indentation hardness, dislocation mobility, and AFM methods. It has been found that polymers formed in pristine and oxygenated fullerite exhibit different physical and mechanical properties. The temperature limits of formation and decomposition of polymers, kinetics of polymerization, depth evolution of polymerized phase and effects of air exposure were studied. In case of pristine fullerite, the obtained results can be explained by polymerization *via* well-known [2+2] photoaddition reaction, which leads to formation of fullerene dimers ($C_{120}$), where the $C_{60}$ molecules are connected by the carbon bonds. However, in oxygenated fullerite the formation of $C_{120}O$ dimmers is suggested. In $C_{120}O$ dimmer the $C_{60}$ molecules are connected by an oxygen bridge. In air atmosphere, the $C_{120}O$ photopolymer is formed in the oxygen-contaminated subsurface layer of 0.8- 1 μm. This phase is found to be thermally stable in the range of 290-330 K. Reduction of the intermolecular distance in fullerene dimers creates internal stress in the polymerized layer. Volume distribution of dimers is considered and columnar growth of dimers along close packed directions is supposed to be preferable from the minimum stress energy condition.

*In cooperation with Institute of Physical Energetics, Latvian Academy of Sciences*.

## ENERGY LOSS AND FLUENCE DEPENDENCY OF ION INDUCED HARDENING IN LIF

**J. Maniks, I. Manika**

The change of hardness and structural modifications in LiF irradiated with 600 MeV Ni ions have been investigated. The ion-induced hardening is related mainly to dispersion strengthening of LiF by the defect aggregates (possibly clusters of lithium, fluorine and/or vacancies). The single defects are found to be of minor importance. Marked hardening is caused by aggregation of single defects due to track overlapping. This contribution becomes significant above the threshold fluence of $\Phi_0=2.4\text{x}10^{10}$ ions/cm$^2$. The additional hardening is observed at the certain ion penetration depth where the threshold energy loss of about 6.6keV/nm is surpassed and formation of defect aggregates via track core damage is initiated.

*In cooperation with GSI, Darmstadt, Germany.*

## SEGREGATION OF LEAD ON CLEAN SURFACE OF SUPERPLASTIC Pb-Sn EUTECTIC

**F.Muktepavela, J.Maniks**

The morphology, structure and chemical composition of the real and atomically clean surfaces of Pb-62%Sn superplastic eutectic alloy have been investigated. The deformation was performed by extrusion with strain rates $10^{-1}$ s$^{-1}$ and $10^{-3}$ s$^{-1}$ at room

temperature in air and vacuum. The interphase boundary sliding (IBS) as the main mechanism of deformation was observed for all samples. However, the structural investigations showed that deformation in a vacuum leads to lower porosity of Pb/Sn interphase boundaries than in air. Using surface analytical tools (SEM with X-ray probe), it was found that atomically clean surface of alloy is enriched by lead. The segregation of lead and overlaying of tin phases with lead are thermodynamically gainful because surface energy of Pb is lower than that of Sn and the value of Pb/Sn interface energy is very small. In the case of deformation in air, the formation of a tin oxide is thermodynamically preferable. The influence of Pb segregation and formation of tin oxides on surface porosity and IBS is discussed.

*In cooperation with Institute of Inorganic Chemistry, Technical University of Riga*

## Scientific publications

### Published in 2003


1. J.Maniks, I.Manika, J.Kalnacs. Photo-induced modifications of the structure and microhardness of fullerite $C_{60}$. In: *Hydrogen Materials Science and Chemistry of Carbon nanomaterials* (Ed. D.V.Schur), IHSE, Kiev, 2003, p.630-633.
2. I.Manika, J.Maniks, K.Schwartz, C.Trautmann, M.Toulemonde. Hardening and long-range stress formation in lithium fluoride induced by energetic ions. *Nucl. Instr. and Meth. B*, 2003, vol.209, p.93-97.
3. F.Muktepavela, M.Vasylyev, A.Czervinski, Z.Rogulski. Investigation of hydrogen embrittlement of Sn-Al alloy during contact with water vapour. *J.Solid State Electrochem*, 2003, vol.**7,** No2, p.83-86.
4. F.Muktepavela, J.Maniks. Mechanical properties of deformed interfaces in bimetallic joints. *Solid State Phenomena,* 2003, vol.94, p. 79-82.
5. J.Maniks, I.Manika, K.Schwartz, M.Toulemonde, C.Trautmann. Formation of dislocations and hardening of LiF crystals irradiated with energetic Bi, Pb and S ions. In: *Proc.SPIE Advanced optical materials*, 2003, vol. 5122, p. 15-22.
6. F.Muktepavela, I.Manika, L.Grigorjeva, V.Skvortsova. Micromechanical properties of AIN and AIN/TiN nanostructured.multilayer coatings. *Proc. SPIE Advanced optical materials*, 2003, vol. 5122, p. 439-444.
7. F.Muktepavela, J.Maniks. Interface diffusion controlled sintering of atomically clean surfaces of metals. In:" Diffusion, Segregation and Stresses in Materials (Ed.B.S.Bokstein and B.B.Straumal)", Defect and Diffusion Forum, Scitec Publications Ltd.,Switzerland, 2003, vol.216-217, p.169-174.
8. F.Muktepavela, M.Vasylyev, S.Stolyarova. Structural and kinetic features of hydrogen desorption process on Al/Sn interphase boundaries. In: *Hydrogen Materials Science and Chemistry of Carbon nanomaterials* (Ed. D.V.Schur), IHSE, Kiev, 2003, p.316-319.
9. V.Mironovs, F.Muktepavela. Technology of manufacturing of machine details from iron-copper powder alloys. In: Сборник докладов "Порошковая металлургия – 2003", Тонпик, Минск, 2003, с.119-123.

**Accepted for publication 2003**

1. J.Maniks, I.Manika, J.Kalnacs. Photo-induced polymerization and stress effects in fullerite $C_{60}$. *Fullerenes, Nanotubes and Carbon Nanostructures*.
2. J.Maniks, I.Manika, J.Kalnacs. Photo-induced modifications of the structure and microhardness of fullerite $C_{60}$. *Carbon*.
3. .F. Muktepavela, J. Maniks, N. Zaporina. Diffusion and softening of phase boundaries in superplastically deformed fine-grained eutectics. *Interface Science.*
4. V.Mironovs, F.Muktepavela. Properties of AlB powder obtained by crushing Al-B composite presenting industrial waste. *Powder Metallurgica*.

## Lectures on Conferences

**19th Scientific Conference of Institute of Solid State Physics, University of Latvia, Riga, February 10-13, 2003**

1. L.Gailite, I.Manika, J.Maniks. Modifications of structure and microhardness of LiF crystals irradiated with energetic Ni ions. Abstracts, p.38.
2. F.Muktepavela, J.Maniks, N.Zaporina. Segregation phenomenon on clean surface of superplastic Pb-Sn eutectic. Abstracts, p.39.

**6th Biennial International Workshop "Fullerenes and Atomic Clusters", St.Petersburg, Russia,June 30- July 4, 2003.**

3. J.Maniks, I.Manika, J.Kalnacs. Photo-induced polymerization and stress effects in fullerite $C_{60}$.Abstracts, p.172.

**VIII International Conference "Hydrogen Materials Science and Chemistry of Carbon Nanomaterials (ICHMS'2003)", Crimea, Ukraine, 14-20 September, 2003.**

4. F.Muktepavela, M.Vasylyev, S.Stolyarova. Structural and kinetic features of hydrogen desorption process on Al/Sn interphase boundaries.
5. J.Maniks, I.Manika, J.Kalnacs. Photo-induced modifications of the structure and microhardness of fullerite $C_{60}$.

**5th Int. Workshop on Radiation Imaging Detectors, Riga, Latvia, 7-11 September, 2003.**

6. F.Muktepavela, I.Manika, L.Grigorjeva, V.Skvortsova. Effect of **γ**-radiation on micromechanical properties of AlN thin films. Abstracts,p.85-86.

**12th International Baltic Conference "Engineering Materials and Tribology (BALTMATTRIB-2003), Tallin, Estonia, October 2-3, 2003.**

7. V.Mironovs, F.Muktepavela. Technology of manufacturing of machines details from iron-copper powder alloys. Abstracts, p.9-11.

**Workshop[ on Powder Metallurgy and Protective Coatings, Minsk, Belarus, 25 March, 2003.**

8. V.Mironovs, F.Muktepavela. Technology of manufacturing of machine details from iron-copper powder alloys.

**Interfaces In Advanced Materials, Chernogolovka, Russia, 26-30 May, 2003.**

9. F. Muktepavela, J. Maniks, N. Zaporina. Diffusion and softening of phase boundaries in superplastically deformed fine-grained eutectics.

10. F. Muktepavela, I. Manika, M. Vasylyev. Micromechanical properties and failure of AlN, TiN and AlN/TiN nanostructured multilayer coatings.

**Workshop on Strength Problems, St Petersburg, Russia, 12-14 March, 2003.**

11. F.Muktepavela. Diffusion processes under conditions of grain boundary sliding in superplastic eutectics.

# 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, oxyde 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 radioactive and nuclear materials in Latvia
- introduction the quality assurance for the nuclear spectral measure according to ISO/IEC 17025 standard
- 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
- the use of the physical methods ( MORPHOQUANT, EPR and optical absorption and luminescence) in the biophysics and medical physics
- flux pinning in neutron irradiated 123 high temperature superconductors and its relationship to magnetic anisotropy.

**Scientific Staff**

1. Dr.hab. J.Berzins
2. Dr.hab. M.Balodis
3. Dr.hab. V.Bondarenko
4. Dr.hab. A.Afanasjevs
5. Dr. hab. U.Ulmanis
6. Dr.hab. N.Mironova - Ulmane
7. Dr. hab. J. Tambergs
8. Dr. L.Simonova
9. Dr. T. Krasta
10. Dr. D.Riekstina
11. Dr. V.Skvortsova
12. Dr. O.Veveris
13. Dr. A.Petrovs
14. Dr. J. Ruza
15. Dr. G. Smilskalne
16. Dr A.Kuzmins
17. mag. A.Pavlenko

**Technical Staff**

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

**Students**

1. A. Andrejevs
2. A. Dzalbs
3. I. Motmillere

**Visitors from abroad**

Dr. J. Honzatko Institute of Nuclear Physics, Prague, Czech Republik (7 days).

**Scientific visits abroad**

Dr. hab. A.Afanasjev Argonne Lational Laboratory, USA (5 months).
Dr. hab. A.Afanasjev Notre Dame University, Notre Dame,USA (5 month).
Dr. hab. J. Berzins European Commisssion Euratom, Brussels,Belgium (10 days).
Dr. hab. J. Berzins IAEA, Wienna, Austria (15 days).
Dr. hab. V. Bondarenko Institute of Nuclear Physics, Prague, Czech Republik ( 20 days).

Dr. hab. N.Mironova - Ulmane Institute of Physics, Tartu, Estonia ( 1 month ).
Dr. hab. N.Mironova – Ulmane Conference Spain Badajoz (1 week)
Dr. hab. N.Mironova - Ulmane Germany Minhen (1 week)
Mag. A.Pavlenko - IAEA (11 month)
Dr. V.Skvortsova Confernce Belarus Minsk (1 week)
Dr. J. Ruza International Conference, Växjö, Sweden (1 week)

## Cooperation

**Latvia**

1. Medical Academy of Latvia (Dr. hab., Prof. M.Eglite, Dr. hab. Prof. I. Cema, Dr.T.Zvagule).
2. Ltd. "RAPA".
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. Instityute of Wood Chemistry ( Dr. hab. G. Dobele Dr.hab. G. Telesheva, Dr.hab T. Dizbit)

**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).

**Czech Republic**

1. Nuclear Research Institute, Řež (Dr. J.Honzatko).
2. Department of Nuclear Physics, Charles University (Prof. J. Kvasil).

**Estonia**

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

**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. Institue of Physics of the Ukrainian Academy of Science, Kiev (prof. S. Nepijko).
1. Atomic Institute of Austrian Universities, Vienna (Prof. H.Weber).

**Croatia**

1. Ruder Boško

**Poland**

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

**Russia**

1. Pedagogical University, Kaluga, (prof.K.Nikiforov), Russia
2. Institute of Chemical Physics, (prof. V.Petinov), Chernogolovka, Russia

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

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

## Main Results

### THE K- ISOMER STUDIES IN TUNGSTEN ISOTOPES

**I. Tomandl, J. Honzatko, V. Bondarenko, J. Berzins**

Knowledge of the absolute transition rates is of great importance not only for probing the nuclear structures but also for many applications in various fields. Conditions under which the certain nuclear state becomes isomeric depends on the many factors. For example, an existence of the many long-lived half lives in Hf-W region is caused by the so known K-selection rules. This situation arises in consequence that the K-projection of the nucleonic spins on the symmetry axis in deformed nuclei is a good quantum number so the nuclear transition violating the K-rule behaves as forbidden. Thermal neutron capture facility installed at the Rez research reactor allows to collect information on the coincident gamma-rays as well as the time distribution of the coincident events in the wide time interval. An analysis of the delayed coincidences is more important in cases where the long-lived isomers were established. The feasibility of this method was tested in the A~180 region where many K-isomers were known previously. Besides of several known nanosec. isomers new long lived isomer was established. The isomer population-depopulation modes were proved by setting the gates on the timing curve that is allowed to determine the sequence order of the gamma quanta in cascades. Several factors affected on the shape of the time distribution are considered.

### THERMAL NEUTRON CAPTURE CROSS SECTIONS OF TELLURIUM ISOTOPES

**I. Tomandl, J. Honzatko, T. von Egidy, H.-F. Wirth, T. Belgya, M. Lakatos, L. Szentmiklosi, Zs. Revay, G.L. Molnar, R.B. Firestone, V. Bondarenko**

Reaction cross sections belong to the basic quantities in nuclear physics. Their precise values are important for the evaluation of many experiments as well as various applications. New values for thermal neutron capture cross sections of the tellurium isotopes $^{122}$Te, $^{124}$Te, $^{125}$Te, $^{126}$Te, $^{128}$Te and $^{130}$Te are reported. These values are based on a combination of newly determined partial gamma-ray cross sections obtained from experiments on targets contained natural Te and gamma intensities per capture of individual Te isotopes. Isomeric ratios for the thermal neutron capture on the even tellurium isotopes are also given.

## NUCLEAR STRUCTURE OF $^{157}$Gd

**V. Bondarenko, A.V. Afanasjev, F. Becvar, J. Honzatko, M.-E. Montero-Cabrera, I. Kuvaga, S.J. Robinson, A.M.J. Spits. S.A. Telezhnikov**

The energy levels of $^{157}$Gd have been investigated using the (n,gamma )and (n,n' gamma )reactions. As a result of the analysis of the gamma-ray spectra from 16 isolated neutron resonances, a level scheme with a complete set of levels with spins J=1/2, 3/2 has been established up to 1.86 MeV excitation energy. A part of the level scheme is interpreted in more detail on the basis of Coriolis and Delta N=2 coupled Nilsson configurations. Slightly different sets of shape parameters are deduced for negative- and positive-parity levels. A large excess of unassigned 1/2 and 3/2 levels evidently requires an explanation in terms of inclusion of new additional degrees of freedom.

## THEORETICAL INVESTIGATION OF FINITE NUCLEI WITHIN MICROSCOPIC THEORIES

**A.V. Afanasjev**

The studies are concentrated in following directions and the following results were obtained.

The systematic study of deformation, rotational and quasi-particle properties of nuclei around $^{254}$No within the cranked relativistic Hartree+Bogoliubov theory has been performed. Based on this study [4,5] it was concluded that spherical nuclei with Z=120 and N=172/184 are doubly magic superheavy nuclei. In order to shed a light on the differences in predictions of different microscopic and phenomenological modelsfor superheavy nuclei, the detailed investigation of self-consistency effects in superheavy nuclei is in progress.

The study of the effects of proton-neutron pairing in rotating N ~ Z nuclei has been performed. Our investigations covering these nuclei in the mass range A=58-80 showed strong evidences for the existence of the isovector T=1 neutron-proton pairing [7]which is consistent with isospin independence of the nucleon-nucleon interaction. On the other hand, we have not found any evidence for the existence of the isoscalar T=0 neutron-proton pairing [7,8,9,10] A large overview article devoted to this topic is in preparation.

Nuclear astrophysics studies are concentrated on the investigation of the r-process abundances using the masses of nuclei obtained within the relativistic mean field theory and the investigation of the dependence of pycnonuclear fusion reactions on the properties of neutron-rich nuclei.

Independent studies and the collaborations with experimental groups from USA, Canada and United Kingdom with the aim to understand the high-spin properties of rotating nuclei are continued. They involve a number of important physical questions such as the termination of smooth terminating, normal deformed $^{87}$Nb [10], magnetic and anti-magnetic
rotational bands $^{105}$In, $^{110,112}$Te, rotational properties of nuclei in actinide region, the properties of the triaxial superdeformed bands in the A= 160-170 mass region (in particular, $^{163}$Tm and neighboring nuclei) and of the superdeformed bands around $^{108}$Cd, the rotational properties of nuclei at the neutron-drip line (study within the framework of the CRMF theory) etc.

We continue the development of tilted (two-dimensional) cranking RMF theory with the goal of subsequent study of magnetic rotation and other properties (including impact of currents) of the so-called magnetic and shears bands. Investigation of the microscopic nature of nuclear magnetism within the RMF theory and of its impact on different

properties of the nuclei along the beta-stability and the proton and neutron-drip lines is in progress.
On the invitation of the Editors of the Physics Reports we are writing a review article discussing the theoretical developments of the relativistic Hartree+Bogoliubov theory and its applications to nuclei under extreme conditions.

## APPLICATIONS OF GROUP PLETHYSM, TECHNIQUE FOR THE CLASSIFICATION OF NUCLEAR STATES

**J.A.Castilho Alcaras[1], J.Tambergs, A.Andrejevs, O.Katkevičius[2], J.Ruža, T.Krasta**

The group plethysm operation technique was developed which allowed to perform calculations of nuclear states classification by unified method for two types of algebraic nuclear models. The classification of states corresponding to the ground SU(3) configuration, taking into account unitary U(A-1), U(3) symmetries and permutation S(A) symmetry, has been carried out in unitary scheme basis for the strictly restricted dynamics model. The precise classification evaluations [11,12] of such kind have been finished in mass number region $4 \leq A \leq 80$, as well as, the approximate evaluations for $81 \leq A \leq 198$ region nuclei involving 1278 experimentally observed nuclides [13]. The corresponding precise classification calculations for $A \geq 81$ region nuclei are in progress now. The group plethysm technique has been applied also for the classification of nuclear states in several versions of interacting boson model [14]. Namely, the classification evaluations have been carried out for the standard s,d-boson model version IBM-1, the proton and neutron boson model version IBM-2, for two versions (IBM-3, IBM-4), where the isospin degree of freedom has been taken into account as well as for the extended variants of this model, involving the g-boson (IBM-1 G) and the negative parity f-bosons (IBM-1 F).

[1] Instituto de Fisica Teorica, Universidade Estadual Paulista, Sao Paulo, Brazil
[2] Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania

## SYSTEMATIC STUDY OF THE $^{194}$Ir NUCLEAR LEVEL SCHEME

**M.Balodis, T.von Egidy*, H.-F.Wirth***

During 2003, an essential progress has been achieved summarizing the $^{194}$Ir spectroscopic information from the neutron capture reactions [1,2], as well as from the (d,α) and (d,p) reaction spectra [3]. A careful analysis of the thermal neutron capture low-energy gamma-ray and conversion electron energies and intensities has been performed. It results in the yet unpublished multipolarity data for the 500-700 keV transition energies. Spectra from the (d,α) and (d,p) reactions, obtained using deuterons from the Tandem Accelerator Munich, Germany, help to establish a number of new levels. Now, instead of 38 levels from the ground state to 543 keV, we have 60 levels up to 740 keV, with spins-parities up to $4^-$ resp. $5^+$.

[1] M.Balodis, P.Prokofjevs, N.Krāmere, L.Simonova, J.Bērziņš, T.Krasta, et al. Nucl.Phys.A641 (1998) 133-187
[2] N.Krāmere, priv.comm. (2000)
[3] H.-F.Wirth et al., priv.comm. (2002-2003)

*Techn. Univ. and Univ. Munich, Germany

## QUALITY ASSURANCE/ QUALITY CONTROL FOR TESTING OF RADIOACTIVITY

**D. Riekstina, J. Berzins, O. Veveris, J.Alksnis**

The laboratory of Radiation physics are elaborated and applied the gamma-nuclear spectroscopy methods for the establishing natural and artificial radionuclides in different objects The quality of results is ensured by the precision in the quality control and assurance. It is achieved by implementation of the new Latvian standard EN ISO/IEC 17025:2000. The quality control in the laboratory involves: 1) the regular and long-term use of the reference materials in controlling and monitoring the equipment, acquired data processing with statistical methods; 2) the use of only calibrated equipment; 3) the regular participation in the intercomparison exercise (LNMC in Latvia, IAEA, RISO laboratory in Denmark), that makes it possible to estimate and find possible occurred error sources and carry out corrective manipulations; 4) the internal audits – analysis of identical samples by different performers using different equipment; 5) the estimation of uncertainty sources and calculation of uncertainties within the given interval of credibility.
Only credible and justified results can be the basis for further use in any field, thus making it possible to make legitimate decisions.

## INVESTIGATION OF METAL BIOACCUMULATION IN PINES SYLVESTRIS NEEDLES BY DIFFERENT ANALYTICAL TECHNIQUES

**D. Riekstina, A. Ludborzs, I. Taure, O. Veveris, A. Viksna**

The concentrations of the following nutric, trace and toxic elements: K, Rb, Ca, Sr, Co, Zn, Fe, Mn, Al, La, Na, Sb, Sc, Cd and Pb in 3 age classes pine needles and 15 elements in soils were established using INAA, TXRF and ET AAS. The pine needles and soil samples were taken from 7 different sites throughout Latvian territory. It was established, that the concentration of K, Rb, Co in the needles does not depend on the concentration of these elements in the soils, only the concentration of Sr in the pine needles strongly depends on the concentration of this element in the soil.

Concentration of K, Rb, Fe, Mn (for low concentrations), decreases with the age classes of the needles, while concentration of Co, Mn (for high concentrations), Zn, Na, Ca, La increases with the age classes of the needles. Concentration of Al, Sc, Sb is impossible to interpret unequivocally. For some elements: Al, Ca, K, Mn, the variation depending from the soil pH and the branch orientation (DA, DR) was observed.

## VIBRATIONAL AND MAGNETIC EXCITATIONS IN DILUTED ANTIFERROMAGNETIC SYSTEM $Ni_CMg_{1-C}O$

**N.Mironova-Ulmane, A.Kuzmin, G.Mariotto*, E.Cazzanelli****

$Ni_cMg_{1-c}O$ system is a nice example of diluted antiferromagnet. It forms a continuous series of solid solutions, whose magnetic properties vary with the composition from antiferromagnetic-like behaviour with the Néel temperature $T_N$=523 K for pure NiO to paramagnetic-like behaviour for pure MgO. For intermediate compositions with $c>0.3$, the paramagnetic-to-antiferromagnetic phase transition occurs upon cooling.

In this work, we performed a Raman spectroscopy study of polycrystalline $Ni_cMg_{1-c}O$ solid solutions in a wide range of compositions ($0.3<c<1$) and temperatures ($6\ K<T<450\ K$). A contribution of phonon and one(two)-magnon scattering in the Raman spectra was identified, and their variations with composition and temperature were investigated. We found that dilution of NiO by magnesium ions influences strongly both vibrational and magnetic properties of the system. In particular, the substitutional disorder results in an increase of one-phonon scattering contribution and a decrease of the two-magnon excitation energy as could be expected. At the same time, the one-magnon scattering at the Brillouin zone-centre shows upon dilution unpredicted behaviour resulting in an abrupt change of the one-magnon energy for small magnesium concentrations [24,25,26].

EC FP5 TARI Project (2001-2004) "Magnons in diluted antiferromagnetic materials (midam)".
* INFM and Dipartimento di Fisica, Università di Trento, Povo (Trento), Italy
** INFM and Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (Cosenza), Italy

## THERMOLUMINESCENCE CENTERS CREATED SELECTIVELY IN MGO CRYSTALS BY FAST NEUTRONS RADIATION PROTECTION DOSIMETRY

**S.Dolgov, T.Kärner, A.Luschik, A.Maaroos, N.Mironova –Ulmane, S.Nakonechny**

The EPR, luminescence and thermoluminescence of neutron-irradiated MgO single crystals , undoped and doped with Al, Be, Cr have been measured. The ivestigationshows that a selective detection of fast neutrons in mixed neutron-gamma fields, based on the registration of interstitial-vacancy processes in MgO by thermoluminescence, is possible. The sensitivity of such detectors is, however, still low but it can be improved by selecting MgO crystals with more effective centres of hole recombination luminescence and with a lower level of background high-temperature thermoluminescence [23].
In cooperation with Institute of Physics, Tartu,Estonia

## PECULLARITIES OF DEFECTS FORMATION IN MgO CRYSTALS WITH TRANSITION METEL IMPURIETES

**V.Skvortsova, N. Mironova-Ulmane, U.Ulmanis**

The absorption spectra of neutron irradiated MgO consists of three bands associated with radiation defects. Additionally to radiation defects there are also absorption bands due to transition from ground state to the excited states of nickel, manganese, chromium and iron impurities ($c>0.1$ mass.%). The intensity of 570 nm absorption band is considerably smaller in MgO with impurities than in pure MgO crystal under the same fluence of the fast neutron, whereas the intensity of 357 nm absorption band is smaller in pure MgO. From annealing results temperature intervals of radiation defects stability were found. The MgO with nickel impurity annealing shows two new absorption bands 347 and 480 nm. We assume that these absorption bands detected after annealing belong to complex $Ni^{3+}$- $V_{Mg}$. A change of the valence state from $Ni^{2+}$ to $Ni^{3+}$ take place by interaction of $Ni^{2+}$ with $O^-$ -centre which arise as a result of hole localization on the one

of the oxygen ions neighbours of a Mg vacancy. The charge is compensated by positive ion vacancies. From the behaviour of ~570 nm and ~357 nm absorption bands intensities during annealing the activation energies of the corresponding defects are determined. Obtained values of activation energy for pure MgO are 0.91 and 0.55eV, for MgO with nickel impurity – are 0.71 and 0.81 eV accordingly. This allows assume that the transition ions play important role in the vacancies and interstitials migration.

## RETROSPECTIVE DOSIMETRY FOR CHERNOBYL CLEAN-UP WORKERS

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

Retrospective ESR dosimetry on teeth enamel of Chernobyl clean-up workers demonstrated underestimation of officially documented doses at factor 2-10 claiming the incorporated $^{90}Sr$ as possible source for internal irradiation. Elevated concentration of toxic elements in blood discovered by Inductively Coupled Plasma Mass Spectrometry (ICP MS) was an additional factor affected health status of clean-up workers.

## CRITICAL INDEXES FOR MAGNETIC PHASE TRANSITION IN Ni FINE PARTICLES

**A.Petrov, I.Kudrenickis, M.Maiorov[1]**

Critical behaviour of the spontaneous magnetisation, the initial susceptibility and the Curie temperature for spherical nickel particles in dependence on their sizes have been experimentally investigated. The sizes of the nickel particles were close to the single-domain size $d_s \cong 60$ nm.

Magnetic phase transition in the Ni particles is remaining with decreasing their sizes, at the same time the values of critical parameters are changing as compared to massive Ni crystal. The experimental values of the statical critical indexes $\beta$ and $\gamma$ $\{ M_s \sim |-\varepsilon|^{\beta}, \ \chi \sim |-\varepsilon|^{-\gamma}$, where $\varepsilon = (T - T_c)/ T_c\}$ are changing to the values given by the theory of the mean field. It is possible these values of the critical indexes are the effective ones not the asymptotic values.. The change of the critical index $\gamma$ observed in our experiments corresponds to the theoretical behaviour of this index in dependence on the physical system's dimension. The size of particles is revealed itself on the value of the Curie temperature due to the influence of particle surface.

[1]Institute of Physics, University of Latvia.

# Scientific Publications

### Published in 2003

1. I. Tomandl, T. von Egidy, J. Honzatko, V. Bondarenko, H.-F. Wirth, D. Bucurescu, V.Yu. Ponomarev, G. Graw, R. Hertenberger, Y. Eisermann, S. Raman *Nuclear Structure of $^{131}$Te studied with (n,gamma) and (d,p) reactions.* Nuclear Physics A 717 (2003) 149.
2. V. Bondarenko, A.V. Afanasjev, F. Becvar, J. Honzatko, M.-E. Montero-Cabrera, I. Kuvaga, S.J. Robinson, A.M.J. Spits. S.A. Telezhnikov: *Nuclear structure of $^{157}$Gd.* Nuclear Physics A 726 (2003) 175--209.
3. I. Tomandl, J. Honzatko, T. von Egidy, H.-F. Wirth, T. Belgya, M. Lakatos, L. Szentmiklosi, Zs. Revay, G.L. Molnar, R.B. Firestone, V. Bondarenko: *Thermal Neutron Capture Cross Sections of Tellurium Isotopes.*Physical Review C68 (2003)067602.

4. A.V.Afanasjev T.L.Khoo, S.Frauendorf, G.A.Lalazissis,I.Ahmad, *Probing the gateway to superheavy nuclei in cranked relativistic Hartree-Bogoliubov theory,*Proc. Int. Conf. on ``Frontiers of Nuclear Structure", (Berkeley, California, 2002), AIP Conference Proceedings v. 656 (Eds. P. Fallon and R. Clark)Melville, New York, 2003 p.379.
5. A.V.Afanasjev, T.L.Khoo, S.Frauendorf, G.A.Lalazissis, I.Ahmad,*Cranked relativistic Hartree-Bogoliubov theory:Probing the gateway to superheavy nuclei*, Phys. Rev. C 67 (2003) 024309.
6. N.S.Kelsall, ... A.V.Afanasjev et al, *High-spin Studies of N~Z Nuclei in the mass 70 region* Proc. Int. Conf. on ``Frontiers of Nuclear Structure", (Berkeley, California, 2002), AIP Conference Proceedings v. 656 (Eds. P. Fallon and R. Clark) (Melville, New York, 2003) p.261-268.
7. C. D. O'Leary, ... A.V. Afanasjev it et al, *Evidence for isovector neutron-proton pairing from high-spin states in N=Z* $^{74}$*Rb,* Phys. Rev. C 67 (2003) 021301(R).
8. N.S. Kelsall, ..., A.V. Afanasjev, it et al, *High-spin structure of N ~ Z Nuclei in the A=72 region,* EuroPhysical Journal A, in press.
9. A.V. Afanasjev and S. Frauendorf,*Neutron-proton pairing in rotating N=Z nuclei:dominance of the isovector component*, Nuclear Physics A, in press.
10. J. Pavan, ..., A.V. Afanasjev et al, *Lifetime Measurements and Terminating Structures in* $^{87}$*Nb,* Phys. Rev. C 67 (2003) 034316.
11. J.A.Castilho Alcaras, J.Tambergs, T.Krasta, J.Ruža, O.Katkevičius *The Plethysm Techni que Applied to the Classification of Nuclear States*. – Brazilian Journal of Physics, vol. 32, N 2B (2002), pp. 641-670.
12. J.A.Castilho Alcaras, J.Tambergs, T.Krasta, J.Ruža, O.Katkevičius *Classification of Basis States for (p-f) Nuclei (41≤A≤80) with Minimal Configuration Energy*. - Brazilian Journal of Physics, vol. 33, N1 (2003), pp. 98-103.
13. A.Andrejevs, J.Tambergs, J.Ruža, J.A.Castilho Alcaras, O.Katkevičius Classification of Nuclear States in Unitary Scheme Basis for Strictly Restricted Dynamics Models. – Proceedings of the 11-th International Symposium Capture Gamma-Ray Spectroscopy and Rotated Topics Pruhonice 2-6 September 2002. Eds.: J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, pp. 417-423.
14. J.A.Castilho Alcaras, J.Tambergs, T.Krasta, J.Ruža, O.Katkevičius *Plethysms and interacting boson models.* – Journal of Mathematical Physics, vol. 44, N11 (2003) pp. 5296-5319.
15. J.Tambergs, T.Krasta, O.*Dumbrajs Quantum Chaos and Symmetries in Nuclear Spectroscopy.* – Proceedings of the 11 Int. Symp. on Capture Gamma-Ray Spectroscopy and Related Topics. Pruhonice 2-6 September 2002. J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, pp. 417-423
16. A.Andrejevs, J.Tambergs, J.Ruža, J.A.Castilho Alcaras, O.Katkevičius *Classification of Nuclear States in Unifary Scheme Basis for Strictly Restrictly Dynamics Models*. - Proceedings of the 11 Int. Symp. on Capture Gamma-Ray Spectroscopy and Related Topics. Pruhonice 2-6 September 2002. J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, pp. 629-632
17. A.Dzalbs, A.Andrejevs, J.Tambergs, J.Ruža, J.A.Castilho Alcaras, O.Katkevičius *Strictly Restricted Dynamics Model Calculations with Quadrupole Interaction*. - Proceedings of the 11 Int. Symp. on Capture Gamma-Ray Spectroscopy and Related Topics. Pruhonice 2-6 September 2002. J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, pp. 645-648
18. J.Ruža *On the reality of EPR paradox*. – Preprint submitted in : arXiv: quant-ph/0304014 v 1, 2 Apr. 2003 (7 pages) and paper submitted (9.10.2003) for publication in: Proceedings of International Conference in Quantum Theory: Reconsideration of Foundations-z, June 1-6, 2003, International Center for Mathematical Modeling, Vaxjo University, Sweden.

19. D. Riekstina, A. Ludborzs, I. Taure, O. Veveris, A. Viksna : *Investigation of metal bioaccumulation inPines sylvestris needles by different analytical techniques,* Ekology No **2,** (2003) p. 56-59.
20. O. Veveris, D. Riekstina**,** I. Taure, A. Skujina: *Forest ecosystem as accumulator of radionuclides*, J. Ekology No **2** (2003) p. 53-55.
21. D. Riekstina, J. Berzins, O. Veveris, J.Alksnis: *Quality assurance/ Quality control for testing of radioactivity*, Proceedings of IRPA Regional Congress on Radiation Protection in Central Europe, Bratislava, Slovakia, September 22-26 2003, p. 851-856.
22. I. Taure, D. Riekstina, O. Veveris: *Neutron activation analysis. (*Accepted for publication in Letters of Latvian University).
23. S.Dolgov, T.Kärner, A.Luschik, A.Maaroos, N.Mironova –Ulmane, S.Nakonechny *Thermoluminescence Centers Created Selectively in MgO Crystals by Fast Neutrons* Radiation Protection Dosimetry Vol.100 No 1-4 , pp. 127 –130 (2002)
24. E. Cazzanelli, A. Kuzmin, G. Mariotto and N. Mironova-Ulmane. *Raman scattering by phonons and magnons in $Ni_cMg_{1-c}O$ solid solutions,* Proc. SPIE 5122 (2003) 68-73.
25. A.Kuzmin, N. Mironova-Ulmane and S. Ronchin, *Origin of visible photoluminescence in NiO and $Ni_cMg_{1-c}O$ single-crystals*, Proc. SPIE 5122 (2003) 61-67.
26. E. Cazzanelli, A. Kuzmin, G. Mariotto and N. Mironova-Ulmane, *Study of vibrational and magnetic excitations in $Ni_cMg_{1-c}O$ solid solutions by Raman Spectroscopy.* J. Phys.: Condensed Matter 15 (2003) 2045-2052.
27. V.Skvortsova, N. Mironova-Ulmane, U.Ulmanis. Effect of Electric Field on Transport of Radiation Defects in MgO, "Mass and Change Transport in Inorganic Materials" Advances in Science and Technology No 37 P.Vincenzini. V. Buscaglia (Editors) Techna 2003 pp. 41-48.
28. P.Alexa, J.Honzatko, I.Tomandl, V.Bondarenko, J.Berzins, T.von Egidy, H.-F.Wirth, R.Hertenberger, Y.Eisermann, G.Graw, V.A.Khitrov, A.M.Sukhovoj. *Interplay of quasiparticle and vibrational states in W isotopes,* Proceedings of the 11 Int. Symp. on Capture Gamma-Ray Spectroscopy and Related Topics. Pruhonice 2-6 September 2002. J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, p.178.
29. J.Bērziņš, V.Bondarenko, T.Krasta, F.Hoyler, K.Fohl, H.G.Borner, B.Krusche, S.J.Robinson. P.Schillenbeck. *Non-rotational states of $^{164}Dy$,* Proceedings of the 11 Int. Symp. on Capture Gamma-Ray Spectroscopy and Related Topics. Pruhonice 2-6 September 2002. J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, pp.637-640.
30. J.Honzatko, and I.Tomandl, V.Bondarenko, T.von Egidy and H.-F.Wirth, R.Hertenberger, Y.Eisermann and G.Graw, D.Bucurescu and N.Marginean, V.Yu.Ponomarev. *Nuclear structure of 127Te studied with (n,) and (d,p) reactions and interpreted with IBFM and QPM,* Proceedings of the 11 Int. Symp. on Capture Gamma-Ray Spectroscopy and Related Topics. Pruhonice 2-6 September 2002. J.Kvasil, P.Cejnar, M.Krtička. World Scientific 2003, pp.686-689.

## Lectures on Conferences

**19th Scientific Meeting of Institute of Solid state Physics, University of Latvia, Riga, February 10.-13., 2003.**

1. D. Riekstina, O. Veveris, J. Berzins, Testing of radionuclides, quality assurance and control, p. 15.
2. J. Honzatko, I. Tomandl, V. Bondarenko, J. Berzins, L.Simonova, T. von Egidy, H.-F. Wirth, R. Hertenberg,,Y. Eisermann, G. Graw, P. Alexa, The nuclear structure studies in $^{185}W$ with neutrons capture and neutron transfer reactions, p. 16.

3. T. Krasta, O. Katkevičius, J. Ruza, J. Tambergs, J.A. Castiljo Alcaras, A. Dzalbs, A.Andrejevs, Studie of p-shell nuclear isospin multiplets, p. 17.
4. V.Skvorcova, Annaeling investigation in magnesium oxides crystals, p.42.

**International Conference "EcoBalt 2003", Rīga, May 15-16, 2003**

1. D. Riekstiņa, O. Vēveris**,** Application of ion resins for separation of radionuclides from water, p.47.

**5th International Workshop on RadiotionImaging Detectors, Riga, September 7-11, 2003**

1. A.Pavlenko, N.Mironova-Ulmane, D. Riekstina, T.Zvagule, I.Cema, Quality of Dental X-ray Image Depending on Calcium Content, p. 74.

**The IRPA Regional Congress on Radiation Protection Neighbouring contries of Central Europe, Bratislava, Slovakia, September 22-26, 2003**

1. D. Riekstina, J. Bērzins, O. Veveris, J.Alksnis

Quality assuarance/ Quality control for testing of radioactivity, p. 98.

**1st International Meetingon Applied Physics APHYS-2003, Badajoz, Spain, October 13-18, 2003**

1. N.Mironova-Ulmane, A.Pavlenko, D. Riekstina, M.Eglite, E.Curbakova, T.Zvagule, N.Kurjane, R.Bruvere, N.Gabruseva, A.Volrate, Chernobyl clean-up workers: 17 years of follow-up in Latvia, p.71.

**5 th International Workshop on Radiation Imaging Detection. September 7-11 Riga, Latvia.**

1. A..Pavlenko, N.Mironova-Ulmane, D.Riekstina, T.Zvagule, I.Cema. Quality of Dental X-ray Image Depending on Calcium Content. P.74
2. F.Muktepavela, I.Manika, L.Grigorjeva, V.Skvortsova. Effect of radiation on Micromehanical Properties of AIN Thin . P.85
3. N.Mironova-Ulmane,A. Pavlenko M.Eglite, E. Curbakova, T.Zvagule. Chernobyl clean-up workers: 17 years of follow-up in Latvia 1 st International Meeting on Applied Physics Spain Badajoz October 13-18 2003 p.71.
4. V. Skvortsova, N.Mironova-Ulmane, U.Ulmanis, D.Riekstina Pecullarities of defects formation in MgO crystals with transition metel impurietes. International Scietific conference "Actual Problems of solid State physics p.151.
5. N. Mironova-Ulmane Quality of Dental X-ray Image Depending on Calcium Content.

**International Workshop on Biological Dosimetry Methods. Riga 22-23 April 2003**

1. N. Mironova-Ulmane. Biophysical methods of dosimetry. (invited)

**Tarty University Institute of physics Tarty Estonia 6 Marth 2003**

1. N. Mironova-Ulmane. Radiation and Health. (invited)

**International Scietific conference "Actual Problems of solid State physics"**

1. Vera Skvortsova. Pecullarities of defects formation in MgO crystals with transition metel impurietes. 2003.

**International Conference on Magnetism "ICM 2003, Roma, Italy, 27.07-01.08.2003"**

1. A.Petrov, I.Kudrenickis, M.Maiorov. Critical indexes for magnetic phase transition in Ni fine particles, Abstract No.5V-pm-13, p.739.

**Workshop NEMEA (Neutron Measurements and Evaluations for Applications) 5--8 November, Budapest, 2003.**

1. I. Tomandl, J. Honzatko, V. Bondarenko, J. Berzins The K- isomer studies in tungsten isotopes.

## Lectures at Universities, Institutes …

J. Tambergs

Latvian University, Faculty of Phycis and Mathematics: 1) Basic principles of nuclear and particle physics; 2) Basics principles of general relativity and cosmology

Latvian University, Faculty of Theology: 1) Biblical and scientific conceptions of the Universe; 2) Dialogue between religion and science.

J. Ruza

Riga Technical University: General physics.

# LABORATORY OF ORGANIC MATERIALS

Head of the Laboratory: Dr.habyl.phys. I.Muzikante

## Research Area and Main Problems

The laboratory's research interests cover polar organic materials for application in optics and molecular electronics. Research area is optical, electrical and photoelectrical properties of new advanced organic materials and structures. Studies include energy structure and charge carrier transport of low mobility organic solids; charge carrier trapping phenomena, surface potential investigations and optically induced switching effect in organized polar organic films.

**Scientific Staff**

1. Dr.habil.phys. I.Muzikante
2. Dr.phys. M.Rutkis
3. Dr.phys. E.Fonavs
4. Dr.phys. O.Vilitis

**Students**

1. R.Dobulans
2. J.Latvels
3. A.Vembris

**Visitors from abroad**

1. Mc.Eng. B.Stiller, Potsdam University, Potsdam, Germany (1 week)
2. Dr. A.Apostoluk, Angers University, Angers, France (2 weeks)
3. Dr.habil. M.Bouvet, P.M.Curie University, Paris, France (1 week)
4. Dr. S.Dabos-Seignon, Angers University, Angers, France (1 week)

**Scientific visits abroad**

1. Dr.h. I.Muzikante, Potsdam University, Potsdam, Germany (1.5 month)
2. Dr. E.Fonavs, Potsdam University, Potsdam, Germany (1 month)
3. A.Vembris, Angers University, Angers, France (20 days)
4. Dr.h. I.Muzikante, Angers University, Angers, France (1 week)
5. R.Dobulans, P.M.Curie University, Paris, France (1 month)
6. Dr.h. I.Muzikante, P.M.Curie University, Paris, France (1 week)

## Cooperation

**Latvia**

1. Department of Material Science and Applied Chemistry, Riga TU (Prof. O.Neilands, Prof. V.Kampars)
2. Latvian Institute of Organic Synthesis (Dr. E.Markava)
3. Institute of Chemical Physics, University of Latvia, (Dr. D.Erts)
4. Institute of Physical Energetics, Latvian Academy of Sciences (Dr. I.Muzikante)

**Lithuania**

Institute of Physics and University of Vilnius (Prof. L.Valkunas)

**Germany**

Lehrstuhl Physik kondensierter Materie, Universität Potsdam, Potsdam (Prof. L.Brehmer)

**France**

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

**Taiwan**

Institute of Atomic and Molecular Sciences of Academia Sinica, Taipei, Taiwan: (Prof. S.H. Lin*)*

**Japan**

Institute for Chemical Research, Kyoto University, (Prof. N.Sato).

## Main Results

### OPTICALLY INDUCED OPTICAL AND ELECTRICAL PROPERTIES OF POLAR PHOTOCHROMIC ORGANIC MATERIALS

**I.Muzikante, E.Markava, O.Neilands**

Polar organic materials have received considerable attention because of their large dipole moments and optical nonlinearities. Organic materials for photonic applications contain chromophore dipoles, which consist of acceptor and donor groups linked by a bridge of delocalized π-electron system. Both calculation and experimental data show reversible highly dipolar photoinduced intramolecular charge transfer in betaine type molecules and trans/cis isomerizarion in azobenzene derivatives, accompanied by the change of sign and value of the dipole moment. The switching phenomenon is important for the for the optoelectronic effects including second harmonic generation.

The number density of the embedded chromophores, their hyperpolarizability and their degree of noncentrosymmetrical orientational order determines the macroscopic effect of switching. This net polarization is usually achieved by aligning the chromophores dipoles. From this point of view the preparation of highly ordered films are very important. The most popular are Langmuir-Blodgett multilayers (LB), self-assembled monolayers (SAM) and polymer films of these compounds. The polar molecules are oriented by corona poling in doped polymer films.

The arrangements of the polar molecules in the films may be clarified through the surface potential measurements. The surface potentials are governed by dipole moment of the ordered polar molecules in the film and are related to chemical structure, packing densities, molecular orientations of the molecules. The reversible surface potential changes under optical irradiation are observed. Experimentally obtained photoinduced changes of the surface potential are in range between some milivolts and tens of volts in dependence of the molecules and their ordering in films.

*In cooperation with Institute of Physical Energetics, LAS (Latvia), Latvian Institute of Organic Synthesis (Latvia) and Riga Technical University (Latvia).*

### STUDIES OF TOPOGRAPHY AND ELECTRICAL PROPERTIES OF POLAR ORGANIC MOLECULES DOPED POLYMER FILMS

**D.Cepīte, E.Fonavs, I.Muzikante, A.Tokmakovs, D.Erts, B.Poļakovs**

The increasing interest in molecular engineering largely arises from the possibility to manipulate the electronic properties of molecule based materials. Besides, organic

materials are of great importance due to possible formation of thin flexible devices. The macroscopic physical properties of film are determined by the degree of orientational ordering destroying the central symmetry. Corona poling is applied to achieve aligning of the dipoles with a high static electric field in host-guest polymer film.
A host-guest polymer films with highly polar molecules were investigated. N-(1,3-indandion-2-yl)pyridinium betaine (IPB) as guest polar molecule and PMMA as host were chosen.
The surface of both the IPB/PMMA and PMMA films is smooth within the area range of 1×1 μm. The roughness $S_q$ is evaluated to be within 0.39–0.44 nm for PMMA films and within 0.49–0.62 nm for IPB/PMMA films. Regularly distributed pinholes are observed in the structure of virgin IPB/PMMA films. The PMMA and host-guest films with polar molecules show an increase of the surface potential after corona poling suggesting that ordering of polar molecules and groups increase. Orientation and displacement of polar molecules and groups under applied electric field may increase the roughness of the film surface. The observed formations of island structures on the surface after corona poling may have increased by several times the value of $S_q$.
The surface potential of polarized host-guest films decreases after being heated over the glass transition temperature of PMMA and is close to that of virgin samples with randomly distributed polar molecules. The surface of the polymer films becomes smoother the roughness being close to that of virgin samples. The island patterns of surface structure emerging at corona poling become less pronounced but remain after thermal annealing.

*In cooperation with Institute of Physical Energetics, LAS, (Latvia) and Institute of Chemical Physics, University of Latvia (Latvia).*

## THE RELAXATION PROCESSES IN POLAR MOLECULE DOPED POLYMER (PMMA AND PS) MATRICES

**R.Dobulans, E.Fonavs, I.Muzikante, A.Tokmakovs**

Relaxation processes in nonlinear optical polymers are of considerable interest for obtaining a better understanding of properties of potential devices from these materials.
Betaine-type molecules (IPB) were incorporated in casted host-guest (HG) polymer film. IPB molecules posses in the ground state a considerable permanent dipole moment of 4.5D. Two different polymers – isotactic polymethylmetacrylate (PMMA) and polystyrene (PS) were chosen. The PMMA has dipole moment of 1.39D caused by ester group in side chain. PS is relatively nonpolar polymer with dipole moment ~0.8D. Besides, the glass transition temperatures of polymers are different, namely, for PMMA it is ~50°C and PS - ~105°C.
Temperature dependence of the surface potential $U_S(T)$ of both polymer and HG poled films was measured in the range from RT up to 125°C. The value of $U_S(T)$ of IPB/PMMA poled film increased on heating reaching a maximum at ~50°C. After the maximum, the value of the surface potential decreases with temperature close to zero. At temperature around ~ 85°C the other peak of $U_S(T)$ appeared. The maximum ~50°C is observed also in $U_S(T)$ dependence of poled PMMA film. In the case of PS film no maximum in $U_S(T)$ curve was observed. When polar IPB molecules are incorporated in PS matrix, the maximum at ~82°C appeared. The influence of α- and β-relaxations of PMMA on the thermal dependence of surface potential is observed. The thermal dependence of the surface potential of poled films shows a drop-off of the surface potential at temperature, which is related to the glass transition temperature of the host-guest system. The decay of the surface potential of poled IPB/PMMA films is

characterized by short time (~6 hours) and long time (~43 hours) relaxations processes in polymer matrix

*In cooperation with Institute of Physical Energetics, LAS (Latvia)*

## PHOTOINDUCED CHANGES OF OPTICAL PROPERTIES OF BETAINE DYE DOPED POLYMER MATRIX.

**A.Vembris, I.Muzikante, A.Tokmakov**

Optically induced intramolecular electron transfer (PIET) is important in photosynthesis and in photoelectrical properties. The investigated betaine type molecules possess large permanent dipole moment, which change in sign and value due to excitation in the intramolecular charge transition band (380-410nm). The films were prepared as polymer doped systems by solvent casting. Poly(methylmetacrylate) (PMMA) was applied as polymer. As guest molecule N-(1,2-diphenylpyrazolidine-3,5-dion-4-yl)pyridinium betaine was chosen. The optical density of the intramolecular charge transition band of betaine decreased on irradiation with light with the same wavelength.
Switching of surface potential caused by irradiation within the intramolecular charge carrier transfer band is observed. The process is reversed after the irradiation is turned off. The response to irradiation is exponential with a characteristic response time of $\tau_{res}$ = 3.1±1.3 min. Both the intensity of intramolecular charge transfer band and optically induced changes of surface potential decrease with the irradiation cycles. The characteristic decay time of betaine in the polymer film is of the order of 6 min. The decay may be caused by photo-oxidation of betaine molecules and is irreversible.
The photo-oxidation may be avoided by covering the host-guest film with a polymer layer of eliminating the contact of betaine molecules with ambient oxygen. The optical absorption of samples covered with a protective layer of a modified polyvinyl alcohol (PVA) do not show any decrease of optical density of the intramolecular charge carrier transfer band at irradiation with light of the same wavelength.

*In cooperation with Institute of Physical Energetics, LAS (Latvia)*

## THIN FILMS OF PHTHALOCYANINE DERIVATIVES FOR OZONE SENSING

**M.Bouvet, I.Muzikante, E.Fonavs, A.Tokmakov, R.Dobulans**

Vacuum-evaporated thin films of phthalocyanine (Pc) derivatives have been studied for chemical sensing to gases. The changes of electrical properties of metal phthalocyanines can be influenced by absorption of oxidation or reducing gases on film. Applicability for gas sensor is determined by response, stability and reproducibility of physical properties to gas. The most of the studies concerning phthalocyanines-based gas sensors are related to oxidation with $NO_2$, which is a fairly good oxidizing agent. Ozone ($O_3$) is an important oxidizing agent present in the atmosphere. The conductivity measurements of thin films of copper phthalocyanine (PcCu) has been shown to be influenced by the presence of $O_3$.
In these studies nickel phthalocyanine (PcNi) as p-type material and fluorinated PcCu ($F_8$PcCu) as n type material was used.
The variation of the density of charge carriers due alternate exposing to the nitrogen stream and ozone was studied by the technique of the Kelvin probe. Energy structures of molecules in solid state may be investigated under air on the basis of the Kelvin probe

method. It is shown that vacuum sublimed films of phthalocyanine in contact with metal form Schottky barrier which height is determined by the difference in work function between a molecular solid film and a metal. The vibrating Kelvin probe has well-established technique for measuring work-function changes of a material. Since the work function of the molecular films is defined as the difference between the vacuum level above the sample surface and the Fermi level in the sample, Kelvin probe measurements are sensitive to environment.
Thin films of PcNi and $F_8$PcCu were prepared by vacuum evaporation Vacuum-evaporated thin films were prepared on glass substrate coated with a thermally vacuum-evaporated polycrystalline gold film. The evaporation temperatures were 400ºC for PcNi and 440ºC for $F_8$PcCu. The film thickness lay in the range $L$= 0.2-1 μm. The changes of surface potential was measured by Kelvin probe equipment described elsewhere.
The changes of surface potential as a function of time of thin films of PcNi and $F_8$PcCu under $O_3$ and $N_2$ stream are observed.

*In cooperation with Institute of Physical Energetics, LAS (Latvia) and Université Pierre et Marie Curie, Paris (France).*

## OPTICAL AND ELECTRICAL PROPERTIES OF ORIENTED THIN FILMS OF OLIGOMER CONTAINING BETAINE TYPE MOIETY IN SIDE CHAIN

**O.Neilands, I.Muzikante, E.Fonavs, A.Tokmakovs, D.Cepite, A.Vembris, B.Stiller, L.Brehmer, A.Apostoluk, J.M.Nunzi**

Organic dye-doped materials have received considerable attention because of their large dipole moments and optical nonlinearities. Amorphous dipole electrets for photonic applications contain chromophore dipoles (A-π-D), which consist of acceptor (A) and donor (D) groups linked by a bridge of delocalized π-electron system. Non-linear optical and electrical properties are obtained by dipole orientation of active units.
A novel oligomer with N-(indan-1,3-dion-2-yl)pyridinium betaine (IPB) as side group was investigated. As a result of the asymmetry of charge distribution in IPB molecule the permanent dipole moment in ground state is of 4.5D [1,2]. Betaine molecules undergo a reversible optically induced change of the value and sign of the dipole moment in the photoinduced electron transfer (PIET) spectral region. In the case of IPB the value of PIET is in range 380-400nm. So far IPB molecules in oriented Langmuir-Blodgett multilayers and corona-poled host-guest systems were investigated [3,4].
The positive high-electric field corona poling was used to generate dipole orientation of casted films containing IPB oligomers. The poling temperature of the casted films was constant in the range 65-100°C, which is above to glass transition temperature $T_g$ = 62°C. The surfaces of the film surfaces obtained by AFM were smooth with average roughness (rms) between 30 and 80 Å. From AFM images follow that during corona poling the roughness of films remain. Whereas the changes of surface potential on irradiation with light at 375nm increased more then 10 time for the corona poled films. An effect of second harmonic generation (SHG) only in corona poled samples was observed.

*In cooperation with Riga Technical University (Latvia), Institute of Physical Energetics, LAS (Latvia), Potsdam University, Potsdam (Germany) and Angers Université, Angers (France).*

## OPTICAL PROPERTIES OF SOME NOVEL AZOBENZENES IN THIN LAYERS

**E.Markava, D.Gustina, I.Muzikante, L.Gerca, A.Tokmakov, E.Fonavs, B.Stiller, L.Brehmer**

Thin ordered films containing azobenzene moieties are frequently investigated as optical switching elements in microelectronics or as high density data storage active media. The photoisomerisation of azobenzene residues from the trans- to the cis-form is generally suppressed or prohibited in the Langmuir-Blodgett film systems owing to the close packing of the azobenzene amphiphiles in the layers and the resulting lack of free volume available for the process. Several strategies have been employed to obtain ideal thin film intended for molecular switching such as introducing of spacer molecules in mixed monolayers of azobenzene derivatives, formation of monolayers from azobenzene copolymers or adding of bulky hydrophobic substituents.

In the last years we are searching for new azobenzene derivatives, which are able to form photoactive LB multilayers. In the design of a new molecular structure we have developed our investigations in the field of modified azobenzene derivatives showing high cis/trans photoreactivity due to looser packing of azo unites in the LB films as a result of steric requirements of the bulky hydrophobic groups.

We have newly synthesized amphiphilic azobenzene derivative containing N, N-dicyclohexyl sulfonamide moiety in order both to improve the monolayer stability on air/water interface and to avoided the well known problem of too dense packing of azobenzene chromophores in layer resulting in loss of photochromism. We have observed the fast reversible photoisomerisation in LB multilayer on alternating irradiation with UV and visible light. The time response both of optical density of main absorption band at 360nm and changes of surface potential caused by trans-to-cis isomerization last about 16s. The reversible process induced by irradiation with visible light is slower more than 4min. The time dependence of surface potential is not possible to described by simple exponential function. Such behavior may be explained by reorientation of molecules in LB films due to dipole-dipole interactions, which govern structural changes of the film. Following the reorientation of polar molecules, which changes the dipole moment of the film, the slower process of changes of surface potential is observed

*In cooperation with Latvian Institute of Organic Synthesis (Latvia), Institute of Physical Energetics, LAS (Latvia), Potsdam University, Potsdam (Germany).*

## Scientific publications

### Published in 2003

1. E.Markava, D.Gustina, I.Muzikante, L.Gerca, A.Tokmakov, E.Fonavs, B.Stiller, L.Brehmer, *Optical properties of some novel azobenzenes in thin layers*, SPIE Proceedings, Advanced Optical Materials, 2003, Vol.**5122**, pp.210-215.
2. A.Gruodis, V.Ališauskaitė, S.Juršėnas, L.Valkunas, I.Muzikante, *Excitonic states in the polar molecular crystals*, SPIE Proceedings, Advanced Optical Materials, 2003, Vol.**5122**, pp.224-231.

3. A.Tokmakov, A.Vembris, A.Jurgis, I.Muzikante, O.Neilands, *Optically induced degradation of some betaine dyes*, SPIE Proceedings, Advanced Optical Materials, 2003, Vol.**5122**, pp.238-243.
4. I.Muzikante, O.Neilands, E.Markava, *Optically induced electrical properties of new advanced organic materials*, SPIE Proceedings, Advanced Optical Materials, 2003, Vol.**5122**, pp.179-187.
5. O.Neilands, I.Muzikante, *The Search for Highly Polar Betainic Type Molecules for Electro-optical Applications*, Organic Nanophotonics, Proceedings of the NATO Advanced Workshop, NATO Science Series II, 2003, Vol.**100**, pp.447-462.
6. R.Karpitz, V.Gulbinas, L.Valkunas, S.Jursenas, I.Muzikante, *Excited state dynamics of N-(4-azaindan-1,3-dion-2-yl)pyridinium betaine in solutions*, SPIE Proceedings, Advanced Optical Materials, 2003, Vol.**5122**, pp.232-237.
7. I.Muzikante, D.Cepite, E.Fonavs, A.Tokmakov, D.Erts, B.Polakov, *Incorporated oriented polar molecules in PMMA polymeric films: characterization by Kelvin probe technique and atomic force microscopy*, Latv.J.Physics and Technical Sci., 2003, No.3, pp.49-55.

**Accepted for publication 2003**

1. R.Dobulans, D.Cepite, E.Fonavs, I.Muzikante, A.Tokmakov, D.Erts, B.Polakov, *Studies of host-guest thin films of corona poled betaine type polar molecules by Kelvin probe technique and atomic force microscopy*, Macromolecular Symposia, 2003
2. O.Neilands, N.Kirichenko, I.Muzikante, E.Fonavs, L.Gerca, S.Jursenas, R.Valiokas, R.Karpicz, L.Valkunas, *Detection of blue light by self-assembled monolayer of dipolar molecules*, UV Solid-State Light Emitters and Detectors, Proceedings of the NATO Advanced Workshop, NATO Science Series II, 2003

## Lectures on Conferences

**Latvijas universitātes Cietvielu fizikas institūta 19.zinātniskā konference, Rīga, Latvija, 2003.gada 10.-12.februāris**
**19th Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, Latvia February 10-12, 2003:**

1. D.Cepite, E.Fonavs, I.Muzikante, A.Tokmakovs, D.Erts, B.Polakov, *Topogrāfijas un elektriskās struktūras pētījumi polimēra matricai ar polārām organiskām molekulām, Studies of Topography and Electrical Properties of Polar Organic Molecules doped Polymer Films*, Abstracts, p.55.
2. R.Dobulans, E.Fonavs, I.Muzikante, A.Tokmakovs, *Polimēra (PMMA un PS) un tajā ievietoto polāro organisko molekulu sistēmas relaksācijas procesi, The Relaxation Processes in Polar Molecules doped Polymer (PMMA and PS) Matrices*, Abstracts, p.36.
3. A.Vembris, I.Muzikante, A.Tokmakovs, *Fotoierosinātas betaina krāsvielu optisko īpašību izmaiņas polimēra matricā, Photoinduced Changes of Optical Properties of Betaine Dye doped Polymer Matrix*, Abstracts, p.37.

**7th International Conference on Frontiers on Polymers and Advanced Materials (ICFPAM-7) and NATO Advanced Research Workshop "Smart and Functional Organic Materials", Bucharest, Romania, June 10-15, 2003:**
I.Muzikante, O.Neilands, E.Markava, *Optically induced optical and electrical properties of polar photochromic organic materials*, Abstracts, p.57.

**NATO Advanced Research Workshop (ARW) "UV Solid-State Light Emitters and Detectors", Vilnius, Lithuania, June 17-19, 2003:**
O.Neilands, I.Muzikante, E.Fonavs, L.Gerca, S.Jursenas, R.Valiokas, R.Karpicz, L.Valkunas, *Detection of blue light by self-assembled monolayer of dipolar molecules*, Program and Abstracts, p.25.

**The 10th International Symposium on Olfaction and Electronic Nose (ISOEN '03), Riga, Latvia, June 26-28, 2003:**
M.Bouvet, I.Muzikante, E.Fonavs, A.Tokmakov, R.Dobulans, *Thin films of phthalocyanine derivatives for ozone sensing*, Book of Abstracts, pp.242-243.

**COST Chemistry Action D19 International Workshop on Nanochemistry, Zakopane, Poland, 28-31 August 2003:**
O.Neilands, I.Muzikante, E.Fonavs, L.Gerca, S.Jursenas, R.Karpicz, L.Valkunas, R.Valiokas, *Self-assembled monolayer preparation of dipolar coloured molecules onto gold surface and studies of electro-optical properties*, Abstracts

**COST Action P8 "Materials and Systems for Optical Data Storage and Processing", Angers, France, September 3-5, 2003:**
I.Muzikante, *Nanoscale addressing of reversible isomerizable chromophores* (without abstract)

**International Workshop on Processing and Characterization of Nanomaterials, 2003, Warsaw, Poland, October 8-10:**
*I.Muzikante, Optically induced electrical properties of organized organic thin films*, Abstracts, p.23.

**The 2nd Workshop of Advanced Spectroscopy of Organic Materials for Electronic Applications, Nagoya, Japan, October 21-25, 2003:**
J.Tsutsumi, H.Yoshida, N.Sato, I.Muzikante, O.Neilands, *Comparison of solid-state structures and properties between a zwitterionic compound and its aza derivative compounds*, Abstracts, P-51.

# 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).

2. Provide physical measuring and manufacturing process automation.
3. Also solve the other problems, not afore-mentioned.

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## 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. *DataPro* Ltd
9. *Apollo AS* Ltd
10. *AlarmLat* Ltd
11. *Mikoniks* Ltd
12. *Energoremonts* *Rīga* Ltd
13. Joint-stock company "Poligons".

**Denmark**
DanBalt Electronics

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

**Estonia**
OÜ Terg A&K

The prospects of the instruments look at appendix.

**Our Clients**

1. Latvijas Krājbanka;
2. Latvijas Pasts;
3. SIA „LatRosTrans";
4. Latvijas Kuģniecība;
5. Latvijas Gāze;
6. Latvian Environment Agency;
7. Latvian Hydrometeorological Agency;
8. SIA „Augstceltne";
9. CSDD (Road Traffic Safety Directorate);
10. SIA "Avantime Amusement Technology";
11. Joint-stock company *Latvenergo.*
12. Latvia's Ministry of Foreign Affairs etc.

## Lectures on Conferences

**19th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2003**

1. D.Gusevs, I.Gvardina, A.Kristiņš, J.Lapiņš, *Experience of distributed Lon Works automation system using.* Abstracts, p.82.
2. P.Annus, A.Kristiņš, *Remote control of the objects.* Abstracts, p.83.
3. D.Gisevs, A.Kristiņš, M.Spriņgis, J.Tibergs, J.Veinbergs, *Automation of optical signal measuring.* Abstracts, p.84.
4. D.Gusevs, V.Jeremejevs, V.Narnicka, *Using of digital phase filtering to secure data transmission.* Abstracts, p.85.

# TESTING LABORATORY

Head of Laboratory Dr.Phys. J.Kļaviņš

ISSP commenced the evaluation of product conformity assurance since 1996, when the Department of Science of the Ministry of Education and Science rendered support from Market demanded research financing resources for the ISSP in Product testing and quality control pursuant to the requirements of the EU. Some of the staff members of the ISSP participated in the number of projects related to the testing and compliance assurance. Among projects was the establishment of the Testing laboratory (TL). The scope of this project includes a lot of activities. (1) TL preliminary measuring equipment has been supplemented by purchasing several new devices - equipment for determination of the waterproofness of building materials, computerized laboratory and analytical balances etc. (2) The already existing equipment has been repaired. (3) The premises of the laboratory have been repaired and equipped accordingly. (4) In the meantime 7 staff members of the ISSP have completed the training course "Preparing the Testing Laboratory Pursuant the Latvian and European Standards", organized by Certification Centre of Latvian Academy of Sciences, some of staff members – courses in Germany and England. (5) The quality system has been implemented in the laboratory. (6) TL is operating and currently performs testing according to 6 standard methods. New methods are being acquired.

On January 12, 2001 Latvian National Accreditation Office (LATAK) completed the accreditation of the Testing Laboratory at the Institute of Solid State Physics. It means that the quality system of one of the Institute units is recognized as comformit to international standard LVS EN 45001.

All the ISSP TL spheres applied for accreditation were accredited. They are: (1) concrete watertightness; (2) adhesion and cohesion of adhesives of ceramic linings; (3) release of lead and cadmium from enemalled metallic ware, (4) from ceramic ware, glass – ceramic ware, glass dinner ware, (5) glass hollow ware and (6) ceramic cookware subjected to heating and as in 3, 4, 5, 6 in contact with food.

In the 2001 TL sphere was extended with (7) the test for determination of breaking strength of glass fiber yarns, (8) the test for determination of breaking strength and alkaline durability of glass fiber mesh, (9) the test for determination of density of hardened concrete, (10) the test for determination of moisture content of building materials.

Test methods and corresponding standards in the scope of accreditation are:

1. Testing hardened concrete. Part 8: Depth of penetration of water under pressure. EN 12390:2000
2. Testing of adhesives for ceramic linings; testing of the deformation of bondings; dispersion adhesives. DIN 53265:1988
3. Ceramic ware, glass-ceramic ware and glass dinnerware in contact with food. Release of lead and cadmium. Part 1: Test method. ISO 6486-1: 1999
4. Vitreous and porcelain enamels. Release of lead and cadmium from enamelled ware in contact with food. Part 1: Method of test. ISO 4531-1: 1998
5. Glass hollowware in contact with food. Release of lead and cadmium. Part 1: Test method. ISO 7086-1: 2000
6. Ceramic cookware in contact with food. Release of lead and cadmium.

Part 1: Method of test. ISO 8391/1 – 1986

7. Textile glass - Yarns - Determination of breaking force and breaking elongation. ISO 3341: 2000
8. Standard Test Method for Determining Tensile Breaking Strength of Glass Fiber Reinforcing Mesh for Use in Class PB Exterior Insulation and Finish Systems (EIFS), after Exposure to a Sodium Hydroxide Solution. ASTM E2098: 2000
9. Testing hardened concrete - Part 7: Density of hardened concrete. EN 12390-7: 2000
10. Hygrothermal performance of building materials and products - Determination of moisture content by drying at elevated temperature. EN ISO 12570: 2000

Other test methods:

1. Floorings. Testing of watertightness. SIS 923511:1974
2. Ceramic tiles - Part 3: Determination of water absorption, apparent porosity, apparent relative density and bulk density. ISO 10545-3: 1995

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2. Dr.hab. M.Spriņģis

## Cooperation

1. Latvian National Accreditation Bureau LATAK
2. Latvian Association of Testing Laboratories
3. Certification Center of Latvian Academy of Sciences
4. Testing Laboratory of fresh and hardened concrete of "Kalnozols Building", Ltd

# ORGANIZED CONFERENCES

## 19th Scientific Conference of the Institute of Solid State Physics, University of Latvia

### Riga, February 10 – 13, 2003

The anual Scientific Conferences of the ISSP are held at the Institute of Solid State Physics in February the 10 – 13 and is a part of Scientific Conference of University of Latvia (UL).

The 19th Conference worked in 6 sections:
- structure and phase transitions (15 reports),
- non – linear optical properties and problems of optometry (10 reports),
- optical spectroscopy and luminescence (17 reports),
- materials and applications (12 reports),
- nuclear reactions and "EURATOM"projects (13 reports),
- nanomaterials and nanotechnologies (15 reports).

Alltogether 74 reports of 15 – 30 minutes were presented. Apart from staff members of ISSP and the Department of Optometry, represesantives of the Faculty of Physics and Mathematics UL, the Riga Technical University, and of the Institute of Inorganic Chemistry participated in the Conference.

The aim of the Conference was to inform the physicists community of Latvia about the most important results obtained in the previous year.

Abstracts of the scientific reports presented at the Conference were published in Latvian and English and were available to participants before the meeting.

Conference chairman
Prof. A.Krumins

**The 10th International Symposium on Olfaction and Electronic Nose (ISOEN`2003) was organized by ISSP of UL in Riga, June 25-28, 2003.**

Main Topics of Symposium:
1. Sensor Technology
2. Electronic Noses - Principles And Measurement Technology
3. Electronic Tongue - Principles And Measurement Technology
4. Data Analysis Algorithms And Problems
5. Application In Food And Food Processing
6. Agricultural Applications
7. Industrial And Environmental Applications
8. Medical And Microbiological Applications
9. Adulteration And Authenticity Test Applications

More participants were from Latvia (25), Russia (11), Italy (10), Germany (9), Ukraine (7), United Kingdom (5), France (4), USA (4), but there were also 2 participants from Argentina, Ireland, Spain and 1 from Belgium, Denmark, Finland, Israel, Japan, Korea, Lithuania, Norway, Poland, Sweden and The Netherlands.

93 participants come together to discuss the main results in sensor and sensor array technologies, e-nose minituarisation, odour description in electronic files and unified description language formation, e-nose application in different fields, making emphasis on product adultaration and environment pollution pproblems. Latest developments and new results were reported in 49 oral and 28 poster presentations, as well as in many discussions through out the symposium.

The Symposium Abstracts were published before the meeting in special book on 281 pages (A4 format). Manuscripts of the prepared reports were edited during 12 months after meeting and will be published in 2004 in special issue of the International Journal from Elsevier “Sensors&Actuators, B: chemical sensors”; editors J. Kleperis and A. D`Amico.

Chairman J.Kleperis

# APPENDIX