Institute of Solid State Physics
University of Latvia

ANNUAL REPORT

2004

Riga 2005

Annual Report 2004, Institute of Solid State Physics, University of Latvia.
Editor: A.Krumins. Composed matter: A.Muratova. Set up at the Institute of Solid State Physics, University of Latvia, *Kengaraga Str.8, Riga LV – 1063, Latvia*.

Riga, Institute of Solid State Physics, University of Latvia, 2005, p. 192

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INTRODUCTION

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

Four laboratories from the Institute of Physics of the Latvian Academy of Sciences, working in the field of solid state physics joined our Institute in 1995. Twenty scientists of the former Nuclear Research Centre joined the ISSP in 1999 and established Laboratory of Radiation Physics. In current year scientists from Latvian Institute of Physical Energetics joined ISSP and established Laboratory of Organic Materials (Table 2).

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

The research of the ISSP includes:

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

The highest decision-making body of the Institute is the **Council** of 23 members elected by the employees of the Institute. Presently Dr. phys. L.Trinklere is the elected chairman of the ISSP Council. The Council appoints director and its deputy.

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

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 2004. 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 246,7 thous. lats (Ls) (exchange rate: 1 Ls ~ 1,43 EUR), see Table 1 and Fig.1.

Additional funding from the **state budget** in 2004 was 123.5 thous. Ls. The main part of this funding was used for purchasing the scientific equipment (112 thous. Ls) on

condition, that a part of expenditures is covered by EC 6th Framework Programme expenses. Further, an aditional support from state budget was used for participation in international conferences (9.0 thous. Ls).

Table 1

INCOME OF ISSP, THOUSAND Ls, FROM 1993 - 2004

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

2004 was successful for **national contracts.** The market oriented contracts reached 85.6 thous. Ls, but contracts with Latvian companies including SMEs – 80.9 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 – 2004 is given in Table 1 and Figure 1.

The main source for **international funding** was the EC 6th Framework programme contracts:

- for the Centre of Excellence CAMART – 14.0 thous. Ls;
- X-TIP project – 43.4 thous. Ls;
- for Green Rose project – 24.5 thous. Ls;
- for POLECER project - 7.0 thous. Ls.

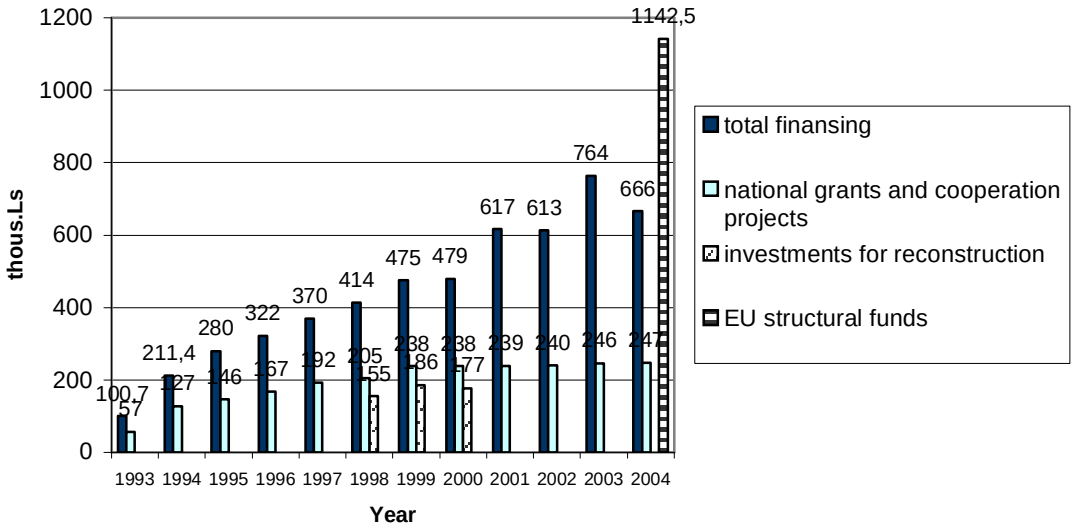
Additional funding was provided by Taivan - Lithuania – Latvia joint agreement – 6.3 thous. Ls .

The Institute obtained 8.0 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 members 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 2004.

Fig.1. Grants, investments in reconstruction and total financing of the ISSP



Main achievments in 2004:

1. The Institute succeeded in receiving a notable grant 1142,5 thous. Ls from EU Structural funds for modernisation of scientific infrastructure (Fig.1). This money will be used for purchasing modern technological, and research equipment. The part of this equipment is listed in Appendix;
2. Promotion of the research activities due to Project of Centre of Excellence CAMART (see the next chapter);
3. Dr.habil.phys. J.Berzins was elected a member of the Latvian Academy of Science;
4. Dr.habil.phys. M.Ozolins was elected as an professor of department of Optometry University of Latvia. He is the first professor at University in medical physics;
5. Dr.habil.phys. U.Rogulis was elected as an assistant professor of Physics Department University of Latvia;
6. G.Krumina and R.Pokulis were acquired degree of doctor of physics University of Latvia;
7. Prof. Dr.A.Truhin received Latvian Academy of Science and ALFA corporation year's award in physics;
8. Succesfull organization of 15th International Conference on Defects in Insulating Materials, July 11-16, 2004, Riga, Latvia, chairman Dr.habil.phys. I.Tale;
9. Dr.Habil.phys. E.Kotomin was one of organizers of following workshop:
    - NATO – ASI "International school on radiation effects in solids", Erice, Italy, 17 – 29 July, 2004;
    - Workshop "Computational Electochemistry", Santorini, Greece, September 26 – 29, 2004.
10. The reconstruction of terrase of main building of Institute (managed by Dr.phys. J.Klavins)

11. About 40 young researchers, mainly students from Physics Department University of Latvia, have been associated with the scientific projects.

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 6th Framework Programme, EU Structural fund, COST Programme, and to many foreign Universities and institutions.

Prof. Dr. A.Krumins

Table 3

International Advisory Board of the Institute

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

Table 2

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2004

International Supervisory board

Council of Institute
Dr.phys. L.Trinklere

Director
Dr.hab. A.Sternberg

Deputy director
Dr.hab. A.Krumins

RESEARCH DIVISIONS AND LABORATORIES

Crystal Physics Division
Dr. P.Kulis

Disordered Material Physics Division
Dr.hab.D.Millers

Ferroelectric Physics Division
Dr.hab. A.Sternberg

Semiconductor Materials Division
Dr. A.Lusis

Lab. of Didactic Systems
Dr. J.Kuzmin

Lab. of Nonlinear Processes Theory
Dr.hab. J.Kotomin

Lab. of Optical Recording
Dr. J.Teteris

Lab. of Wide Band Gap Materials
Dr.hab. B.Berzina

Lab. of Surface Physics
Dr.hab. J.Maniks

Lab. of Optical Materials
Dr.hab. I.Lacis

Lab. of Radiation Physics
Dr.hab. J.Berzins

Lab. of Organic Materials
Dr.hab. I.Muzikante

ADMINISTRATION AND SERVICES

Finance and Accounting
A.Jozepa

Mechanical Workshop
J.Katkevics

Domestic services
R.Siatkovskis

Division of Electronic Engineering
Dr. A.Kristins

Library
L.Rihtere

Testing Laboratory
Dr. J.Klavins

ACTIVITIES OF THE CENTRE OF EXCELLENCE

2004 was the last 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 was 703 000 EUR or 400 000 Ls for three years and the **funding had 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 and organization of workshops (35%);
- purchase of equipment and materials necessary for foreign colleagues during their visits (9%);
- overhead expenses (25%).

Undoubtedly, "Centre of Excellence" (CE) label has raised the **prestige of the Institute, the international one as well as the national.**

Attracting visitors from EU and other countries, the CE project facilitaded and extended international scientific cooperation. If formerly only rare single scientists paid durable work visits to the Institute, then now, thanks to the support of the EC, the work visits of foreign scientists were rather frequent. E.g. in the years 2001 – 2004, 66 foreign scientists and 9 PhD students from different European countries worked at the laboratories of the Institute, 60 of them for a longer time as one month (Table 4). 68 Institute fellows had in 2001 – 2004 foreign research trips supported by the CE funds.

Such a **high mobility** of the scientists has been never before noticed during the whole history of the Institute. Intensive exchange of know-how, research methods and numerous productive joint researches was a natural product of the great number of working trips. Centre of Excellence funds enabled for the first time the Institute to accept foreign postdocs (2).

Table 4

Long term visits to CAMART 2001 – 2004

From old EU Member States:	
Germany:	8
Italy:	6
Sweden:	3
Finland:	3
Spain:	3
France:	3
Austria:	2
Netherlands:	2
UK:	1
Belgium:	1
Portugal:	1
Total:	**33**

From new EU Member States:	
Lithuania:	10
Czech Rep.:	9
Poland:	7
Estonia:	6
Hungary:	3
Total:	**35**

From Other States:
Israel: 1

Due to EC funding, several **international scientific events and scientific seminars** of Institute were organised. (Table 5). These meetings upgraded the level of education in the scientific field of the project and were stimulating for the Institute's staff, as well for the visitors from European partner institutions. The CE project stimulated attracting of **young researchers** and modernisation of study programms in physics.

Table 5

Conferences and Workshops, organised by CAMART (2001 – 2004):

- The regional seminar on Solid State Ionics, Jurmala, Latvia, September 22 – 26, 2001;
- The International Conference "Advanced Optical Materials and Devices", Riga, Latvia, August 19 – 22, 2002;
- The Workshop of International Advisory Board of Institute, Riga, Latvia, August 19, 2002;
- The 10th International Symposium on Olfaction and Electronic Nose, Riga, Latvia, June 25 – 28, 2003;

Centre of Excellence funds enabled to improve the scientific infrastructure of the Institute. Due to financial support from Latvian government, on condition that a part of expenses is covered by CE funds, in 2002 – 2004 there was purchased scientific equipment by 325 000 EUR (Table 6).

Table 6

SCIENTIFIC EQUIPMENT, PURCHASED IN 2002 – 2004 DUE TO FINANCIAL SUPPORT OF:
§ LATVIAN GOVERNMENT (300 000 EUR)
§ CENTRE OF EXCELLENCE (25 000 EUR)

1. ARS closed cycle cryostat
2. Portable handheld gas chromatograph
3. Ar laser tube
4. Tektronix digital storage oscilloscope
5. Scanning probe microscope Smena H
6. Supercomputer, consisting of Cluster of 5 Compaque PC_s
7. IR spectrometer Bruker Equinox 55
8. AMKO spectrometer with CCD camera
9. Digital EMG system for evoked brain potentials study
10. Dual phase lock – in amplifiers
11. Magnetooptical cryostat.

The CE status assisted to obtain funds from EC 6^{th} Framework programme as well (Table 7). Fruitfull was the cooperation in Network of Centres of Excellence "Interfacial Effects, Novel Properties and Technologies of Nanostructured Materials"

Table 7

ENHANCED PARTICIPATION OF THE INSTITUTE IN OTHER AREAS OF 6TH FRAMEWORK PROGRAMME

1. STREP Project "Nanoscale mapping and surface structural modification by joined use of x-ray microbeams and tip assisted local detection" (Dr.habil. J.Purans)
2. Collective Research Project "Removal of Hazardous Substances in Electronics: Processes and techniques for SMEs" (Dr.A.Lusis)
3. Marie Curie Large Conference ICDIM 2003 (Dr.habil. I.Tale)
4. NE Project "Multifunctional and Integrated Piezoelectric Devices" (Dr.V.Zauls)
5. EURATOM project "Investigation of metal ions in fusion plasmas using emmision spectroscopy" (Prof.Dr. I.Tale)
6. EURATOM project "Study of the dynamics of edge localised modes in the ASDEX Upgrade and JET tokamaks" (Prof.Dr.V.Kuzovkov)
7. EURATOM project "Development of ferroelectric thin films for radiation resistant diagnostic componenets" (Dr.A.Sternberg)

Many thanks to everybody who contributed to final report, as well as to Directorate N – International Scientific Co-operation of European Commission (Mrs. J.Vennekens – Capkova) that support us.

Prof. Dr.A.Krumins
Scientific coordinator of CAMART

CRYSTAL 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

Technical Staff

1. Mg. J. Jansons
2. E. Tale
3. M. Veispale

PhD Students

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

Students

1. Dz. Berzins
2. A. Gulans
3. I. Gromuls
4. G. Marcinshs
5. M. Piesins
6. A. Sharakovsky
7. A. Voitkans
8. P. Zarans

Visitors from abroad

1. Dr. J. Rosa, Institute of Physics Academy of Science of the Czech Republic, Prague, Czech Republic (60 days);
2. Prof. A. Luschik, Institute of Physics, University of Tartu, Estonia, (1 week);
3. Prof. J.-M. Spaeth, Department of Physics, Faculty of Sciences,University of Paderborn, Germany, (2x1 week)
4. Dr. S. Schweizer, Department of Physics, Faculty of Sciences,University of Paderborn, Germany, (1 week);

Scientific visits abroad

1. Dr. hab. phys. U. Rogulis - University of Paderborn, Germany (4 months);
2. Dr. hab. phys. I. Tale - University of Paderborn, Germany (4 weeks);
3. Dr. hab. phys. I. Tale, University of Rostock, Germany (1 week);
4. Dr. hab. phys. I. Tale, University of Erlangen, Germany (1 week);
5. Dr. hab. phys. I. Tale, Vilnius, Lithuania (1 week);
6. Dr. hab. phys. I. Tale, Tartu, Estonia (3 days);
7. Dr. hab. phys. I. Tale, Pittsburgh, Pennsylvania USA (1 week);
8. M. Piesinhs, Pittsburgh, Pennsylvania USA (1 week);
9. A. Sharakovsky, Instituto Superior Tecnico (IST), Lisbon Portugal (6 weeks);
10. I. Gromuls, Instituto Superior Tecnico (IST), Lisbon Portugal (6 weeks);
11. A. Sharakovsky, University of Tartu, Estonia (1 week);
12. A. Sharakovsky, Asdex upgrade seminar, Munchen, Germany (1 week);
13. M. Piesinhs, Haga, The Netherlads(1 week);
14. M. Piesinhs, Palanga, Lithuania (1 week);
15. I. Gromuls, Palanga, Lithuania (1 week);
16. A. Gulans, University of Turin, Turin, Italia (1 week);
17. A. Gulans, University of Oslo, Oslo, Norway (5 weeks).

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

CARRIER LOCALIZATION EFFECT IN POLARIZED InGaN/GaN MULTIPLE QUANTUM WELLS

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

***Graduate Institute of Electro-Optical Engineering and Department of Electrical Engineering, National Taiwan University*

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

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

PR spectra revealed reliable values of built-in field (typically about 0.5 MV/cm for 15% In content). Meanwhile a remarkable Stokes shift between the PR feature and the PL peak position was observed. The Stokes shift increased with both the well width and In-content. We attributed this Stokes shift to solely the localization effect. Temperature

behavior of the Stokes shift and PL linewidth was shown to be consistent with phonon-assisted carrier tunneling (hopping) through the random distribution of states confined in the band potential minima within large In-rich regions. The scale of the band potential profile fluctuations within the In-rich regions and the dispersion in the average band gap energy of the regions were quantitatively estimated from the PL temperature behavior using Monte Carlo simulation of in-plane carrier hopping. These estimations were compared with the observations of the band tail in the PLE measurements.

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

LCAO CALCULATION OF DEFECTS IN GaN

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St.-Petersburg, Russian Federation
****Graduate Institute of Electro-Optical Engineering,*
National Taiwan University, Taipei, Taiwan.

We present an analysis of methods for LCAO calculations of defects in GaN. As a starting point for choice of the calculation method a perfect hexagonal GaN has been considered. Four well known approximations HF, LDA, GGA and B3LYP have been utilized to obtain the main properties of the perfect crystal. Lattice parameters, elastic constants and the band gap have been compared with the experimental, data and the calculated values, referred by other authors. As a consequence, the GGA method has been selected for further calculations. The following obtained set of Ga. characteristics - the lattice parameters a=3.20 Å, c=5.20 Å, the distance between Ga - N planes u-0.377 in c units, the bulk modulus B=206 GPa and the energy gap E_g=2.7 eV reasonably reproduce the experimental data. Following the analysis of requirements to size and configuration of the supercell representing the perfect crystal for modeling of defects, it was shown that in order to eliminate the interaction of a defect with its images a supercell of size at least 96 atoms for calculation of defects is necessary to use. Results of calculation of a number of neutral defects: Ga and N vacancies, Mg and Zn substituting Ga indicated that the size of the 96 atom supercell correctly represents an isolated neutral defect. Atomic relaxations of two nearest neighbours of both impurities and vacancies are found to be ~ 4 - 5%. However, Mulliken atomic charge difference at neighbours of vacancies is greater than at neighbours of impurities. These charge differences are significant only at first two coordination spheres of the defect.

THERMOACTIVATION SPECTROSCOPY OF CHARGE LOCALIZATION STATES IN InGaN/GaN QUANTUM WELLS

M. Piesins*, I. Tale* and C.C. Yang**
**Institute of Solid State Physics, Riga, Latvia;*
**Graduate Institute of Electro-Optical Engineering,*
National Taiwan University, Taipei, Taiwan

Both the carrier trapping and the strain-induced piezoelectric field, which generates the quantum confined Stark effect, has been involved for interpreting observed optical phenomena in QW structures in samples with increasing silicon-doping concentration, such as the photoluminescence peak shift and decay time decrease followed by intensity increase [1-3]. The temperature dependence of photoluminescence has been interpreted assuming capture and thermoactivated delocalization of excitons from QD. [1]. It can be expected that, like other structure defects and impurities, the QD will act as deep capture centers 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. We report detailed characterization of defects in InGaN/GaN quantum well structures. Different methods are utilized to investigate the relative concentration and the thermal activation energy of charge carrier release of various defects - thermostimulated currents (TSC), thermostimulated depolarization currents (TSDC) and deep level transient spectroscopy (DLTS). Structure of samples under investigation is as follows: GaN buffer layer on sapphire, thickness -1.52 μm; 5 pairs of GaN:Si/InGaN MQWs, the thickness of well layer 2.5-3.0 nm; the thickness of barrier layer ~ 7.5 nm; the thickness of GaN cap layer ~ 7.5 nm. The Si concentration in the barrier layer is - 5*lO^{18} cm^{-3}. MQWs and buffer layer are grown at 1075 K and 1375 K respectively. TSC, TSDC and DLTS trap spectroscopy have been performed using closed cycle cryostat in the temperature region starting from ~ 10 K to about 350 K with the linear heating rate being either 0.05 or 0.2 K/s for TSC/TSDC. Polarization of the sample before TSDC measurements have been carried out in an external field (5-50 V on whole structure) either in the course of slow cooling from ~ 300 K, or by the irradiation with photo-activating light at 10 K For TSC investigations sample was irradiated with photo-active light as well. Depending on the photon energy, a selective excitation of either the QW region or the barrier (GaN) region was performed. This allowed to identify the origin of trapping levels in MQWs.

[1] Shih-Wei Feng, Yung-Chen Cheng etal., J. Appl. Phys. 92(8), 4441 (2002),
[2] P.Ramvall, Y.Aoyagi, A. Kuramara, etal..App1. Phys. Lett. 76, 2994 (2000).
[3] E. Oh, C. Sone, O. Nam, H. Park, and Y. Park, Appl. Phys- Lett. 76, 3242 (2000).

X-IRRADIATION INDUCED PHOTO- AND THERMOSTIMULATED LUMINESCENCE OF $CsCdF_3$:Mn CRYSTALS

M. Springis, A. Sharakovsky, I. Tale, U. Rogulis
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Perovskite type fluoride crystals doped with rare-earth ions and other activators are promising materials for laser hosts and detectors of ionising radiation. The radiation-induced effects have been studied in a number of fluorides and the main defects (F- and V_K

-type) have been identified. Considerably less information on radiation effects is available for $CsCdF_3$. Here we present a study of photo- and thermostimulated luminescence (PSL and TSL respectively) of previously X-irradiated $CsCdF_3$ crystal doped with Mn. After X-irradiation of $CsCdF_3$ crystal at 8 K luminescence bands about 300 nm and 550 nm appear, when the crystal is optically stimulated at the same temperature. Several stimulation bands can be revealed for luminescence at 300 nm and 550 nm. According to Molwy-Ivey relation for halide crystals the stimulation band at 340 nm seems to be related to F-type centre absorption band. Subsequent heating of the crystal after X-irradiation at 8 K shows two groups of TSL peaks in temperature regions 8 K – 90 K and 200 K – 300 K. The spectral composition of the peaks involves both the emission band at 300 nm and 550 nm, moreover in spectra at low temperatures 300 nm emission band prevails, while in spectra of the most intense TSL peaks at 245 K and 295 K the emission band at 550 nm is dominant. Performed experiments allow us to suggest that the PSL band at 300 nm should be a result of electron recombination with self-trapped holes (STH), but the luminescence at 550 nm is related to Mn ions. Mechanisms of radiative recombinations as well as thermal stability of both STH and Mn ions are investigated.

RECOMBINATION PROCESSES IN $LiBaF_3$ CRYSTALS

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The creation of radiation defects in $LiBaF_3$ crystals at 10 K and the processes of their thermostimulated recombination are investigated. The methods of optical absorption, thermal bleaching of colour centers, thermostimulated and optically stimulated luminescence are used. The radiation defects anneal in a multi-stage process accompanied with thermo-luminescence at 20, 46, 105, 130, 170, 210 and 270 K. Differences in the optical absorption spectra measured before and after the TSL peaks are obtained and recombination parameters are determined. The TSL peak at 20 K arises from the delocalization of H-centers. The presence of two TSL peaks related to V_K-centers at 105 and 130 K indicates that 60˚ and 90˚ migration hops occur. The absorption band of H-centers is at 3.8 eV, but V_K-centers are characterized with two absorption bands at 3.2 and 4.3 eV.

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

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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

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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 x 10^7 K), the average electron temperature – 8,9 keV (1,04 x 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

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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.

HARDENING IN LiF IRRADIATED WITH SWIFT Kr IONS AND RECOVERY OF PROPERTIES UNDER ANNEALING

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Formation of radiation defects and defect aggregates in LiF upon irradiation with 10.1 $MeV.u^{-1}$ chromium ions, depth distribution of damage products, and their thermal stability were studied using the indentation microhardness, optical absorption spectroscopy and chemical etching techniques. The ion-induced hardening, which scales with the range of ions and correlates with the calculated energy loss along the path of Kr ions in LiF, was observed. Formation of a dislocation forest and an additional hardness increase in the vicinity of the irradiated layer due to the long-range shear and bending stresses resulting from the expansion of the irradiated part of the crystal were ascertained. Using annealing at temperatures from 450 to 800 K, recovery of optical absorbance, structure, and mechanical properties was studied. The results confirm the non-uniform depth distribution of the damage products responsible for hardening. The highest effect of hardening is observed

and thermally more stable defects are created in a certain ion path range around the Bragg maximum where the energy loss exceeds a threshold of about 10 keV.nm^{-1} for track core damage.

EPR OF F-TYPE CENTRES IN $LiBaF_3$

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

EPR HYPERFINE STRUCTURE OF THE Mo-RELATED DEFECT IN $CdWO_4$

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The hyperfine structure (hf) of the electron paramagnetic resonance (EPR) spectrum of Mo-related impurity defects in $CdWO_4$ crystal observed previously is reconsidered with account for interactions with two different groups of neighbouring Cd nuclei. The best fit of calculated EPR spectrum to the experimental is obtained with account for 2 groups of 3 and 2 equivalent Cd nuclei, respectively.

OPTICAL AND MAGNETO-OPTICAL STUDIES ON Mn-ACTIVATED $LiBaF_3$

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The photoluminescence of Mn-doped $LiBaF_3$ shows a weak Mn^{2+} emission band at 710 nm; the corresponding excitation bands are between 210 and 620 nm. After X-irradiation the PL spectrum shows two new bands peaking at 600 and 670 nm which are tentatively assigned to perturbed Mn^{2+} emissions; the intensity of all PL bands is increased. The magnetic circular dichroism (MCD) and the MCD-detected electron paramagnetic resonance (EPR) have shown that F-type centres are found after X-irradiation. The EPR

spectra indicate that there is a spatial correlation between the F-type centre and the Mn^{2+} dopant.

Scientific publication

Published in 2004

1. I.Tale, *Optical and magnetic resonance spectroscopy of stimulated recombination processes in defect studies*, – Radiation Measurements, **V38**, No.4-6, 639-644, 2004.
2. 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, **V38**, No.4-6, 663-666, 2004.
3. P. Kulis, I. Tale,I. Gromuls, M. Nikl, N. Ichinose, K. Shimamura, *Thermostimulated recombination processes in $LiBaF_3$ crystals*, – Radiation Measurements, **V38**, No.4-6, 723-726, 2004.
4. M. Secu, S. Schweizer, U. Rogulis, J.-M. Spaeth, A. Edgar, G.V.M. Williams, *Radiation defects in Ce^{3+}-activated fluorobromozirconate glass-ceramics X-ray storage phosphor*, – Radiation Measurements, **V38**, No.4-6, 739-742, 2004.
5. M. Springis, A, Sharakovsky, I.Tale, *Thermally and optically stimulated radiative processes in $LiBaF_3$ crystals*, – Radiation Measurements, **V38**, No.4-6, 611-614, 2004.
6. U. Rogulis, J.-M. Spaeth, E. Elsts, A. Dolgopolova, *Tl- related radiation defects in CsI:Tl*, – Radiation Measurements, **V38**, No.4-6, 389-392, 2004.
7. V. Ogorodnik, U. Rogulis, I. Tale, A. Veispals, *EPR of F-type centres in $LiBaF_3$,* - Latvian Journal of Physics and Technical Sciences, 2004 , vol. 2, pp. 62-67.
8. U. Rogulis, E. Elsts, *EPR hyperfine structure of the Mo-related defect in $CdWO_4$,* - Phys Stat. Sol. (c) vol. 2, No.1, p. 69-72, 2005.
9. B. Henke, M. Secu, U. Rogulis, S. Schweizer, J.-M. Spaeth, *Optical and magneto-optical studies of Mn-activated LiBaF3,* - Phys Stat. Sol. (c) vol. 2, No.1, p. 380-383, 2005.
10. I. Manika, J. Maniks, P. Kulis, L. Gailite, *Hardening in LiF induced by fast Ni ions and recovery of properties under annealing,* - Phys Stat. Sol. (c) vol. 2/1 p. 430-433, 2005.
11. A. Gulans, R.A. Evarestov, I. Tale, C.C. Yang, Ab *inito calculations of charged point defects in GaN,* - Phys Stat. Sol. (c) vol. 2, No.1, p. 507-510, 2005.
12. M. Springis, A. Sharakovsky, I. Tale, U. Rogulis, *X-irradiation induced photo- and thermostimulated luminescence of $CsCdF_3$:Mn crystals,* - Phys Stat. Sol. (c) vol. 2, No.1, p. 511-514, 2005.
13. A.N. Truhin, P. Kulis, J. Jansons, T.I. Dyuzheva, L.M. Lityagina, N.A. Bendeliani, *Host-defect luminescence of stishovite,* - Phys Stat. Sol. (c) vol. 2, No.1, p. 584-587, 2005.

Accepted for publication in 2004

1. I. Tkach, U. Rogulis, S. Greulich-Weber, J.-M. Spaeth, *W-Band Fabry-Perot microwave resonator for optically detected electron paramagnetic resonance and electron nuclear double resonance of paramagnetic defects in solids*, - Scientific Instruments, 2004 (accepted for publication).

2. A. Gulans, I. Tale, R. Evarestov, C.C. Yang, *LCAO calculation of defects in GaN,* - Phys Stat. Sol. (c) (accepted for publication).
3. M. Piesins, I. Tale, C.C. Yang, *Thermoactivation spectroscopy of charge localization states in InGaN/GaN quantum wells*, - Phys Stat. Sol. (c) (accepted for publication).
4. I. Tale, M. Springis, A. Sharakovskis, C.C. Yang, *Spectroscopy of charge localization states in InGaN/GaN multiquantum wells,* - Phys Stat. Sol. (c) (accepted for publication).
5. A. Zukauskas, K. Kazlauskas, G. Tamulaitis, J. Mickevicius, S. Jursenas, G. Kurilcik, S. Miasojedovas, M. Springis, I. Tale, Y.-Ch.Cheng, H.-Ch. Wang, Ch.-F. Huang, C.C. Yang, *Carrier localization effect in polarized InGaN/GaN multiple quantum wells,* - Phys Stat. Sol. (c) (accepted for publication).
6. I. Manika, J. Maniks, P. Kulis, L. Gailite, *Hardening in LiF irradiated with swift Kr ions and recovery of properties under annealing,* - SPIE Proceedings (accepted for publication).
7. A. Sharakovsky, M. Springis, U. Rogulis, I. Tale, *Photostimulated recombination processes in X-ray irradiated CsCdF3:Mn crystals,* - SPIE Proceedings (accepted for publication).

Lectures on Conferences

20th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 16–18, 2004

1. A. Sharakovsky, I. Gromuls, R. Gomes, *The equipment for spectroscopic diagnostics of Ga impurities in the Isttock fusion plasmas,* - Abstracts of the 20th Scientific Conference of Institute of Solid State Physics UL, Riga, 2004, p.37, (oral presentation).
2. I. Tale A. Sharakovsky, I. Gromuls, *The problems of evaluation of the parameters of laser ablation plasma for development of Ga-impurity emission etalon source*, - Ibid. p. 39, (oral presentation).
3. A. Sharakovsky, I. Gromuls, I. Tale, *The emission spectroscopy for evaluation of concentration of the metal vapor in tokamak plasma,* - Ibid. p. 40, (oral presentation).
4. P. Kulis, I. Tale, U. Rogulis, M. Springis, A. Veispals, *The Li-containing compounds as storage materials for slow neutron imagining,* - Ibid. p. 41, (oral presentation).
5. I. Gromuls,P. Kulis, I. Tale, M. Nikl, N. Ichinose, K. Shimamura, *Thermostimulated recombination processes in $LiBaF_3$ crystals,* - Ibid. p. 83, (oral presentation).
6. A. Sharakovsky, M. Springis, M. Nikl, *The role of localized holes in recombinative luminescence of $LiBaF_3$ crystals,* - Ibid. p. 84, (oral presentation).
7. L. Dimitrocenko, M. Springis, U. Rogulis, *Read-out processes of stored radiation energy in $LiBaF_3$ crystals*, - Ibid. p. 85, (oral presentation).
8. V. Ogorodnik, U. Rogulis, I. Tale, A. Veispals, *EPR of F-type centre in $LiBaF_3$*, - Ibid. p. 86, (oral presentation).
9. E. Elsts, U.Rogulis, *EPR hyperfine structure of the Mo-related defects in $CdWO_4$*, - Ibid. p. 87, (oral presentation).
10. M. Piesins, *Methodics of DLTS measurements and processing of results,* - Ibid. p. 93, (oral presentation).

The Fourth International Conference on Advanced Optical Materials and Devices (AOMD-4), July 6-9, 2004, Tartu, Estonia

1. I. Manika, J. Maniks, P. Kulis, L. Gailite, *Hardening in LiF irradiated with swift Kr ions and recovery of properties under annealing,* - Abstracts of The Fourth International Conference on Advanced Optical Materials and Devices (AOMD-4), July 6-9, 2004, Tartu, Estonia, p. 40. (poster presentation).
2. A. Sharakovsky, M. Springis, U. Rogulis, I. Tale, *Photostimulated recombination processes in X-ray irradiated CsCdF3:Mn crystals,* - Ibid. p. 41, (poster presentation).

The 15-th International Conference on Defects in Insolating Materials ICDIM-2004, July 11-16, 2004, Riga, Latvia

1. M. Secu, U. Rogulis, B. Henke, S. Schweizer, J.-M. Spaeth, *Optical and magneto-optical studies on Mn-activated $LiBaF_3$,* - Book of abstracts of the 15-th International Conference on Defects in Insolating Materials ICDIM-2004, July 11-16, 2004, Riga, Latvia, p. 34, (oral presentation).
2. I. Manika, J. Maniks, P. Kulis, L. Gailite, *Hardening in LiF induced by energetic ions and recovery of structure and properties under annealing,* - Ibid. p. 81, (poster presentation).
3. U. Rogulis, E. Elsts*, EPR hyperfine structure of the Mo-related defect in $CdWO_4$,* - Ibid. p. 98, (poster presentation).
4. A. Gulans, R.A. Evarestov, I. Tale, C.C. Yang, *Ab inito calculations of charged point defects in GaN,* - Ibid. p. 113, (poster presentation).
5. A.N. Truhin, P. Kulis, J. Jansons, T.I. Dyuzheva, L.M. Lityagina, N.A. Bendeliani, *Host-defect luminescence of stishovite,* - Ibid. p. 115, (poster presentation).
6. A. Sharakovsky, I. Tale, M. Springis, S. Jursenas, C.C. Yang, *Spectroscopy of charge localization states in InGaN/GaN multiquantum wells,* - Ibid. p. 132, (poster presentation).
7. M. Springis, A. Sharakovsky, I. Tale, U. Rogulis, *X-irradiation induced photo- and thermostimulated luminescence of $CsCdF_3$:Mn crystals*, - Ibid. p.137, (poster presentation).

International Workshop on Nitride Semiconductors IWN-2004, July 19-23, Pittsburgh, Pennsilvania USA

1. I. Tale, R. Evarestov, C.C. Yang, *LCAO calculation of defects in GaN,* - Abstract book of the International Workshop on Nitride Semiconductors IWN-2004, July 19-23, Pittsburgh, Pennsilvania USA, p. 32. (poster presentation).
2. M. Piesins, I. Tale, C.C. Yang, *Thermoactivation spectroscopy of charge localization states in InGaN/GaN quantum wells*, - Ibid. p. 32, (poster presentation).
3. I. Tale, M. Springis, A. Sharakovsky, C.C. Yang, *Spectroscopy of charge localization states in InGaN/GaN multiquantum wells,* - Ibid. p. 78, (poster presentation).
4. A. Zukauskas, K. Kazlauskas, G. Tamulaitis, J. Mickevicius, S. Jursenas, G. Kurilcik, S. Miasojedovas, M. Springis, I. Tale, Y.-Ch.Cheng, H.-Ch. Wang, Ch.-F. Huang, C.C. Yang, *Carrier localization effect in polarized InGaN/GaN multiple quantum wells,* - Ibid. P. 84, (poster presentation).

The 6-th International Summer Scool-Conference "Advanced materials and technologies", Palanga, Lithuania, 27-31 August 2004

1. M. Piesins, I. Tale, *Application of Deep-level Transient Spectroscopy in characterization of GaN based diode structure,* - Book of Abstracts of the 6-th International Summer Scool-Conference, Palanga, Lithuania, August 27-31, 2004, p. 45, (poster presentation).

DISORDERED MATERIAL PHYSICS

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

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Defect studies Group
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Research Area and Main Problems

The transient optical absorption due to electron polaron states in complex oxides $LiNbO_3$ $KNbO_3$, $SrTiO_3$, $KTaO_3$, YVO_4 have been studied. The electron polarons are identified to be Nb^{4+} ions in various oxygen environments in niobates. It is shown that the position of the absorption band depends on Nb environment.

The role of rare earth dopants in electron-hole trapping and relaxation process in complex oxides $Gd_3Ga_5O_{12}$, $LaGaO_3$, YAG, YAP have been studied.

The luminescence spectra and decay kinetics for ZnO and ZrO_2 nanopowders (grain size 10-70 nm) obtained by microwave driven hydrothermal synthesis were studied using time-resolved luminescence spectroscopy. The FTIR reflection spectra for investigation of nanopowders have been developed.

The experimental setup used pulse electron accelerator as an irradiation source. The electron pulse duration was 10 ns, electron energy was 270 keV and average density of electron beam was 10^{12} el.cm^{-2}. Xe-flash lamp working in pulse mode served as a probe light source for the absorption measurements. The signal from photomultiplier or IR detector was registered by digital oscilloscope TEKTRONIX TDS 5052.

The experimental set-up described above allows to investigate induced transient absorption and luminescence spectra as well as luminescence decay kinetics and induced absorption relaxation kinetics.

The optical properties of silicon dioxide-based glasses were studied by using Fourier-transform infrared spectrometer, visible-to ultraviolet spectrophotometer, vacuum-ultraviolet spectrometer and electron paramagnetic resonance spectrometer. Samples were irradiated by KrF and F_2 excimer laser light.

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4. Dr.hab.phys. D.Millers, Poland (14 days).
5. Dr.hab.phys. D.Millers, Poland (5 days)
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8. Dr.hab.phys. L.Skuja, USA (6 days)
9. Dr.hab.phys. L.Skuja, France (4 days)
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The main results

RADIATION DEFECTS IN UNDOPED AND Nd-DOPED $LaGaO_3$ CRYSTALS

T. Dudareva, L. Grigorjeva, D. Millers

Radiation induced defects have been studied in undoped and Nd-doped (6 mol% and 12 mol%) $LaGaO_3$ crystals. Wide absorption band (2.2 – 2.8 eV) was observed after crystal irradiation with x-rays at 300 K. Induced defects have been annealed in air at ~450 K. Similar absorption band was observed in transient absorption spectra after ns-pulsed electron beam excitation. The radiation defect creation efficiency is higher in undoped $LaGaO_3$ crystal. It is shown that small concentration of Nd-doping increases the $LaGaO_3$ crystal radiation hardness.
In transient absorption spectra along with 2.7 eV band the absorption bands at 1.5 eV and 2.2 eV were observed. The decay process of transient absorption has been studied.
The luminescence spectra and luminescence decay times for $^4F_{3/2} \rightarrow {}^4I_{9/2}$ and $^4G_{7/2} \rightarrow {}^4I_{9/2}$ transitions in Nd-doped crystals have been studied. Decay time decreases and additional fast decay component appears with Nd concentration increase. The interaction of Nd atoms with defects and Nd atoms aggregation processes has been discussed.

X-RAY AND PULSED ELECTRON BEAM EXCITED LUMINESCENCE AND OPTICAL ABSORPTION IN $KTaO_3$ CRYSTALS

D. Millers, L. Grigorjeva, V. Trepakov, S. E. Kapphan, L. A. Boatner

Nature of the electronic excitations, mobile charge curriers and charge transfer processes remain a hot topic for ABO_3 perovskite-like oxides. X-ray, pulsed electron beam excited time-resolved luminescence and transient absorption in $KNbO_3$, $SrTiO_3$ and $LiNbO_3$ crystals had been subject of our previous studies. The luminescence bands at 2.8 eV ($SrTiO_3$) and 2.75 eV ($LiNbO_3$) were attributed to the formation and recombination of electron and hole polarons. The present study is focused on nominally pure and Li-, Cu-doped $KTaO_3$ single crystals. $KTaO_3$ has an obvious advantage over $SrTiO_3$ in respect to polarons formation due to larger lattice constant (3.905 *Å* in $SrTiO_3$ and 3,989 *Å* in $KTaO_3$). It is found that under electron beam excitation the dominant luminescence band centred at ~ 2.75 eV for all $KTaO_3$ specimens. Another weak luminescence peaks at ~1.8 eV. The luminescence decay kinetics within these two bands is quite different indicating that the two different excited states are involved. In the transient absorption spectrum the optical density spreads to the long-wavelength side up to 0.75 eV. In nominally pure $KTaO_3$ the main absorption band peaks at <1.0 eV and ~1.7 eV, whereas in $KTaO_3$:Li at ~1.1 eV and 1.7 eV. The transient absorption decay varies over the spectrum revealing several short-lived centres involved into transient absorption formation.

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INTRINSIC LUMINESCENCE IN YTTRIUM TRIFLUORIDE

V.Pankratov, M.Kirm, H.von Seggern

Luminescence and excitation spectra as well as their temperature dependence were investigated for nominally pure yttrium trifluoride powders using synchrotron radiation. Broad emission bands in VUV-visible spectral range were observed under excitation above 11 eV in YF_3 at 10K. At least three emission bands were distinguished peaking at 5.6 eV, 4.5 eV and 3.1 eV. It was shown that the emission bands at 5.6 eV and 4.5 eV are intrinsic but the emission at 3.1 eV is of extrinsic nature. The excitation spectra for the two intrinsic luminescence bands have their individual features, but in both cases a sharp peak at the fundamental absorption edge is observed. This fact as well as a large Stokes shift of intrinsic luminescence (more than 5 eV) and a large width of the emission bands (neat 1 eV) allows us to assign the 4.5 eV and 5.6 eV luminescence to the radiative decay of self-trapped excitons in YF_3. The strong influence of temperature on the intrinsic luminescence, observed at temperatures above 120K, is used to evaluate the activation energy of thermal quenching.

In cooperation with:
Material Science Department, Institute for Electricacal Materials, Darmstadt
University of Technology
Institute of Physics, University of Tartu

LUMINESCENCE SPECTRA AND LUMINESCENCE DECAY KINETICS EXITED BY PULSE ELECTRON BEAM AND NINTROGEN LASER IN $ZnWO_4$ AND $CdWO_4$

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

The luminescence spectra and luminescence decay kinetics in $ZnWO_4$ (nominally pure and doped with Fe and Mo) under pulsed electron beam and pulsed nitrogen laser excitation have been studied. Two-stage intrinsic luminescence decay was observed only under electron beam excitation. It is suggested that different types of self-trapped exciton configuration were created under high-energy excitation. The role of Fe and Mo impurities for scintillation efficiency in $ZnWO_4$ and $CdWO_4$ has been analyzed.

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

OPTICAL INVESTIGATIONS OF TlBr DETECTOR CRYSTALS

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

Shift of fundamental absorption edge, the position of main luminescence bands, the luminescence decay and transient absorption spectra in different types of TLBr crystals were studied. The γ-quanta detectors were made from the same crystals. The detectors parameters was controlled and the role of impurities and crystal defects in detectors quality was studied.

In cooperation with: GIREDMET", B.Tolmachevskiy per.5, Moscow, Russia
Baltic Scientific Instruments, LV-10005, Riga, Latvia

LUMINESCENCE AND FTIR SPECTROSCOPY OF NANOPOWDERS

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

Nanocrystalline oxide powders is important materials and has been found to have commercial applications (sensors, pigments, rubber industry etc.). Nanostructured optical materials including transparent nanostructured ceramics might be possible obtained from nanocrystalline powders. These new materials are promising for applications in lasers and scintillators. The main interesting fundamental problems for the nanocrystalline oxide powders is the exciton quantum confinement effect, the electronic excitation transfer processes, the nanocrystal surface defects, and dopand incorporation.

The ZnO luminescence properties for the nanopowders free standing and embedded in PMMA and PS was studied. The luminescence spectra and intensity depends on nanopowder grain size as well as the synthesis conditions. It is shown that luminescence properties are quite different for ZnO nanopowders obtained by ammonia and urea synthes conditions. Luminescence at ~2.0 eV (due to defect states in ZnO crystals and nanopowders) was suppressed in nanopowders obtained by urea method. During the nanopowder synthesis some uncontrolled impurities were incorporated in nanocrystal

mainly at surface. Luminescence of functional organic groups on nanocrystal surface was observed. FTIR spectroscopy results and luminescence spectra shows that fractions of chemicals used in synthesis process could be found as impurities in nanopowders.
It is suggested that self-assembling functional organic groups blocked the defect states at nanocrystals surface.
The ZrO_2 exist in three polymorphs: monoclinic, tetragonal and cubic. The Zr oxygen surrounding for tetragonal and cubic phase is different. Thus, the luminescence from regular Zr-oxygen complex can be different for tetragonal and cubic phase. The luminescence of nanocrystalline tetragonal and cubic ZrO_2 has been investigated. The luminescence from tetragonal undoped reveals two bands, at ~2.0 eV and 2.7 eV, from cubic ZrO_2 one luminescence band at ~2.7 eV was observed. This luminescence was shown to be intrinsic. The regular zirconium-oxygen complex excited state is suggested to be responsible for intrinsic luminescence.
In cooperation with: High Pressure Research Center of the Polish Academy of Sciences, Warsaw, Poland.

ANOMALOUSLY EFFICIENT CREATION OF STABLE COLOR CENTERS IN WET SILICA GLASS BY HIGH-DOSE FLUORINE-EXCIMER LASER IRRADIATION

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

An anomalous accumulation of room temparature-stable color centers was observed in "wet" synthetic silica glasses under fluorine excimer laser irradiation at 80K. The currently accepted mechanism for defect generation predicts a nearly complete annihilation of defects upon warm-up above 250K, when radiolytic interstitial hydrogen atoms and molecules become mobile and saturate the radiation-induced dangling bonds. Contrary to this, up to 30% of dangling oxygen and silicon bonds induced by 7.9eV photons remained stable at 295K. Their principal origin is most probably the insertion of radiolytic interstitial hydrogen atoms into Si-O bonds excited by photons within the tail region of the fundamental absorption edge.
In cooperation with: Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Agency, KSP, Kawasaki, Japan.

DEFECTS IN OXIDE GLASSES

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

An insight into the present understanding of point defects in the simplest and the most radiation-resistant oxide glass, glassy silicon dioxide (silica) is presented. The defects and their generation processes in glassy and α-quartz forms of silicon dioxide are significantly different. The only defect, confirmed to be similar in both materials, is oxygen vacancy. In silica, additional defects of dangling bond type are generated from precursor sites formed by strained Si-O bonds, and by modifier ions. The optical absorption spectra of silica are dominated by paramagnetic dangling bond type defects: silicon dangling bond ("E'-center") and oxygen dangling bond ("non-bridging oxygen hole center, NBOHC"). Radiation-induced interstitial oxygen atoms exist in peroxy linkage (Si-O-O-Si) form, they

can react with oxygen dangling bonds to create peroxy radicals or dimerize into interstitial O_2 molecules. Hydrogen doping helps to reduce the defect concentration, however, creates new precursors in the form of hydroxyl groups and may stimulate O vacancy generation. Doping by fluorine reduces the number of strained Si-O bonds and results in glass, which has higher vacuum ultraviolet transparency and higher resistance to excimer laser light than pure silica.

In cooperation with: Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Japan and Transparent Electro-Active Materials Project, ERATO, Japan Science and Technology Agency, KSP, Kawasaki, Japan.

Scientific Publications

Published in 2004

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., v. 129, p.691-696 (2004).
2. D.Millers, L.Grigorjeva, W.Lojkowski, T.Strachwski. Luminescence of ZnO *nanopowders.* Radiaion Measurements*,* v.38, p.589-591 (2004).
3. P.Potera, L.Grigorjeva, A.Matkovskii, D.Millers, T.Lukasiewicz, Z.Galazka, T.Wojciechowski. *Time-resolved opticalazbsorption in YAP crystals*. Radiation Measuruments, v. 38, p.371-374 (2004).
4. L.Grigorjeva, D.Millers, M.Shorohov, I.S.Lisitskii, M.S.Kuznecov, S.Zatoloka, V.Gostilo. *Optical investigations of TlBr detector crystals.* Nuclear Instruments and Methods in Physics Research A, v.531, p.197-201 (2004).
5. L.Grigorjeva, D.Millers, V.Trepakov, S.Kapphan. *Luminescence in $SrTiO_3$ and $LiNbO_3$ crystals under high density pulsed electron beam excitation.* Ferroelectrics, v.304, p.117-123 (2004).
6. S.Chernov, L.Grigorjeva, D.Millers, A.Watteri`ch. *Luminescence spectra and decay kinetics in $ZnWO_4$ and $CdWO_4$ crystals*. Phys.Stat.Sol.(b), v.241, No.8, p.1945-1948 (2004).
7. A.Matkowskii, P.Potera, D.Sugak, L.Grigorjeva, D.Millers, V.Pankratov, A.Suchocki. *Stable and transient color centers in Gd_3 Ga_5 O_{12} crystals*. Cryst.Res.Technol., v.39. No.9, 788-795 (2004).
8. K. Kajihara, L.Skuja, M.Hirano, H.Hosono *Role of Mobile Interstitial atoms in defect processes in oxides: Interconversion between oxygen-associated defects in SiO_2 glass.* Phys. Rev. Letters vol.92, No1, p.015504-(1-4) (2004).
9. 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 v.345-346, p.219-223 (2004).
10. 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 v.345-346, p.328-31 (2004).
11. K. Kajihara, Y. Ikuta, M. Oto, M. Hirano, L. Skuja, H. Hosono *UV-VUV laser induced phenomena in SiO_2 glass.* Nucl. Instr. Meth. Phys. Res, vol B218 p. 323 –331 (2004).
12. K. Kajihara, T. Miura, H. Kamioka, M. Hirano, L. Skuja and H.Hosono, *Surface dissolution and diffusion of oxygen molecules in SiO_2 glass.* J. Ceram. Soc. Japan,vol. 112, No10, p.559-562 (2004).

13. 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 v.349, p.205-208 (2004).
14. K. Kajihara, H. Kamioka, M. Hirano, T.Miura, L. Skuja, H. Hosono, *Dissolution and diffusion of oxygen molecules in SiO_2 glass measured by photoluminescence*, Proc. XX Internat. Congr. Glass, Kyoto, Sept.27-Oct.1 2004, paper O-07-11, p.1-4.
15. L. Skuja, K. Kajihara, M. Hirano, H. Hosono, *Anomalously Efficient Creation of Stable Color Centers in Wet Silica Glass by High-Dose Fluorine-Excimer Laser Irradiation.*, Proc. XX Internat. Congr. Glass, Kyoto, Sept.27-Oct.1 2004, paper O-14-052, p.1-6.

In Press

1. V.Pankratov, M.Kirm, H.von Seggern. *Intrinsic luminescence in yttrium trifluoride*. J.of Luminescence, (2004).
2. V.Pankratov, M.Kirm, H.von Seggern. *Exciton emission and defect formation in yttrium trifluoride***.** Phys.stat.sol., (2005).
3. D. Millers, L. Grigorjeva, V. Trepakov, S. E. Kapphan L. A. Boatner. *X-ray and pulsed electron beam excited luminescence and optical absoption in $KTaO_3$ crystals*. Phys.stat.sol., (2005).
4. D.Millers, L.Grigorjerva, W.Lojkowski and A.Opalinska. *Luminescence of ZrO_2 nanocrystals*. Solid State Phenomena, (2005).
5. T.Dudareva, L.Grigorjeva, D.Millers*. Radiation defects in undoped and Nd-doped $LaGaO_3$ crystals.* Phys.Stat.Sol., (2005).
6. A.Matkovskii, P.Potera, L.Grigorjeva, D.Millers, T.Lukasewicz, Z.Galazka. *Transient color centers in complex oxide crystals*. Phys.Stat.Sol. (2005).
7. S.Chernov, D.Millers, L.Grigorjeva. *Luminescence center formation under pulse electron beam excitation in $PbWO_4$ and $ZnWO_4$ crystals*. Phys.Stat.Sol. (2005).
8. L.Skuja, M.Hirano, H.Hosono, K.Kajihara, Defects in Oxide Glasses. phys. stat. sol. (c) vol. 2, No. 1, p. 15 –24 (2005).
9. K. Kajihara, L. Skuja, M.Hirano, H. Hosono, *Decomposition of peroxy radicals in SiO_2 glass with X-rays or KrF laser light.* phys. stat. sol. (c) vol. 2, No. 1, p. 314 –317 (2005).
10. K. Kajihara, L. Skuja, M. Hirano, H. Hosono *In-situ observation of diffusion of hydrogenous species in F_2 -laser-irradiated SiO_2 glass using a pump and probe technique*, Phys.Rev.B.

Lectures at Conferences

Annual Meeting of American Association for the Advancement of Science, Feb.12-16, 2004, Seattle,USA

L. Skuja *The Optical Properties Of Fundamental Defects In Silica Glasses.* Abstract A13.

20. Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, 16-18. February, 2004

1. D.Millers. L.Grigorjeva, *Luminescence properties of oxide nanocrystals* Abstracts, p.67.
2. S.Chernov, D.Millers. Recombinative creation of self-trapped excitons in lead and zink tungstates. Ibid, p.88.
3. T.Dudareva. *Radiation induced defectts in $LaGaO_3$ crystals*. Ibid, p.89.
4. L.Grigorjeva, D.Millers. *Fourier transformation infrared spectroscopy informative resources. Ibid.*, p. 92.
5. A.Siliņš, *Light-emitting defect reactions in glasses. Ibid,* p.77.
6. L. Skuja, K.Kajihara, H.Hosono, M.Hirano. *Interstitial oxygen atoms in radiation processes in glassy SiO_2. Ibid.,* p.78.

The 15th International Conference on Defects in Insulating Materials (ICDIM-2004), July 11-16, 2004, Riga, Latvia

1. V.Pankratov, M.Kirm, H.von Seggern. *Exciton emission and defect formation in yttrium trifluoride***.** Phys.stat.sol., (2005). Abstracts, p.17.
2. A.Matkovskii, P.Potera, L.Grigorjeva, D.Millers, T.Lukasewicz, Z.Galazka. *Transient color centers in complex oxide crystals*. Abstracts, p.52.
3. D.Millers, L. Grigorjeva, V. Trepakov, S. E. Kapphan L. A. Boatner. *X-ray and pulsed electron beam excited luminescence and optical absoption in $KTaO_3$ crystals*. Abstracts, p.58.
4. T.Dudareva, L.Grigorjeva, D.Millers. *Radiation defects in undoped and Nd-doped $LaGaO_3$ crystals.* Abstracts, p.91.
5. S.Chernov, D.Millers, L.Grigorjeva. *Luminescence center formation under pulse electron beam excitation in $PbWO_4$ and $ZnWO_4$ crystals*. Abstracts, p.100.
6. L.Skuja, *Defects in oxide glasses*. Abstracts, p.18.
7. K. Kajihara, H.Kamioka, T,Miura, M.Hirano, L. Skuja, H. Hosono, *Photoluminescence decay of interstitial oxygen molecules in SiO_2 glass*. Abstracts, p.19.

European Material Research Society 2004 Fall Meeting, 6th –10th September, 2004, Warsaw, Poland

1. R.R.Piticesku, C.Monty, L.Grigorjeva. *Hydrothermal synthesis of nanostructured zirconia materials: present state and future prospects.* Abstracts, p.46.
2. T.Strachowski, E.Reszke, L.Perchuc, E. Grzanka, A.Preesz, T.Chudoba, W.Lojkowski, L.Grigorjeva, D.Millers. *Influence of synthesis conditions on the particles size and morphology of zinc nanopowders.* Abstracts, p.202.
3. L.Grigorjeva, W.Lojkowski, D.Millers, T.Strachowski. *Molecular impurities in the luminescent ZnO nanocrystals*. Abstracts, p. 205.
4. D.Millers, W.Lojkowski, L.Grigorjeva, A.Opalinska. *Luminescence of ZrO_2 nanocrystals*. Abstracts, p.218.

6th Internat. Summer School-conference "Advanced materials and technologies", Aug. 27-31, 2004, Palanga, Lithuania
L.Skuja, *Advanced glassy materials for optical fibers, ultraviolet and laser optics*. Abstracts, p.10.

XX International Congress on Glass, Sept.27-Oct.1 2004, Kyoto, Japan
1. L. Skuja, K. Kajihara, M. Hirano, H. Hosono*, Anomalously Efficient Creation of Stable Color Centers in Wet Silica Glass by High-Dose Fluorine-Excimer Laser Irradiation.* Paper O-14-052.
2. Silins, *Light Emitting Defect Reactions In Fused Silica.* Paper O-07-074.
3. K. Kajihara, H. Kamioka, M. Hirano, T.Miura, L. Skuja, H. Hosono, *Dissolution and diffusion of oxygen molecules in SiO_2 glass measured by photoluminescence.* paper O-07-11.

SOLID STATE OPTICS LABORATORY

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

Research area and Main Problems

The electronic excitations, intrinsic and impurity defect of the ordered materials (crystals) and the disordered material (optical glasses) are the main object of Solid State Optics Laboratory of DMP.

Electronic structure and electronic processes of crystalline and glassy materials was studied. The localized states are studied in details. The 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. Raphael Blum, Universite Paris Sud, Orsay, Lab. Labo. Physico-Chimie des Solides, France. 1 month.

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.

Cooperation

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

L.F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia (Dr. N.A.Bendeliani)

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)

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

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

Main Results

LUMINESCENCE AND IRRADIATION DAMAGE OF SILICON DIOXIDE BY ELECTRON BEAM

Anatoly Trukhin, Christian Haut*, Anne-Sophie Jacqueline*, Bertrand Poumellec*

Luminescence and radiation damage under electron beam of germanium-doped crystalline α-quartz, pure silica glass with different deficiency of oxygen and thin film of silicon dioxide on silicon were studied. Luminescence and optical absorption spectra were

measured at room temperature. The profile of the radiation damage was measured. The main effects are:
1. The transformation of the Ge center in crystal to the Ge related oxygen deficient center (GeODC) of glassy state was not found in spite of observation of an amorphous phase of the irradiated germanium doped α-quartz crystal. At small dose (0.1 C/cm^2) an expansion of the irradiated volume was observed. At high dose (>1 C/cm^2) a dilatation of the irradiated surface takes place.
2. In thin film of amorphous silicon dioxide on silicon the bulk NBO and the SiODC luminescence grows practically from a negligible initial level.
3. Pure silica samples with a different level of oxygen deficiency provide luminescence of SiODC centers under e-beam already at a low dose. Strongly deficient sample gives decrease of SiODC luminescence with dose, whereas more stoichiometric sample gives increase of luminescence with dose. The observed dilatation of the surface could be restored after heating to 1000 C. Therefore it is connected with densification of the irradiated volume. The CL spectrum of pure silica has additional red band of the NBO, when densification occurs.
Therefore, beside densification of silica glass volume the three principal centers are recognized through absorption and luminescence in radiation processes under electron beam. These are: SiODC, NBO and E' center.

**In cooperation with: Physico-Chimie de l'Etat Solide, Bat. 414, Université Paris Sud, Orsay 91405 France*

UV CATHODOLUMINESCENCE OF CRYSTALLINE α-QUARTZ AT LOW TEMPERATURES

A. Trukhin[a], P. Liblik*, Ch. Lushchik*, J. Jansons

Two luminescence bands in the UV range were detected in crystalline α-quartz under electron beam excitation (6 kV, 3-5 μA). One band is situated at 5 eV and could be observed in pure samples. Its intensity increases with cooling below 100 K and undergoes saturation below 40 K alongside a slow growth with the time of irradiation at 9 K. The decay curve of the band at 5 eV contains two components, a fast (< 10 ns) and a slow one in the range of 200 μs. The photoluminescence band at 5 eV with a similar temperature dependence was found in previously neutron-irradiated crystalline α-quartz. Therefore, the band at 5 eV was attributed to host material defects in both irradiation cases. The creation mechanism of such defects by electrons, the energy of which is lower than the threshold for a knock-out mechanism of defect creation, is discussed. Another band at 6 eV, containing subbands in different samples, appears in the samples containing aluminum, lithium and sodium ions. This luminescence is ascribed to a tunnel radiative transition in an association of (alkali atom)^o-$[AlO_4]^+$ that is formed after the trapping of an electron and a hole by Li^+ (or Na^+) and AlO_4.
**In cooperation with: Institute of Physics, University of Tartu, Estonia*

INTRINSIC ABSORPTION THRESHOLD OF STISHOVITE AND IT HOST-DEFECT'S LUMINESCENCE

Anatoly N.Trukhin, Tatyana I.Dyuzheva*, Ludmila M.Lityagina*, Nikolai A.Bendeliani*

The optical absorption spectra of the small mono-crystals samples of stishovite and coesite were studied at first. The intrinsic absorption threshold of sitshovite is determined at 8.75 eV, being, probably, highest in the family of different crystalline polymorph modifications of silicon dioxide. The absorption spectrum of stishovite is independing on temperature (studied in the range 290-450 K). The intrinsic absorption threshold of coesite mono-crystal is situated near 8.6 eV at 293 K, coincides within experimental errors with that of □-quartz crystal, and depends on temperature, as use to be for the tetrahedron structured silicon dioxide crystalline modifications. A broad absorption band with a first spread maximum near 7.6 eV sides with intrinsic absorption threshold was found in the stishovite mono-crystal sample. It low intensity (about 10 cm^{-1}) in an as-received sample shows on a defect nature of this band. No analogous band was detected in the sample of coesite.
**In cooperation with: L.F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia*

LUMINESCENCE OF FLUORINE-DOPED AND NON-DOPED SILICA GLASS EXCITED WITH ARF LASER

Anatoly N. Trukhin, Margarita F. Kink*, Yuri A. Maksimov*, Rein A. Kink* Tatyana A Ermolenko*, Ivan I. Cheremisin*

The role of fluorine doping on silica was studied through comparison of luminescence of fluorine doped and fluorine-free samples made on KS-4V technology and excited by ArF laser (6.4 eV) at liquid helium temperatures. The fluorine doped sample possesses very weak absorption band at 7.6 eV on the level of 0.1 cm^{-1} and there the photoluminescence of so call oxygen deficient centers with blue (2.7 eV) and UV band (4.4 eV) could be excited. The same luminescence bands are observable in fluorine-free sample, containing the absorption band at 7.6 eV on the level of 20 cm^{-1}. In fluorine-doped sample the UV band prevails the blue band. The effect is explained as fluorine quenching influence on intra-center transitions probabilities and the fast UV luminescence is less affected than the long-living blue luminescence. The photoluminescence spectral, decay kinetics and temperature dependences were measured under ArF laser (6.4 eV. The main effect is observation of components of decay for UV band in the microsecond range of time, which is slower than usual decay detectable in ns range of time. The blue band also possesses decay in microseconds range of time, being much faster than "normal" decay of this band in millisecond range of time. Decay becomes faster, however intensity increases with increasing of the temperature showing on atomic (ionic) mobile particle participation in recombination processes. The parameters of kinetics are slightly different in fluorine doped and fluorine-free samples. The observed effects were explained in framework of recombination process of defect created under ArF laser excitation.
**In cooperation with: Institute of Physics, University of Tartu, Estonia, Institute of Silicate Chemistry, RAS, St-Petersburg,*

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, Bat. 414, Université Paris Sud, Orsay 91405 France*

LUMINESCENCE OF SILICA GLASS CONTAINING ALUMINUM OXIDE

A. N. Trukhin, J.L.Jansons, K.Truhins

Optical properties of silica glass with different doping of Al_2O_3 up to 1.5 mol. % were studied. Alumina stimulates creation of a luminescence centers with specific band at 3.3 eV. A new band at 8.2 eV appears in luminescence excitation spectra. There is transport of energy to other luminescence centers associated with an impurity (Ag, Ce) at this energy. Alumina stimulates creation of E' centers under γ - irradiation beside trapped hole on AlO_4 tetrahedron as well as creation of a silicon related oxygen deficient center (SiODC) under cathodoexcitation. Visually, the samples look inhomogeneous even after γ - irradiation. The explanation could be heterogeneity of the samples. Alumina doped samples contain alkali ions, which were revealed with the use of silver exchange electrolysis experiments.

LUMINESCENCE OF γ-RADIATION-INDUCED DEFECTS IN α-QUARTZ

M Cannas*, S Agnello*, FM Gelardi*, R Boscaino*, A N Trukhin
P Liblik, C Lushchik**, MF Kink**, Y Maksimov**, RA Kink****

Optical transitions associated with γ-radiation-induced defects in crystalline α-quartz were investigated by photoluminescence excited by both pulsed synchrotron radiation and steady-state light. After 10 MGy γ-dose we observed two emissions at 4.9 eV (ultraviolet band) and 2.7 eV (blue band) excitable in the range of the induced absorption band at 7.6 eV. These two luminescence bands show a different temperature dependence: the ultraviolet band becomes bright below 80 K, the blue band increases below 180 K, but drops down below 80 K. Both emissions decay in a timescale of a few ns under pulsed

excitation, however the blue band could be also observed in slow recombination processes and it afterglows in about 100 s at the end of steady-state excitation. The origin of the observed luminescence bands and the comparison with optical features of oxygen-deficient centres in silica glass are discussed in the framework of different models proposed in literature.

*In cooperation with: Istituto Nazionale per la Fisica della Materia and Dipartimento di Scienze Fisiche ed Astronomiche dell'Università, via Archirafi 36, I-90123 Palermo, Italy;
**Institute of Physics, University of Tartu, Riia 142, 51014 Tartu, Estonia

Scientific publications

1. 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- Vol 129/5 (2004) pp 285-289.
2. A.Trukhin, P. Liblik, Ch. Lushchik, J. Jansons, *UV cathodoluminescence of crystalline α-quartz at low temperatures*, Journal of Luminescence (2004) Vol 109/2 pp 103-109.
3. A.N.Truhins, J.L.Jansons, T. I.Dyuzheva , L. M. Lityagina , N. A.Bendeliani, *Intrinsic absorption threshold of stishovite and coesite*, Solid State Communications, (2004) Reference: SSC7340, Vol 131/1 pp 1-5
4. A. N. Trukhin, M.Kink, J.Maksimov, R.Kink, T. A. Ermolenko and I. I. Cheremisin, *Luminescence of fluorine-doped and non-doped silica glass excited with an ArF laser*, Journal of Non-Crystalline Solids 342/1-3 pp. 25-31
5. Marco Cannas, Simonpietro Agnello, Roberto Boscaino, Franco M.Gelardi, Anatoly Trukhin, *Photoluminescence in γ-irradiated α-quartz investigated by synchrotron radiation,* Radiation Measurements 38 (2004) 507 –510.
6. A.N.Trukhin, J.L.Jansons, K.Truhins, *Luminescence of silica glass containing aluminum oxide*, Journal of Non-Crystalline Solids 347/1-3 (2004) pp. 80-86 Journal of Non-Crystalline Solids 347 (2004)80 -86
7. A. Trukhin, P. Kulis, J. Jansons, T. Dyuzheva, L. Lityagina, N. Bendeliani, *Host-defect Luminescence of Stishovite*, the 15 international conference on defects in Insulating materials (ICDIM 2004), book of abstracts, Riga, Latvia, p.115
8. MCannas, SAgnello, FMGelardi, RBoscaino, A N Trukhin, P Liblik, C Lushchik, M FKink, Y Maksimov and R A Kink, *Luminescence of γ-radiation-induced defects in α-quartz,* J. Phys.: Condens. Matter 16 (2004) 7931–7939.

Lectures in Conferences

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

1. Anatoly Trukhin, Christian Haut, Anne-Sophie Jacqueline, Bertrand Poumellec, *Luminescence and irradiation damage of silicon dioxide by electron beam*, 20. CFI LU Zinātniskās konferences referātu tēzes, Rīga, Latvija, 16.-18. Februāris 2004, 79.lpp.

The 15 international conference on defects in Insulating materials (ICDIM 2004)

1. A. Trukhin, P. Kulis, J. Jansons, T. Dyuzheva, L. Lityagina, N. Bendeliani *Host-defect Luminescence of Stishovite*, the 15 international conference on defects in Insulating materials (ICDIM 2004), book of abstracts, Riga, Latvia, p.115

Lectures at Universities, Institutes, Companies

Trukhin A., *Purity of natural crystalline quartz detected by luminescence,* Irkutsk, Institute of Geochemistry

Awards

A.Truhins. Years' award in physics and engineering applications of Latvian Academy of Science and ALFA corporation for creation of a new direction of scientific investigations Physics of the optical crystals and glasses in Latvia".

PHYSICS OF FERROELECTRICS

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

Research Area

The research issues of the Division of Ferroelectric Physics includes various aspects of theoretical modelling, sample production related material synthesis, processing and characterization of ferroelectrics. Synthesis of ceramics is based on chemical coprecipitation and two stage hot pressing technologies. Production of thin films is made by pulsed laser ablation or sol-gel deposition techniques. Characterization methods include x-ray diffraction, dielectric spectroscopy and hysteresis measurements, atomic force microscopy, optical reflectometry and ellipsometry 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.

Main research topics in 2004

Theoretical Modelling of Relaxation Dynamics of Metastable Systems: Application to Non-Equilibrium Condensed Matter

- Polarization Microstructure in Ferroelectrics: Imaginary Time Schrödinger Treatment.

Synthesis of Ferroelectric Ceramics and Investigation of Microstructure

- New Ceramic Compositions Based on $PbSc_{1/2}Nb_{1/2}O_3 - PbTm_{1/2}Nb_{1/2}O_3$ System;
- Investigation of PLZT Ceramics Processing – Microstructure Relationships;
- Production of Transparent Electrooptic PLZT Ceramics for Vision Science Applications, Synthesized by Hydroxopolymer and Sol-Gel Methods.

Dielectric Properties of Perovskite Ferroelectric Relaxor Thin Films

- Dielectric Impedance Fourier Spectroscopy and Characterization of Functional Films.

Nanoscale Piezoresponse and Electrostatic Force AFM Imaging and Patterning of Ferroelectric and Ferroelectric Relaxor Thin Films

- Piezoeresponse Imaging of Domain Structure and Electric Lithography;
- Surface Electrostatic and Capacitance Imaging.

Determination of Thickness and Refractive Index of Thin Films by Optical Reflectometry and Ellipsometry

- Thickness Effects on Optical Properties of $BaTiO_3$ Thin Films;
- Non-Destructive Diagnostics of Passive Electrode Interface Layers;
- Optical Constants for Data Evaluation of Optical Second Harmonic Experiment Data.

Irradiation Effects on Ferroelectric and Antiferroelectric Thin Films for Future Thermonuclear Reactor Diagnostics Applications

- Intensive Neutron Irradiation Effects on Sol-Gel $PbZrO_3$ and $PbZr_{1-x}Ti_xO_3$ Thin Films;
- Physical Properties of Ferroelectric and Antiferroelectric Thin Films After Electron Irradiation.

Optical Materials for Vision Science

- Light Scattering and Depolarization in PDLC Optical Phantoms Used for Simulation of Eye Cataract;
- Electrically Controlled Eye Occluders Based on Electrically Induced Light Scattering in Vision Science;
- Application of PLZT and PDLC Passive and Active Optical Elements in Infrared Laser Systems for Bio-Optical Experiments and Medicine.

Scientific staff

1. Dr. phys. Eriks Birks
2. Dr. phys. Karlis Bormanis
3. Dr. sc. ing. Maruta Dambekalne
4. Dr. habil. phys. Vilnis Dimza
5. Dr. phys. Jevgeņijs Kaupuzs
6. Dr. phys. Eriks Klotins
7. Dr. habil. phys. Andris Krumins
8. Dr. phys. Anatolijs Mishnovs
9. Dr. habil. phys. Maris Ozolins
10. Dr. habil. phys. Andris Sternberg
11. Dr. phys. Marina Tjunina
12. Dr. phys. Vismants Zauls
13. Dr. habil. phys. Juris Zvirgzds
14. Mg. chem.. Maija Antonova
15. Mg. phys. Laila Chakare-Samardzija
16 Mg. phys. Karlis Kundzins

Technical staff

1. Mg. phys. Maris Kundzins
2. Mg. phys. Maris Livins
3. Mg. phys. Astrida Spule
4. Mg. chem. Marite Kalnberga
5. Mg. chem. Anna Kalvane
6. Ing. Modris Logins
7. Ing. Alberts Tupulis

Doctorants

1. Mg. phys. Ilze Aulika

Students

1. Reinis Arajs
2. Martins Granats
3. Andris Mikuls
4. Peteris Spels
5. Olga Zoldaka

Visitors from Abroad

1. Raivo Jaaniso, Institute of Physics, University of Tartu, Estonia (1 month);
2. Andrey Kholkine, Aveiro University, Portugal (1week).

Scientific Visits Abroad

Mg. **Maija Antonova**

1. 4th International Conference on Advanced Optical Materials and Devices, Tartu, Estonia (1 week).

B. sc. **Ilze Aulika**

1. Atomic Institute of the Austrian Universities, Vienna, Austria (2×1 month).

Dr. phys. **Karlis Bormanis**

1 The International Jubilee Conference "Single Crystals and Their Application in the XXI Century – 2004", VNIISIMS, Alexandrov, Russia (1 week).
2. 4th International Conference on Advanced Optical Materials and Devices (AOMD-4), Tartu, Estonia (1 week).
3. 7th European Conference on Applications of Polar Dielectrics "ECAPD 7", Liberec, Czech Republic (1 week).
4. The XXI International Conference on Relaxation Phenomena in Solids (RPS-21), Voronezh, Russia (1 week).

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

1. 9th International Conference on Electroceramics and their Applications, Cherbourg, France (1 week).
2. 4th International Conference on Inorganic Materials, Antwerp, Belgium (1 week).
3. 4th International Conference on Advanced Optical Materials and Devices, Tartu, Estonia (1 week).

Mg. chem.. **Anna Kalvane**

1. 4th International Conference on Advanced Optical Materials and Devices, Tartu, Estonia (1 week).

Dr. phys**. Eriks Klotins**

1. 9th International Conference on Electroceramics and their Applications, Cherbourg, France (1 week).
2. 20th General Conferenceof the EPS Condensed Matter Division, Prague, Czech Republic (1 week).
3. 1st International Workshop on Smart Materials and Structures, Kiel, Germany (2 days).

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

1. International Exhibition "Hannovere Messe", Hannovere, Germany (1 week).
2. Presentation of Excellence Centre, Prague, Czech Republic (1 week).
3. University of Tartu, Tartu, Estonia (3 days).

Mg. phys. **Karlis Kundzins**

1. MaxPlanck Institute for Plasma Physics and EFDA Close Support Unit, Garching, Germany (11 days).
2. Association Euratom-CEA, Cadarache, France (1 week).

Dr. phys. **Anatolijs Mishnovs**

1. IX European Powder Diffraction Conference, Prague, Czech Republic (1 week).

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

1. Vilnius University, Lithuania (1 week).
2. Tartu University, Estonia (1 week).
3. LRPC Clermont-Ferrand, France (1 week).
4. Murcia University, Spain (1 week).

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

1. European Science Foundation Committee, Brussels, Belgium (2 weeks).
2. ERA – NET Workshop, Brussels, Belgium (3 x 4 days).
3. EFDA Meeting, Brussels, Belgium (1 week).
4. International Exhibition "Hannovere Messe", Hannovere, Germany (1 week).
5. Presentation of Excellence Centre, Prague, Czech Republic (1 week).
6. ERA – NET Workshop, Luxemburg (3 days).
7. International Conference "Plasma-2004", London, United Kingdom (3 days).
8. 7th European Conference on Applications of Polar Dielectrics "ECAPD 7", Liberec, Czech Republic (1 week).
9. 23th Symposium on Fusion Technology, Venice, Italy (1 week).
10. COST Technical Committee of Physics Meeting, Strasbourg, France (3 days).
11. International Conference on Fusion Energy Sources, Paris Polytechnical Institute, Paris, France (4 days).
12. COST - 525 Meeting, Limerick, Ireland (5 days).
13. Meeting on Material Science and Fusion Energy Sources, Brussels, Belgium (2 days).
14. University of Tartu, Tartu, Estonia (3 days).

Dr. phys. **Vismants Zauls**

1. MaxPlanck Institute for Plasma Physics and EFDA Close Support Unit, Garching, Germany (11 days).
2. Association Euratom-CEA, Cadarache, France (1 week).
3. European Network on Polar Electroceramics Meeting at Instituto de Ciencia de Materiales de Madrid (ICMM), Spain (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:
6. Laboratory of Optical Recording (Dr. J. Teteris);
7. Laboratory of Organic Materials (Prof. I. Muzikante);
8. EXAFS Spectroscopy Laboratory (Dr.habil. J. Purans).

Austria

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

Belorussia

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

Estonia

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

Finland

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

France

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

Germany

1. MaxPlanck Institute for Plasma Physics and EFDA Close Support Unit, Garching, (Dr. L. Giannone)
2. Institute of Optics, Berlin Technical University (Prof. H.J. Eichler).
3. Institute for Lasertechnology in Medicine, Ulm University (Prof. R. Steiner).

Japan

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

Lithuania

1. Vilnius University, Vilnius (Prof. J.Grigas, Prof. J. Banys).
2. Vilnius University Laser Research Centre (Prof. R. 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, Mg. W. Smiga).
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. Kholkine).

Russia

1. Ural State University, Ekaterinburg (Prof. V. Shur).
2. Volgograd State Architectural and Engineering Academy, Volgograd (Dr. phys. A. Burkhanov).
3. Russian Academy of Science, Moscow (Prof. A. Medovoi).
4. Joint Institute for Nuclear Research, Dubna (Dr. S. Tiutiunnikov, Dr. V.V. Jefimov).
5. Moscow State University, Moscow (Prof. B.A. Strukov).
6. Tver State University (Dr. O.V. Malyshkina).
7. 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).
2. CIEMAT, Madrid (Dr. E. Hodgson).

Sweden

1. Liquid Crystal Group, Chalmers TH, Gotheborg (Prof. L. Komitov).
2. Medical Laser Centre Lund University (Prof. S. Svanberg).

Ukraina

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

Main Results

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

E. Klotins

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This research deals with new applications for methods of quantum statistics in non-equilibrium condensed matter and is addressed to nonadiabatic behavior of macroscopic metastable systems. Namely, the canonical solutions of Schrödinger equation for pure quantum problems are reformulated for application to the probability distribution of the order parameter. Key advantages of this mathematical technique inherited from its quantum counterparts are the norm conservation and the obtaining an auxiliary function from which

observable quantities can be computed. Preliminary results [1] concern dynamic hysteresis of electric polarization in a model system specified by Ginzburg-Landau energy functional and its extensions toward weak nonlocality [2]. A more realistic approach addressed to finite size and spatially inhomogeneous systems goes beyond this canonical representation and models an assembly of coarse grained metastable particles with attractive interaction. A solution exhibiting specific features of phase instability - ground state bifurcation and divergence of relaxation time – in presence of the metastability, nonlocality, high driving and thermal noise is found the first time in [3,4]. Available extensions of the physical background include supplementary terms in the energy functional. Examples are electroelastic interactions [5], the spatial extended problems in general [6], and the connection with first principle results. Above mentioned analysis is illustrated by polarization switching [7].

References

[1] E. Klotins, J. Hlinka and J. Kaupužs. *Semiadiabatic High-Field Polarization Response in Ferroelectrics I: Hysteresis and Nonlinear Susceptibility*. (Ferroelectrics, in press).

[2] E. Klotins. *Relaxation Dynamics of Metastable Systems: Application to Polar Medium.* PHYSICA A, 2004, Vol. **340**, pp. 196 – 200.

[3] E. Klotins , V. Shvartsman, I. Bdikin, and A. Kholkin. *Imaginary Time Schrödinger Treatment for Microstructure Modeling in Ferroelectrics.* (In process of preparing the ISIF 2004 Proceedings for publication).

[4] E. Klotins. Theory and Modeling of Polarization Switching in Ferroelectrics. *(accepted for Journal of Electroceramics).*

[5] J. Hlinka, E. Klotins. *Application of Elastostatic Green Function Tensor Technique to Electrostricton in Cubic, Hexagonal and Orthorhombic Crystals*. J. Phys.: Condens. Matter, 2003, Vol. **15**, pp. 5755-5764.

[6] J. Kaupužs, J. Rimshans. *Polarization Kinetics in Ferroelectrics with Regard to Fluctuations.* Reprint arXiv:cond-mat/0405124, 05/2004.

[7] E. Klotins. *Symplectic Integration Approach to Nonadiabatic Polarization Response in Ferroelectrics.* (PHYSICA E , submitted).

NEW FERROELECTRIC MATERIALS ON THE BASIS OF $PbSc_{1/2}Nb_{1/2}O_3 – PbTm_{1/2}Nb_{1/2}O_3$

M. Dambekalne, M. Kalnberga, M. Livinsh, A. Mishnovs, and A. Spule

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Original binary solid solutions system of $(1-x)PbSc_{1/2}Nb_{1/2}O_3$-$xPbTm_{1/2}Nb_{1/2}O_3$ [(1-x)PSN-xPTmN)] have been produced.

Our purpose was to investigate possibility to synthesize solid solutions of (1-x)PSN-xPTmN, to study formation process and sequence of phases during thermal treatment, structure and properties.

Synthesized powders of (1-x)PSN-xPTmN solid solutions, obtained by solid state reactions from high purity grade oxides Sc_2O_3, PbO, Nb_2O_5 and chemically pure thulium hydrocarbonate $Tm_2(CO_3)_3{\cdot}3H_2O$ were used for producing ceramic samples.

Differential thermal and X-ray diffraction analysis were used to investigate sequence of phases formed during thermal treatment from 200 ^oC till 1000 ^oC phase constitution.

It was found that the three sharp endothermic effects on all thermograms of the compositions tested in the interval from 100 ^{o}C to 670 ^{o}C are due to the processes of decomposition of $Tm_2(CO_3)_3.3H_2O$ which take place in 3 stages: at 160 ^{o}C (evaporation of moisture), 320 ^{o}C (evaporation of crystallized water) and 580 ^{o}C (decomposition of the carbonates). The total loss of mass (33.8%) is in a good agreement with the calculated value (34.5 %). The decomposition process of thulium hydrocarbonate was completed at 670 ^{o}C. Decomposition of thulium hydrocarbonate proceeds simultaneous-ly with the formation of the first intermediate compound - $2PbO{\cdot}Nb_2O_5$ as suggested by a pronounced exothermic effect at 670 ^{o}C (for pure PTmN) and 630 ^{o}C (for solid solution). The reactivity of Tm_2O_3, released at decomposition of thulium hydrocarbonate, is enhanced considerably, and formation process of PTmN and solid solutions of PSN-PTmN is more intensive. Two-staged synthesis was used to facilitate the interaction of precursors and so eliminate the undesired pyrochlore phase: the first one was made for 1-2 hours at 960 ^{o}C –1110 ^{o}C depending on composition, the second - for 2 hours at 980 ^{o}C –1250 ^{o}C. The highest calcinations temperature is in case of PSN 1250 ^{o}C, lowest in case of PTmN.

Ceramic samples were hot pressed under the pressure of 20 MPa during 1-4 hours, the temperature being adjusted within the 1150 ^{o}C –1200 ^{o}C interval, depending on the particular component ratio, for 0.5-2.5 hours. At room temperature PSN has a rhombohedral distortion of the unit cell: a = 4.080 Å, $\alpha = 89.89^{0}$. Pure PTmN is an antiferroelectric. Transition from the antiferroelectric phase to paraelectric phase is observed at T_{max} = 303 ^{o}C. Solid solutions of (1-x)PSN - xPTmN with x = 0-0.5 have perovskite structure, solid solutions with x = 0.6-1.0 has a tetragonal structure. The system has morphotropic phase boundary extending over the x=0.5-0.60 interval. The value of dielectric permittivity of (1-x)PSN - xPTmN decreases rapidly with the concentration of thulium: from ε = 40000 (PSN) up to ε = 335 (PTmN).

INVESTIGATION OF PLZT CERAMICS MICROSTRUCTURE

M. Dambekalne, M. Antonova, M. Livinsh, B. Garbarz-Glos[1], and W. Smiga[1]
Institute of Solid State Physics, University of Latvia, Riga, Latvia
[1] Institute of Physics, Krakow Pedagogical University, Poland

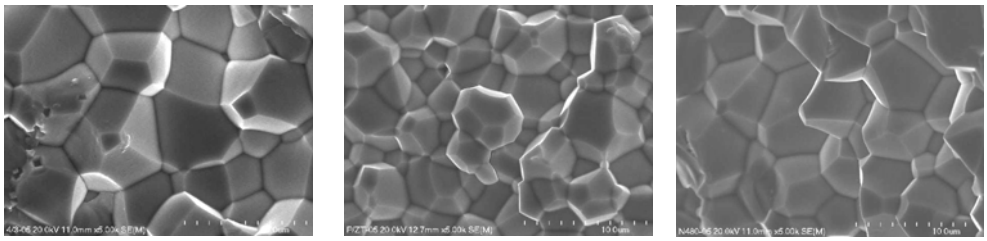
The purpose of the present study was to investigate the influence of the technological factors - composition, sintering temperature and soaking time on the microstructure and quality $Pb_{1-x}La_x(Zr_{0.65}Ti_{0.35})O_3$ (PLZT) ceramics. For producing the ceramic samples were used powder synthesized by original two-stage co-precipitation method from mixed solutions of corresponding inorganic salts solution. Transparent PLZT ceramic samples of large size (Ø $\geq$ 60 mm) were produced by two-stage hot pressing sintering: the first stage was performed at 930 ^{o}C –980 ^{o}C for about 1h in forvacuum at 20 MPa pressure, the second – at 1150 ^{o}C –1200 ^{o}C for 20 h at pressure 20 MPa in air atmosphere. The optical transmittance of ceramic plates (thickness 0.3 mm) measured at wavelength of λ = 630 nm reached 67-69 %. Best results of ceramics density have been obtain by using liquid phase sintering by means of PbO excess, about 3 wt.%.

The microstructure of PLZT ceramics was observed by emission scanning electron microscope (SEM) and stoichiometry of compositions - by scanning microanalyser.

SEM images of PLZT with different content of lanthanum **(**x=0.130; x=0.0975 and x=0.085) were presented in Figures 1a, b and c. As a result of following thermal regimes the fine-grained material with the average grain size of 5-7 μm was obtained. Homogeneity

varies slightly among the different compositions, slightly more - uniform grain size. However, the difference between the homogeneity and grain size of the different compositions is not significant enough to conclude any influence of composition. The fine-grained microstructure is quite uniform, with internal and grain-boundary porosity virtually nonexistent.

The influence of the thermal conditions is very important in the formation of high-quality PLZT ceramics. An excess lead significantly increased density and transparency of ceramics. The excess lead slightly increases the grain size and slightly decreases inhomogeneity of the grains. The most important effect on the size and homogeneity of grains has sintering time. Long sintering times promote mass transport and considerable increases in the grain size. Samples fabricated similarly, but sintered at higher temperatures (>1200 ^{o}C) exhibited a microstructure with a little larger grain size (up to 10 μm), but no significant improvement in optical quality. Chemical analysis of PLZT ceramics by emission microanalyzer for Pb, Zr, Ti and La agreed well with the nominal composition of PLZT.



a) b) c)

Figure 1. SEM micrographs of the PLZT ceramics with different content of lanthanum: a) x=0.130; b) x=0.0975; c) x=0.085.

OPTICAL PROPERTIES AND SURFACE MORPHOLOGY OF PLD DEPOSITED $BaTiO_3$, $Ba_{0.8}Sr_{0.2}TiO_3$ AND $SrBi_2Ta_2O_9$ THIN FILMS

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Institute of Solid State Physics, University of Latvia, Riga, Latvia

Ferroelectrics (FE) thin films have attracted much attention due to their potential applications such as high dielectric constant capacitors, non-volatile memories, infrared sensors and electro-optic devices. Their FE and dielectrics properties have been extensively investigated, while their optical properties have been relatively rarely studied. However, the optical constant, e.g., refractive index and extinction coefficient has great importance for wave guiding and other optical applications.

The optical properties of barium titanate $BaTiO_3$ (BT), barium strontium titanate $Ba_{0.8}Sr_{0.2}TiO_3$ (BST) and strontium bismuth tantalite $SrBi_2Ta_2O_9$ (SBT) thin films by pulsed laser deposition (PLD) have been investigated. Thin films have been deposited on various substrates: a) silicon Si, b) silicon / strontium ruthenium oxide $Si/SrRuO_3$, c) silicon / silicon dioxide / titan / platinum $Si/SiO_2/Ti/Pt$, and d) silicon / silicon dioxide / titan / platinum / strontium ruthenium oxide $Si/SiO_2/Ti/Pt/SrRuO_3$.

The ellipsometric measurements were performed with variable-angle null-ellipsometer “ЛЭМ - 3М” (at He-Ne laser wavelength λ = 632.8 nm, angles set from 45° to

75°). 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.

Optical constants and thickness were determined by fitting the multilayer model function (program was made by HP VEE programming language) to the measured ellipsometric and reflectometric data.

Decrease of the refraction coefficient and band gap energy (for direct allowed electron transition) with thickness increase has been established for BT film on Si and $Si/SiO_2/Ti/Pt$ substrates. Such dependence of optical properties and film thickness cold be illuminated by different structures formation at the various thickness of FE [1-3]. The refraction coefficient for all FE thin films on Si substrates has been observed lower than for films on $Si/SrRuO_3$, $Si/SiO_2/Ti/Pt$ and $Si/SiO_2/Ti/Pt/SrRuO_3$ substrates, what could be related with inconsistency of lattice parameters and expansion coefficients between FE thin films and substrates [1-3].

The changes in band gap energy can be created because of defects (such as oxygen) and impurities as well. The impurity may form discrete localised energy levels in the forbidden gap [4-7]. If its concentration increase, the impurity wave functions can overlap to form an impurity band in which the electrons or holes are free to move. These impurities significantly influence the reflection properties of the films and contribute to the fluctuations of the energy level in the internal potential, which would increase absorption beyond the absorption edge in the absorption spectra. Any such defect state can act as a recombination centres if it is capable on trapping carriers of one type and subsequently capture of carriers of the opposite type, thereby enabling them to recombine for increasing absorption possibility. The main probability is oxygen vacancies: they can trap electrons, leading to donor level in the thin films, which will form addition energy levels in the band gap.

The interface with thickness form 1.5 nm till 11.5 nm between Pt bottom electrode and FE film have been established with ellipsometry. The complex refractive coefficient shows dependency of thickness: the refractive coefficient increase but extinction coefficient decrease with thickness increase (Figure 1.).

In this report optical reflectometry and ellipsometry techniques have been shown as an efficient non-destructive tools for measuring thickness and refractive index of transparent FE thin films. The obtained results of this work are practically significant in the studies of thin films for applying them as microactuators, photonic and sensore devices, which occur in the Ferroelectric Physic Division of the Institute of Solid State Physics.

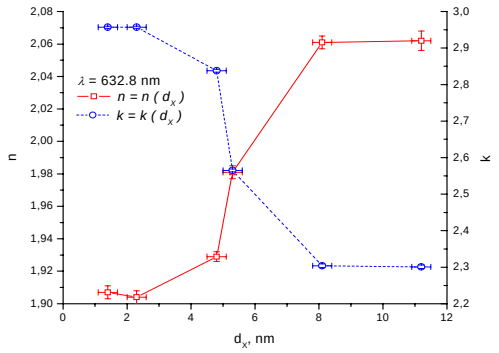

Figure 1. Refractive coefficient n and extinction coefficient k as the function of interface thickness of FE thin films.

References

[1] I. Aulika, V. Zauls, K. Kundzins, M. Kundzins, and S. Katholy. *Study of Trans-parent Ferroelectric Thin Films by Optical Reflectometry and Ellipsometry.* Journal of Optoelectronics and Advanced Materials, 2003, Vol. **5**, No. 3, pp. 755–761.

[2] I. Aulika, V. Zauls, K. Kundzins, and M. Granats. Optical Properties and Surface Morphology of PLD Deposited $BaTiO_3$, $Ba_{0.8}Sr_{0.2}TiO_3$ and $SrBi_2Ta_2O_9$ Thin Films. *The 6-th International Conference-School: Advanced materials and technologies, Palanga, Lithuania, August 27-31, 2004, Abstracts, p. 38.*

[3] I. Aulika, V. Zauls, K. Kundzins, and M. Kundzins. *Thickness Effects on Optical Properties of $BaTiO_3$ Thin Films*. 20th Scientific Conference, Institute of Solid State Physics, University of Latvia, February 16 –18, 2004, Riga, Latvia. Abstracts, p. 52.

[4] R. Thielsch, K. Kaemmer, and B. Holzapfel. Thin Solid Films, 1997, Vol. **301**, p. 203.

[5] M. Losurdo, D. Barreca, P. Capezzuto, G. Bruno, and E. Tondello. Surf. Coat. Tech., 2002, Vol. **151**, p. 2.

[6] P. Pasierb, S. Komornicki, and M. Radecka. Thin Solid Films, 1998, Vol. **324**, p. 134.

[7] Hu-Yong Tian, Wei-Gen Luo, and Ai-Li Ding. Thin Solid Films, 2002, Vol. **408**, p. 200.

ATOMIC FORCE MICROSCOPY INVESTIGATION OF INDUCED SURFACE POLARIZATION BY PIEZORESPONSE AND ELECTROSTATIC IMAGING TECHNIQUE

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Operation of Atomic Force Microscope (AFM) using modified multi-pass regimes allows direct poling of ferroelectric / relaxor thin films in voltage lithography mode and immediate testing of local surface potential and piezoresponse. Methods of local piezoresponse measurement (PFM) in contact mode and several modifications of electrostatic force microscopy (EFM) in noncontact mode have been developed as mutually beneficial when applied to ferroelectric film surface investigation in multi pass sequence. The attention was paid to examine and eliminate crosstalk between different contributions (mainly surface topography, surface potential, and sub-surface capacitance between sample and tip) to the signals measured in electrostatic Kelvin surface potential and capacitance imaging modes to develop versatile characterization method for ferroelectric samples. 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 and some spin coated DMABI-PMMA host-guest polymer films. 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 were 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 or surface potential profiles can be interpreted in terms of size effects on local polarization, presence of defects, charge accumulation and local conductivity.

THICKNESS EFFECTS AND INTERFACE LAYERS IN THIN FILMS REVEALED BY OPTICAL REFLECTOMETRY AND ELLIPSOMETRY

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Optical reflectivity and ellipsometry were used as effectice nondestructive methods to investigate layered ferroelectric heterostructures. 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 45^0 to 75^0, step 5^0). 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 optimization procedure was developed for reflectometric and ellipsometric data evaluation. Passive interface layer of a few nanometer thickness between Pt electrode and active ferroelectric film has been clearly observed and characterized by ellipsometry. The variation of refractive index and absorption coefficient has been observed for pulsed-laser deposited (PLD) $BaTiO_3$ (BT) thin films on $Si/SiO_2/Ti/Pt/SrRuO_3$ substrate with different thickness. The refractive index slightly decreases and absorption coefficient spectra 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.

PHYSICAL PROPERTIES OF FERROELECTRIC THIN FILMS AFTER ELECTRON AND NEUTRON IRRADIATION

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Electron irradiation damage have been observed oriented in $PbZrO_3$ (PZ) and $PbZr_{0.53}Ti_{0.47}O_3$ (PZT) sol-gel and pulsed laser deposited (PLD) thin films with a thickness from 250 nm to 1000 nm, deposited on $SrRuO_3/Pt/Ti/SiO_2/Si$ and $Pt/Ti/SiO_2/Si$ substrates. PZ and PZT thin films have been exposed to electron fluency up to 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 HP4284 LRC meter. 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. Ferrolelectric or antiferroelectric behavior of the films was evaluated by polarisation-electric field hysteresis loops measured on a modified Sawyer-Tower circuit at frequency 15 Hz testing system. 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 ε decreases, it's temperature increases and hysteresis loop becomes asymmetric for PZ thin films after electron irradiation. Decrease of ε and remanent polarisation have been observed for PZT films 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.

As a result 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 $Pt/TiO_2/Si$ substrate. The PZ and PZT heterostructures have been exposed to high fluency 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; $T_{irrad} < 60$ °C in TRIGA MARK II reactor, Atomic Institute of the Austrian Universities in Vienna. Decrease of dielectric permittivity ε, 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.

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**.**

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

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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 α according to the polarization of the incident light.

Depolarization (if assume that depolarization prevails over circular polarization for such symmetry) at small scattering angles θ 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: LandoltC 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.

References

[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.

Scientific publications
Published in 2004

1. K. Bormanis, A. Sternberg, and M. Kalnberga. *Microscopic studies of the Surface Morphology of High Temperature Superconductor Thick Layers*. Physica C, 2004, Vol. **408-410**, p. 844-845.
2. K. Bormanis, A.I. Burkhanov, A.V. Shil'nikov, A. Sternberg, S.A. Satarov, and A. Kalvane. *Features of Dielectric Polarisation in the PSN-PT Ferroelectric Ceramics*. Journal of Optoelectronics and Advanced Materials, March 2004, Vol. 6, No. 1, pp. 341-344.
3. K. Bormanis, M. Dambekalne, M. Antonova, M. Livinsh, L. Shebanovs, and A. Sternberg. *New Ferroelectric Materials on the Basis of* $PbSc_{1/2}Nb_{1/2}O_3$-$PbLu_{1/2}Nb_{1/2}O_3$ *Solid Solutions*. Journal of the European Ceramic Society, 2004, Vol. **24**, pp. 1557-1560.
4. 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,** p. 37/[253].
5. J.M. Bueno, E. Berrio, M. Ozolinsh, and P. Artal. *Degree of Polarization as an Objective Method of Estimating Eye Scattering.* J. Opt. Soc. Am. 2004, Vol. **21**, pp. 1316-1321.
6. A.I. Burkhanov, A.V. Shil'nikov, S.A. Satarov, K. Bormanis, A. Sternberg, and A. Kalvane. *Specifics of Polarisation Switching in* $PbNi_{1/3}Nb_{2/3}O_3$-$PbTiO_3$-$PbZrO_3$ *Ferroelectric Ceramics*. Journal of the European Ceramic Society, 2004, Vol. **24**, pp. 1541-1544.
7. M. Dambekalne, M. Kalnberga, M. Livinsh, and K. Bormanis. *Production and Properties of (1-x)PSN – xPLYbN Solid Solutions*. Key Engineering Materials, 2004, Vols. **264-268**, pp. 1353-1356.
8. V.V. Efimov, S.S. Khasanov, B.N. Mavrin, N.N. Novikova, A.V. Shilnikov, A.I. Burkhanov, V.V. Sikolenko, A. Sternberg, S.I. Tiutiunnikov, D.M. Többens, and V.A. Yakovlev. *Structure and Lattice Dynamics in PLZT 8/65/35 Ceramics Irradiated by High-Current Pulsed Electron Beam.* Ferroelectrics, 2004, Vol. **302,** p. 327/[573].
9. E. Klotins, J. Hlinka, and J. Kaupuzs. *Semiadiabatic High-Field Polarization Response in Ferroelectrics I: Hysteresis and Nonlinear Susceptibility*. Ferroelectrics, 2004, Vol. **301**, p. 79.
10. E. Klotins, and A. Sternberg. *Free-Energy Functional Technique for Finite Ferroelectric Bodies*. Ferroelectrics, 2004, Vol, 299, pp. 35-41.

11. E. Klotins. *Relaxation Dynamics of Metastable Systems: Application to Polar Medium*. Physica A , 2004, Vol. 340, pp. 196-200.
12. G. Krumina, M. Ozolinsh, and V.A. Lyakhovetskii. *Stereovision by Visual Stimulus of Different Quality.* In: Ocular Biomechanics, Helmholtz Research Institute for Eye Diseases, Moscow, 2004, pp. 282-289.
13. A. Krūmiņš, A. Šternbergs. *Cietvielu fizikas institūts*. Latvijas Universitātes rakstu Jubilejas izdevums, 2004, 296.-300. lpp.
14. J. Levoska and M. Tyunina. *Chemical Ordering and Epitaxy in Relaxor and Ferroelectric $PbSc_{0.5}Pb_{0.5}O_3$ Thin Films.* Ferroelectrics, 2003, Vol. **291,** p. 11/[227].
15. M. Ozolinsh, and G. Papelba. *Eye Cataract Simulation Using Polymer Dispersed Liquid Crystal Scattering Obstacles.* Ferroelectrics, 2004, Vol. **304,** pp. 207–212.
16. A.V. Shil'nikov, S.A. Satarov, A.I. Burkhanov, K. Bormanis, A. Sternberg, and A. Kalvane. *Dielectric Properties of $PbSc_{1/2}Nb_{1/2}O_3$ - $PbTiO_3$ Ceramics.* Ferroelectrics, 2004, Vol. **302**, p. 319/[565].
17. V.Ya. Shur, G.G. Lomakin, E.L. Rumyantsev, S.S. Beloglazov, D.V. Pelegov, A. Sternberg, and A. Krumins. *Fractal Clusters in Relaxor PLZT Ceramics: Evolution in Electric Field.* Ferroelectrics, 2004, Vol. **299**, pp. 75-81.
18. V. Shvartsman, M. Tyunina, J. Levoska, and A. Kholkin. *Local Electromechanical Properties of $PbMg_{1/3}Nb_{2/3}O_3$ Thin Films Studied by Piezoelectric Force Microscopy.* Ferroelectrics, 2004, Vol. **302,** p. 323/[569].
19. M. Tyunina, K. Kundzinsh, V. Zauls, and J. Levoska. *Ferroelectric Behavior in Epitaxial Films of Relaxor $PbMg_{1/3}Nb_{2/3}O_3$.* Ferroelectrics, 2004, Vol. **302**, p. 285/[531].
20. M. Tyunina and J. Levoska. *Glassy State in Relaxor Ferroelectric Thin Films.* Ferroelectrics, 2003, Vol. **291**, p. 93/[309].
21. А.И. Бурханов, С.А. Сатаров, А.В. Шильников, К. Борманис, А. Штернберг, А. Калване. *Особенности диэлектрического отклика сегнетоэлектрической керамики PSN-PT.* Физика диэлектриков (Диэлектрики 2004): Материалы X международной конференции. –Издательство РГПУ им. Герцена, 2004. с. 72-74.
22. А.И. Бурханов, А.В. Шильников, А.В. Алпатов, К. Борманис, А. Штернберг, А. Калване. *Низко- и инфранизкочастотные диэлектрические свойства сегнетопьезокерамики системы 0,5PZN-0,5PSN при различных значениях измерительного поля***.** Физика диэлектриков (Диэлектрики 2004): Материалы X международной конференции. Издательство РГПУ им. Герцена, 2004. с. 74-75.
23. А.И. Бурханов, С.А. Сатаров, А.В. Шильников, К. Борманис, А. Штернберг, А. Калване. *Диэлектрические свойства разупорядоченой сегнетоэлектрической керамики PSN-PT.* Изв. РАН, Сер. Физ. 2004, т. **68**, №7, с. 976-978.
24. А.И. Бурханов, А.В. Алпатов, А.В. Шильников, К.Борманис, А. Штернберг, А. Калване, М. Дамбекалне. *Амплитудно-частотные зависимости диэлектрической проницаемости системы xPZN-(1-x)PSN.* Материалы Международной научно-практической конференции «Фундаментальные проблемы радиоэлектронного приборостроения» (INTERMATIC-2004), 7-10 сентября 2004 г., Москва. МИРЭА – ЦНИИ «Электроника», 2004, часть 1., с. 81-84.

Submitted in 2004

1. I.S. Baturin, V.Ya. Shur, D.K. Kuznetsov, N. Menou, C.H. Muller, and A. Sternberg. *Influence of Irradiation on the Switching Behavior in PZT Thin Films.* Material Science & Engineering B.
2. J. Banys, J. Macutkevic, A. Brilingas, J. Grigas, K. Bormanis, A. Sternberg. *Radio and Microvawe Spectroscopy of 0.2PMN-0.4PSN-0.4PZN Relaxor Ceramics.* Ferroelectrics.
3. K. Bormanis, A. Kalvane, A.I. Burkhanov, A.V. Alpatov, M. Dambekalne, and A.V. Shil'nikov. *Dielectric Polarisation of Ferroelectric xPZN - (1-x)PSN Solid Solutions*. Proceedings of AOMD-4: for publishing in Proceedings of SPIE.
4. K. Bormanis, A. I. Burkhanov, A. V. Alpatov, M. Dambekalne, A. Kalvane, A. Sternberg, and A. V. Shil'nikov. *Dielectric Properties of the 0.05PZN – 0.95PSN Ferroelectric Ceramics at Low and Infra-Low Frequencies*. Ferroelectrics.
5. K. Bormanis, S.A. Satarov, A. Kalvane, A.I. Burkhanov, A.V. Shil′nikov, and M. Dambekalne. *Low and Infra-Low Frequency Measurements in Lead Titanate Solid Solutions*. Relaxation Phenomena in Solids 2004, Trans Tech Publications.
6. M. Dambekalne, M. Antonova, M. Livinsh, and A. Sternberg. *PLZT – Synthesis, Sintering and Properties.* J. Solid State Sciences, 2005.
7. E. Klotins, V. Shvartsman, I. Bdikin, and A. Kholkin. *Imaginary Time Schrödinger Treatment for Microstructure Modeling in Ferroelectrics*. Proceedings ISIF 2004.
8. E. Klotins. *Theory and Modeling of Polarization Switching in Ferroelectrics*. Journal of Electroceramics.
9. E. Klotins. *Symplectic Integration Approach to Nonadiabatic Polarization Response in Ferroelectrics*. Physica E.
10. G. Liberts, G. Ivanovs, V. Dimza, and E. Tamanis. *Thermo-Optical Investigation of Sodium-Bismuth Titanate Single Crystal and PLZT Ceramics.* Ferroelectrics.
11. M.N. Palatnikov, I.V. Biryukova, N.V. Sidorov, K. Bormanis, D.V. Makarov, A.V. Denisov, and V.T. Kalinnikov. *Growth and Properties of $LiNbO_3$ Single Crystals Doped with Rare Earth Elements*. Relaxation Phenomena in Solids 2004, Trans Tech Publications.
12. M.N. Palatnikov, N.V. Sidorov, I.V. Biryukova, V.T. Kalinnikov, and K. Bormanis. *Optical Properties of Lithium Niobate Single Crystals.* physica status solidi (c).
13. V.Ya. Shur, E.L. Rumyantsev, G.G. Lomakin, O.V. Yakutova, A. Sternberg, and M. Kosec. *Field Induced Evolution of Nanoscale Structures in Relaxor PLZT Ceramics.* Ferroelectrics.
14. V.Ya. Shur, E.L. Rumyantsev, G.G. Lomakin, O.V. Yakutova, D.V. Pelegov, A. Sternberg, and M. Kosec. *AC Switching of Relaxor PLZT Ceramics*. Ferroelectrics.
15. N.V. Sidorov, M.N. Palatnikov, V.T. Kalinnikov, I.V. Biryukova, and K. Bormanis. *Effects of Ionising Irradiation on Optical Properties of Lithium Niobate Single Crystals.* Ferroelectrics.
16. N.V. Sidorov, M.N. Palatnikov, and K. Bormanis. *Raman Studies of Phase Transitions in Ferroelectric $Li_{0.12}Na_{0.88}Ta_{0.4}Nb_{0.6}O_3$ Solid Solutions*. Submitted: Proceedings of Conference « Single crystals and their application in the XXI century - 2004 »

17. N.V. Sidorov, M.N. Palatnikov, and K. Bormanis. *Ferroelectric-Antiferro-electric Phase Transition in $Li_{0.12}Na_{0.88}Ta_{0.4}Nb_{0.6}O_3$ Ceramics*. Ferroelectrics.
18. В.Я. Шур, Г.Г. Ломакин, Е.Л. Румянцев, О.В. Якутова, Д.В. Пелегов, А. Штернберг, М. Косец. *Переключение поляризации в гетерофазных наноструктурах: релаксорная ЦТСЛ керамика*. ФТТ.

Lectures on Conferences

20th Scientific Conference, Institute of Solid State Physics, University of Latvia, February 16 –18, 2004, Riga, Latvia.

1. S. Fomins, M. Ozoliņš. *Kā izmērīt attālumu starp krāsām. Measuring Distance Between Colours*. Referātu tēzes, 14. lpp.
2. M. Ozoliņš. *Gaismas izkliede un polarizācija redzes eksperimentos. Light Scattering and Polarization in Vision Science Experiments*. Referātu tēzes, 15. lpp.
3. K. Aņisko, M. Ozoliņš. *Vadošā acs un stereoredze. Dominant Eye and Stereovision*. Referātu tēzes, 17. lpp.
4. A. Šternbergs, I. Aulika, V. Zauls, K. Kundziņš, M. Kundziņš, R. Bittner, H.W. Weber, E. Hodgson. *Segnetoelektrisku un antisegnetoelektrisku plānu kārtiņu fizikālās īpašības pēc elektronu apstarošanas. Physical Properties of Ferroelectric and Antiferroelectric Thin Films After Electron Irradiation.* Referātu tēzes, 33. lpp.
5. A. Šternbergs, I. Aulika, V. Zauls, K. Kundziņš, M. Kundziņš, R. Bittner, H.W. Weber. *Intensīva neitronu starojuma iedarbība uz sol – gel $PbZrO_3$ un $PbZr_{1-X}Ti_xO_3$ plānajām kārtiņām. Intensive Neutron Irradiation Effects on sol – gel $PbZrO_3$ and $PbZr_{1-X}Ti_xO_3$ Thin Films*. Referātu tēzes, 34. lpp.
6. I. Aulika, E. Klotiņš. *Pusadiabātiska elektriskā polarizācija segnetoelektriķos: dinamiskā histerēze. Semiadiabatic High Field Polarization Response in Ferroelectrics: Dynamic Hysteresis*. Referātu tēzes, 49. lpp.
7. I. Aulika, E. Klotiņš. *Termisko fluktuāciju efekti segnetoelektriķos: nelineārā dielektriskā uzņēmība. Effect of Thermal Fluctuations on Ferroelectric Response: Nonlinear Susceptibility*. Referātu tēzes, 50. lpp.
8. Ē. Klotiņš. *Polarizācijas mikrostruktūra segnetoelektriķos: Imaginārā laika Šrēdingera tuvinājums. Polarization Microstructure in Ferroelectrics: Imaginary Time Schrödinger Treatment*. Referātu tēzes, 51. lpp.
9. I. Aulika, V. Zauls, K. Kundziņš, M. Kundziņš. *Biezuma ietekme uz plānu $BaTiO_3$ kārtiņu optiskajām īpašībām. Thickness Effects on Optical Properties of $BaTiO_3$ Thin Films*. Referātu tēzes, 52. lpp.
10. E. Birks, I. Aulika, A. Fuith, H. Kabelka, M. Antonova, A. Štrenbergs. *Fizikālās īpašības un fāžu diagrammas PLZT X/85/15 keramikām. Physical Properties and Phase Diagrams of PLZT X/85/15 Solid Solutions*. Referātu tēzes, 53. lpp.
11. M. Dambekalne, M. Antonova, M. Līvinš, M. Plonska, B. Garbarz - Glos. *Dažādu sintēzes metožu izmantošana caurspīdīgās PLZT keramikas iegūšanā. Producing Transparent PLZT Ceramics Using Different Synthesis Methods*. Referātu tēzes, 54. lpp.

12. J. Pelšs, A. Mišņovs, L. Bērziņa, R. Cimdiņš, J. Bossert. *Niobiju saturošas stikla keramikas strukturālās pārvērtības termiskā apstrādē. Structural Transformation of Nb Containing Glass-Ceramics at Thermal Treatment.* Referātu tēzes, 58. lpp.
13. K. Kundziņš, V. Zauls, A. Holkins, M. Tjuņina. *Inducētas lokālās polarizācijas pētījumi segnetoelektriskos materiālos ar modificētu atomspēka mikroskopu. Investigation of Locally Induced Polarization by Modified Atomic Force Microscopy Technique*. Referātu tēzes, 69. lpp.
14. V. Zauls, C. Flueraru, S. Šrāders. *Fāzes jutīga otrās optiskās harmonikas ģenerācijas metode nelineāri optisku organisku molekulu ansambļu orientācijas pētījumiem. Investigation of NLO Molecular Arrangements by Phase Sensitive Optical Second Harmonic Generation*. Referātu tēzes, 73. lpp.
15. U. Kanders, J. Kļaviņš, N. Zeltiņš, K. Bormanis. *Būvkonstrukciju energo-efektivitātes modelēšana un U-faktora noteikšana atsevišķiem būvelementiem pirms iebūvēšanas un ekspluatācijas periodā. Modeling of Energy Efficiency of Building Constructions and Their U-value Determination Before Installation and Post – Evaluation of Thermal Performance of Envelopes.* Referātu tēzes, 112. lpp.

APS March Meeting 2004, Montreal, Canada, March 22-26, 2004.

1. V.Ya. Shur, G.G. Lomakin, O.V. Yakutova, and A. Sternberg. *Study of Intrisic Inhomogeneity in Relaxor PLZT x/65/35 Ceramics by Analysis of Switching Current.* Abstract Log Nr. 11983, session W 19, Multiferroics I.

The 16th International Symposium on Integrated Ferroelectrics, ISIF2004, Korea, April 05 – 08, 2004.

1. E. Klotins, V. Shvartsman, I. Bdikin, and A. Kholkin. *Imaginary Time Schrödinger Treatment for Microstructure Modeling in Ferroelectrics.*

X Международная конференция по физике диэлектриков «ДИЭЛЕКТРИКИ – 2004», Санкт-Петербург, Россия, 23-27 мая 2004.

1. Бурханов А.И., Сатаров С.А., Шильников А.В., Борманис К., Штернберг А., Калване А. *Особенности диэлектрического отклика сегнетоэлектрической керамики PSN-PT.* Материалы X международной конференции «Диэлектрики 2004», с.72-74.
2. Бурханов А.И., Шильников А.В., Алпатов А.В., Борманис К., Штернберг А., Калване А. *Низко- и инфранизкочастотные диэлектрические свойства сегнетопьезокерамики системы 0,5PZN-0,5PSN при различных значениях измерительного поля***.** Материалы X международной конференции «Диэлектрики 2004», с.74-75.

International Conference on Electroceramics and their Applications "ELECTROCERAMICS IX", Cherbourg – France, 31 May – 3 June 2004.

1. M. Dambekalne, M. Antonova, M. Livinsh, V. Belov, and A. Sternberg. *Producing of PLZT Powders by Two-Stage Chemical Method.* Programme & Abstracts, p. 27.

2. V. Shur, G. Lomakin, O. Yakutova, A. Sternberg, A. Krumins, and M. Kosec. *Field Induced Evolution of Nanoscale Structures in Relaxor (5-12)/65/35 PLZT Ceramics.* Programme & Abstracts, p. 221.
3. E. Klotins, J. Hlinka, and J. Kaupuzs. *Theory and Modeling of Polarization Switching in Ferroelectrics.* Programme & Abstracts, p. 225.
4. J. Banys, J. Macutkevic, A. Brilingas, K. Bormanis, A. Sternberg, and V. Zauls. *Dielectric Dispersion and Distribution of the Relaxation Times of The Relaxor 0.4PSN-0.3PMN-0.3PZN Ceramics*. Programme & Abstracts, p. 245.
5. K. Bormanis, N. Sidorov, A. Sternberg, M. Palatnikov, N. Golubjatnik, and I. Birjukova. *Ferroelectric - Antiferroelectric Phase Transition in* $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$ *Ceramics*. Programme & Abstracts, p. 249.
6. J. Banys, J. Macutkevic, S. Lapinskas, A. Brilingas, R. Grigalaitis, A. Sternberg, and K. Bormanis. *Distribution of the Relaxation Times of Relaxor Ceramics.* Programme & Abstracts, p. 384.

The International Jubilee Conference "Single Crystals and Their Application in the XXI Century – 2004", VNIISIMS, Alexandrov, Russia, June 8-11, 2004.

1. K. Bormanis, V.A. Latovin, A. Kalvane, A.V. Shil'nikov, and A.I. Burkhanov. *Frequency Dispersion of Dielectric Permittivity of Relaxor (Pb,Sr,Bi)*TiO_3 *Solid Solutions*. Abstracts, p. 33.
2. K. Bormanis, M.N. Palatnikov, N.V. Sidorov, and I.V. Biryukova. *Growth and Properties of* $LiNbO_3$ *Single Crystals Doped With Rare Earth Elements.* Abstracts, p. 34
3. K. Bormanis, A.I.Burkhanov, S.A.Satarov, A. Kalvane, A. Sternberg, and A.V. Shil'nikov. *Low Frequency Measurements in Lead Titanate Ferroelectric Solid Solutions*. Abstracts, p. 35-37.
4. M.N. Palatnikov, N.V. Sidorov, K. Bormanis, and V.T. Kalinnikov. *Structural Perfection of Stoichiometric Lithium Niobate Single Crystals.* Abstracts, p. 38
5. N.V. Sidorov, M.N. Palatnikov, and K. Bormanis. *Raman Studies of Phase Transitions in Ferroelectric* $Li_{0.12}Na_{0.88}Ta_{0.4}Nb_{0.6}O_3$ *Solid Solutions.* Abstracts, p. 39.

4th International Conference on Advanced Optical Materials and Devices (AOMD-4), Tartu, Estonia, 5 – 9 July, 2004.

1. Karlis Bormanis, Maruta Dambekalne, Maija Antonova, Maris Livinsh, and Marite Kalnberga. *Ferroelectric Solid Solutions on the Basis of Lead Complex Niobates*. Abstracts, edited by A. Rosental, p. 36.
2. Karlis Bormanis, Anna Kalvane, Andris Sternberg, Anver Burkhanov, Arkadiy Shil'nikov, and Vasiliy Latovin. *Dielectric Polarisation of Ferroelectric (Pb,Sr,Bi)*TiO_3 *Solid Solutions*. Abstracts, edited by A. Rosental, p. 37.
3. Maruta Dambekalne, Maija Antonova, Maris Livinsh, Malgorzata Plonska, Zygmunt Surowiak, and Karlis Bormanis. *Producing of Transparent PLZT Ceramics*. Abstracts, edited by A. Rosental, p. 37.

The 15-th International Conference on Defects in Insulating Materials "ICDIM-2004", Riga, Latvia, July 11-16, 2004.

1. K. Bormanis, A. Sternberg, A. Kalvane, A.I. Burkhanov, A.V. Shil'nikov, and V.A. Latovin. *Dielectric Properties and Lattice Defects of Ferroelectric (Pb,Sr)TiO_3-$Bi_{2/3}TiO_3$ Solid Solutions*. Book of Abstracts, p. 60.
2. K. Bormanis, M. Palatnikov, V. Sidorov, and V. Kalinnikov. *Spectroscopic Criteria of Composition and Degree of Structural Perfection of Lithium Niobate Single Crystals of a Stoichiometric Composition.* Book of Abstracts, p. 61.
3. V.V. Efimov, B.N. Mavrin, A.V. Shil'nikov, A. Sternberg, S.I. Tiutiunnikov, and D.M. Többens. *Mechanism of Pulsed Electron Irradiation of the PLZT X/65/35 Ceramics*. Book of Abstracts, p. 85.
4. A.I. Burkhanov, A.V. Alpatov, A.V. Shil'nikov, K. Bormanis, A. Sternberg, and A. Kalvane. *The Effects of Frequency and Amplitude of the Measuring Field on Dielectric Properties of the xPZN–(1-x)PSN System.* Book of Abstracts, p. 126.

Frontiers of Quantum and Mesoscopic Thermodynamics (Satellite of the 20th General Conference of the EPS Condensed Matter Division), Prague, Czech Republic, July 19-23, 2004.

1. E. Klotins, J. Hlinka. *Symplectic Integration Approach to Nonadiabatic Polarization Response in Ferroelectrics.* Book of Abstracts, p.85.

8th International Symposium on Ferroic Domains and Micro- to Nanoscopic Structures, Tsukuba, Japan, August 24-27, 2004.

1. I.S. Baturin, V.Ya. Shur, D.K. Kuznetsov, N. Menou, C.H. Muller, and A. Sternberg. *Influence of Irradiation on the Switching Behavior in PZT Thin Films.* Abstracts, p. 54.
2. V.Ya. Shur, G.G. Lomakin, O.V. Yakutova, A. Sternberg, and M. Kosec. *Switching Behavior of Nanoscale Domain Structure in Relaxor (5-12)/65/35 PLZT Ceramics: Analysis of the Switching Current Data.* Abstracts, p. 62.

The 6-th International Conference-School: Advanced materials and technologies, Palanga, Lithuania, August 27-31, 2004.

1. I. Aulika, V. Zauls, K. Kundzins, and M. Granats. *Optical Properties and Surface Morphology of PLD Deposited $BaTiO_3$, $Ba_{0.8}Sr_{0.2}TiO_3$ and $SrBi_2Ta_2O_9$ Thin Films.* Abstracts of Advanced materials and technologies, p. 38.
2. Andris Sternberg. *Fusion and International Thermonuclear Experimental Reactor (ITER).* CD-version, PDF file, 102 p.
3. Vismants Zauls. *Optical Second Harmonic Generation for Material Analysis*. CD-version, PDF file, 78 p.

IX European Powder Diffraction Conference (EPDIC IX), Prague, Czech Republic, September 2-5 , 2004.

1. A.Mishnevs. *Crystallite Size Analysis in the Range of 10-100 mkm for Organics by X-ray Diffraction.* Book of Abstracts, Material Structure, Vol. 11, 1a, p.121 (2004).

7th European Conference on Applications of Polar Dielectrics "ECAPD 7", Liberec, Czech Republic, September 6-9, 2004.

1. J. Banys, J. Macutkevic, J. Grigas, A. Brilingas, K.Bormanis, and A.Sternberg. *Dielectric Properties of New Relaxors PMN-PSN-PZN Ceramics*. Program and Abstract book, p. 63.
2. M. Tyunina, and J. Levoska. *Epitaxial Films of Relaxor Ferroelectric* $PbMg_{1/3}Nb_{2/3}O_3$ *in Strong Electric Fields*. Program and Abstract book, p. 89.
3. J. Levoska, M. Tyunina, I. Jaakola, and S. Leppävuori. *Evolution of Strain and Dielectric Properties in* $Ba_{1-X}Sr_XTiO_3$ *Epitaxial Thin-Film Heterostructures*. Program and Abstract book, p. 148.
4. J. Levoska, and M. Tyunina. *Compositional Evolution of Properties in Epitaxial Films of Relaxor* $PbMg_{1/3}Nb_{2/3}O_3 - PbTiO_3$. Program and Abstract book, p. 154.
5. G. Liberts, Ģ. Ivanovs, V. Dimza, and E. Tamanis. *Thermo – Optical Investigation of Sodium-Bismuth Titanate Single Crystal and PLZT Ceramics*. Program and Abstract book, p. 202.
6. A.I. Burkhanov, A.V. Shil'nikov, A.V. Alpatov, K. Bormanis, A. Sternberg, and A. Kalvane. *Dielectric Properties of the 0.5PZN-0.5PSN Ferroelectric Ceramics at Low and Infra-Low Frequencies*. Program and Abstract book, p. 219.
7. A.I. Burkhanov, S.A. Satarov, A.V. Shil'nikov, K. Bormanis, A. Sternberg, and A. Kalvane. *Dielectric Response in Ferroelectric PSN-PT Ceramics*. Program and Abstract book, p. 220.
8. M.N. Palatnikov, N.V. Sidorov, V.T. Kalinnikov, and K. Bormanis. *Anomalous Behaviour of Periodic Domain Structure in Doped* $LiNbO_3$ *Single Crystals at 300-400 K*. Program and Abstract book, p. 221.
9. M.N. Palatnikov, N.V. Sidorov, I.V. Biryukova, V.T. Kalinnikov, and K. Bormanis. *Effects of Ionising Irradiation on Optical Properties of* $LiNbO_3$ *Single Crystals*. Program and Abstract book, p. 222.

The 4th International Conference on Inorganic Materials, Antwerp, Belgium, September 19-21, 2004.

1. M. Dambekalne, M. Antonova, M. Livinsh, and A. Sternberg. *PLZT – Synthesis, Sintering and Properties*. Abstract book, P121, p. 220.

The II EOS Topical Meeting on Physiological Optics, Granada, Sept. 2004.

1. J.M. Bueno, E. Berrio, M. Ozolinsh, and P. Artal. *Impact of Ocular Scattering on Visual Performance.* Abstracts, p.24.
2. M. Ozolinsh, M. Colomb, and G. Ikaunieks. *Colour Stimuli Perception in Adverse Viewing Conditions*. Abstracts, p.25.

«Basic Problems of Optics», Topical Meeting on Optoinformatics, St.Petersburg, October, 2004.

1. M. Ozolinsh, G. Ikaunieks, J.M. Bueno, E. Berrio, A. Kozachenko, and G. Andersson. *Human Eye Photoreceptor Acuity at Different Colour Contrast Stimuli.* Proc. «Basic Problems of Optics», p.33-35.

Conference OSAV-2204: Optical Sensing and Artificial Vision, St.Petersburg, October, 2004.

1. M. Ozolinsh, S. Fomins, and M. Colomb. *Optotypes for Human Color Contrast Sensitivity Tests.* Proc. Conference OSAV-2204 Optical Sensing and Artificial Vision. St.Petersburg, 2004, p.129.

V Международная конференция «Нелинейные процессы и проблемы самоорганизации в современном материаловедении», Воронеж, Россия, 3.-5. октября, 2004.

1. В.Я. Шур, О.В. Якутова, Г.Г. Ломакин, Д.В. Пелегов, А. Штернберг, М. Косец. *Индуцированная электрическим полем кинетика фрактальных нанокластеров в релаксорной ЦТСЛ керамике.* Материалы V Международной конференции «Нелинейные процессы и проблемы самоорганизации в современном материаловедении», Воронеж, 2004, том **1**, с. 155-156.

The XXI International Conference on Relaxation Phenomena in Solids (RPS-21), Voronezh, Russia, October 5-8, 2004.

1. K. Bormanis, S.A. Satarov, A. Kalvane, A.I. Burkhanov, and A.V. Shil'nikov. *Low and Infra-Low Frequency Measurements in Lead Titanate Solid Solutions.* Abstracts, p. 99.
2. K. Bormanis, A. Sternberg, A.I. Burkhanov, A.V. Shil'nikov, A.V. Alpatov, and A. Kalvane. *Dielectric Properties of the System of xPZN-(1-x)PSN Ceramics*. Abstracts, p. 100.
3. A.I. Burkhanov, K. Bormanis, A.V. Shil'nikov, A.V. Alpatov, A. Sternberg, and A. Kalvane. *Relaxor PZN-PSN Ceramics at Low and Infra-Low Frequencies*. Abstracts, p.101.
4. M.N. Palatnikov, K. Bormanis, and V.T. Kalinnikov. *Circumstances of Lithium Niobate and Tantalate Crystals Growth.* Abstracts, p. 114.
5. V.Ya. Shur, G.G. Lomakin, O.V. Yakutova, A. Sternberg, and M. Kosec. *Study of Nano-Scale Structure Kinetics in Relaxor Ceramics PLZT X/65/35.* Abstracts, p. 118.
6. N.V. Sidorov, P.G. Chufyrev, M.N. Palatnikov, Yu.A. Zheleznov, V.T. Kalinnikov, and K. Bormanis. *Defects, Photorefractive Features and Vibration Spectrum of Lithium Niobate Crystals of Various Compositions.* Abstracts, p. 119.

1st International Workshop on Smart Materials and Structures, Kiel, Germany, October 7-8, 2004.

1. E. Klotins. *Ferroelectric Materials Under High Alternate Driving: Toward Nonadiabatic Response and Spatial Extension*.

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 (transition metal oxides, bronzes, metal hydrates, solid electrolytes, etc.);
- Material preparation methods: thin and thick film technologies, sol-gel process;
- Material characterization by spectroscopic methods (Raman scattering, optical and X-ray absorption, electrical and electrochemical impedance, ESR, etc);
- Solid state ionics 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. Intergrain 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. Research and development of intelligent senor systems and application technologies of them:
   7.1. Software Environment for Electronic Nose and Electronic Nose Module;

7.2. Preparation of sensor elements and testing their sensitivity and selectivity;

7.3. Application technologies of electronic nose for food quality, aging of chemical products, oils, etc.

8. Odour pollution monitoring methods and instrumentation.

Scientific staff

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

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. J. Hodakovska
5. V.Vorohobovs

Students

1. L.Jēkabsone
2. J. Gaidelene

Visitors from abroad

1) Prof. A. Orliukas – Vilnius University;
2) Prof. P. Vidakovic – GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (10 days).
3) Eng. D. Pailharey – GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (10 days).
4) Eng. F. Jandard – GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (10 days).

Scientific visits abroad

1. J.Gabrusenoks: University of Trento, October 2004 (1 Week)
2. J.Gaidelene: GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (10 days).

3. PhD L. Grinberga:
   1) Stavern, Norway, First NORSTORE conference(5 days).
   2) RISO Center, Denmark, Scientific work 3.5 months (4 month);
   3) MH2004, Crakow Poland, September, 2004 (5 days);
   4) Brussels, Belgium, September 2004 (2 days);
   5) Alpbach, Austria, March, 2004 (7 days).

4. Dr. J.Kleperis:
   1) Helsinki, Finland, March 2004 (3 days),
   2) London, England, April 2004 (3 days),
   3) Copenhagen, Denmark, December 2003 (4 days);

4) Dresden, Germany, May 2004 (5 days);
5) Stavern, Norway, First NORSTORE conference, June 2-5, 2004 (5 days);
6) JRC-IE, Petten, The Netherlands, 28-29th of October 2004 (3 days).

5. MSc. J. Hodakovska: Alpbach, Austria, March, 2004 (7 days).

6. Dr. A.Kuzmin: 1) IFN-CNR, Cefsa, Trento, Italy (3 months),
2) GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (14 days).

7. Dr. A.Lusis: 1) Kick off meeting FP6 project PRODEST, Brussels, April 21-26;
2) Eureka project MINATUSE propsal preparation meeting, Brussels, May 7-9;
3) FP6 project SPFCnet propsal preparation meeting, Grenoble, June 3-6:
4) Project "SoC-SME" Steering Committee Meeting, Reikjavik, Sept.10-13;

8. Dr.phys. E. Pentjuss: Project "GreenRoSE" Steering Committee Meeting, Berlin,Sept.11-13;

9. Dr.hab. J.Purans: 1) University of Trento, Trento, Italy (3 months)
2) GPEC, Universite de la Mediterranee (Aix-Marseille II), Marseille, France (14 days).

10. Dr. G.Vaivars: Cape Town University, Cape Town, South Africa (10 month).

11. Dr. G.Vitins: 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

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

Estonia

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

France

1. SOLEIL and LURE, National Laboratores of Synchrotron Radiation (Orsay, France) – Prof. D. Raoux, Prof. J.-P. Itie,Dr. Ph. Parent.
2. GPEC, Universite de la Mediterranee (Aix-Marseille II) (Marseille, France) - Prof. Y.Mathey, Eng. D. Pailharey, Prof. D. Tonneau.
3. IPN, Institut de Physique Nucléaire, Orsay, France - Dr. S.Hubert, Dr.B. Fourest

Germany

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

Great Britain

1. 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.
4. Laboratori Nazionali di Frascati, INFN, Frascati (National Lab. of Synchrotron Radiation) – Prof. E. Burattini, Dr. A. Marcelli

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

Swiss Federal Institute of Technology of 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. "Provisions of System-On-Chip technology for Small and Medium sized Enterprises" Acronym: „SoC-SME" Nordic Industry Fund project No. 02050 (Dr. A.Lusis)
2. "Integration of advanced H storage materials and systems into the hydrogen society"Nordic Energy Research Project NERP No. 46-02 (Dr. J. Kleperis, PhD L. Grinberga).
3. "Removal of Hazardous Substances in Electronics: Processes and techniques for SMEs (GreenRoSE)" EC FP6 Collective research project N^O COLL-CT-2003-500225 (Dr. A. Lusis).
4. "Nano-scale chemical mapping and surface structural modification by joined use of X-ray microbeams and tip assisted local detection (X-TIP)", EC FP6 Specific Targeted Research Project , 2004-2006 (*J. Purans*).
5. "Lanthanide Chemistry for Diagnosis and Therapy", European COST Action D18, 1999-2004 (Head: Dr.hab. J. Purans).
6. "Stable Gadolinium Complexes with fast water exchange for MRI Agents", NATO SCIENCE PROGRAMME - COLLABORATIVE LINKAGE GRANT, 2004-2005 , University of California, Berkeley (Prof. K. N. Raymond:) and ISSP, Riga (Dr.hab. *J. Purans*).
7. "Study of nanocrystalline oxide films for nano-lithographic applications" OSMOSE project within the bilateral collaboration programme between France and Latvia, 2004-2005 (Dr. hab. *J. Purans* and Prof. *Y. Mathey*).

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 PhD studies - L. Grinberga "Ūdeņraža ģenerācija un akumolācija"
   - Supervisor of MS studies - J.Hodakovska„Sensoru selektivitātes īpašības un molēkulu formas reģistrācija"
   - Advance lecture for BS students "Electrocatalyses"
5. E. Pentjuss - Supervisor of BS thesis of A.Efenvalde "Hazardous Substances in Electronics"
6. L. Grinberga, J. Kleperis – popular about science – lectures and demonstrations for visitors of ISSP, students and school children's.

Main results

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

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

The model for performance of thin film electrochemical cells have been worked out, which helps to solve the problem of cycling capacity for ionic devices or electrochemical cells

(ECC) with intercalation electrodes. The model electrode for thin film electrochemical cells are used amorphous WO3 films. The cycling capacity is actual problem for ionic devices or electrochemical cells 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. The developed model was base for drawing up ionic device performance - degradation scheme. 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 of electrochromic cells. 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. 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. 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 symmetry of the vibrations of WO3 crystal have been determined for different polimorphous phases. The infrared and Raman spectra have been applied to calculate the parameters of lattice dynamics for WO3 and ReO3 crystals. In the framework of a rigid-ion model, lattice dynamics for the cubic phase involves only five parameters. These parameters characterize the interaction constants parallel and perpendicular to W-O and O-O bonds and the electric charge of the oxygen ion. The phonon-dispersion curves and the phonon density of states are calculated. The phonon spectra have two characteristic regions. The calculated phonon spectra are used to determine the mean square displacement of tungsten and oxygen ions. The mean square displacement of an oxygen ion show the well-pronounced anisotropy. The mean square relative displacement are calculated for ion pairs W-O and W-W. The obtained results are compared with the experimental data of X-Ray scattering and EXAFS.

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.

EXAFS Spectroscopy Laboratory conducts studies of the local electronic and atomic structure of mainly oxide compounds by X-ray Absorption Spectroscopy (XAS) using synchrotron radiation. The effects of co-doping, ion intercalation, static and thermal disorder, pressure and correlation effects were addressed in a number of systems.

Main topics of our studies in 2004 were related to

- oxygen K-edge studies of layered transition metal oxides;
- in-situ studies of hydrogen intercalation into transition metal oxides;
- investigations of mixed transition metal oxide thin films;
- studies of the rare-earth ions structure in oxide glasses;
- development and evaluation of novel ab initio theoretical approaches for the simulation of x-ray absorption spectra;
- development of new experimental techniques for nano-materials investigation via combination of Scanning Probe Microscopy and XAS.

In particular, the following results were obtained.

X-ray absorption near edge structure (XANES) signals at the oxygen K-edge in polycrystalline α-MoO_3 and amorphous a-MoO_3 thin film were analysed within the full-multiple-scattering (FMS) formalism. Significantly different XANES signals were found for non-equivalent oxygen atoms in low-symmetrical layered-type α-MoO_3 structure. The obtained results are in agreement with the experimental data and allow to interpret all XANES peaks for α-MoO_3. Besides, the FMS XANES simulations, performed for several fragments of α-MoO_3 structure, allowed us to explain the O K-edge XANES in amorphous a-MoO_3 thin film. We found that in spite of the crystallographic structures of α-MoO_3 and a-MoO_3 are strongly different, a cluster, consisting of six MoO_6 octahedra joined by vertices, produces the main contribution into both XANES signals.

In-situ x-ray absorption spectroscopy at the Re L_1 and L_3 edges was used to study a modification of the local atomic and electronic structure around rhenium in perovskite-type ReO_3 upon hydrogen intercalation. The analysis of both EXAFS and XANES parts of the x-ray absorption spectra shows an evidence of the charge disproportionation phenomenon in hydrogenated rhenium trioxide. An interpretation of the Ni K-edge x-ray absorption near edge structure (XANES) in pure NiO and $Ni_cMg_{1-c}O$ solid solutions was given based on three types of ab initio theoretical calculations: the full-multiple-scattering (FMS) approach, the finite difference method (FDM) and the full potential linear muffin-tin orbital (FP-LMTO) method within the LSDA+U approach. The first two methods differ in the cluster potential approximation: the spherically symmetric muffin-tin potential is used in the FMS approach, whereas a non-muffin-tin numerical potential makes the core of the FDM. We found that the FMS and FDM techniques allow rather accurate description of the

experimental XANES signal especially above the absorption edge and produce close results, the FP-LMTO is more accurate close to the absorption edge.

Pressure-induced scheelite-to-wolframite structural phase transition in $SrWO_4$ was studied using two complementary techniques - x-ray absorption spectroscopy and x-ray diffraction (XRD). In situ XRD and W L_3-edge EXAFS measurements were performed using the synchrotron radiation. The experiments were done at room temperature in the pressure range from 0 to 30 GPa using the diamond anvil cell. The XRD results unambiguously show that $SrWO_4$ transforms from the tetragonal scheelite phase to the monoclinic wolframite-type phase at about 11.7 GPa. Locally this transition appears as a change of the tungsten ions coordination from regular tetrahedral to distorted octahedral. The analysis of the EXAFS data suggests that tungsten ions displace from the centres of the tetrahedra by about 0.04 Å and some nearest oxygen atoms relax by about 0.23 Å.

Development of new experimental techniques for nano-materials investigation via combination of Scanning Probe Microscopies (SPM) such as Atomic Force Microscopy (AFM), Scanning Tunnelling Microscopy (STM) and Scanning Near-field Optical Microscopy (SNOM) with XAS were started in collaboration with scientists from other EU countries (France, Italy, Estonia). The method will provide chemical-specific contrast at unprecedented lateral resolution of below 100 nanometers, thus overcoming existing limitations of the two (SPM and XRS) methods and opening a wide range of research opportunities and challenges.

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 based on configurational averaged method was applied to ab initio calculations of EXAFS spectra in glasses. This is one of the most promising approaches capable of accurate account for both thermal and static disorder and thus to overcome many existing problems.

SODIUM ALUMOSILICATE FIBER LEACHING

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The leaching process of the alkali metals alumosilicates have been investigated by IR an Raman spectroscopy. Raman spectra changes give possibility to analyze the leaching different stages 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. 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}). The ≈ 910 cm^{-1} maximum is related to Si-O none-bridge valence bond oscillations. Their intensity grows in this process. Infrared transmission spectra comparatively intense ≈1600, 5200 cm^{-1} bands are observed supposed to relate to H_2 O molecules presence, but ≈4500cm^{-1} one - to Si-OH group bonds oscillations.

Influence of temperature on micropores in leached NaAlSi glass fibres emportent from application poin of view.

Substructure of microporous sodium alumosilicate glass fibres are investigate by AFM and by gas isothermal desorption using gas chromatography. Substructure of porous glass fibres are prepared by leaching of NaAlSi fibres in 1N HCl solution at 95 0C and investigated by using both methods.It is demonstrated that leached NaAlSi glass fibres surface have micropores ranging from 1-2 to 15 nanometers. Insignificant increase (about 50%) of the surface total area after leaching specifies that micropores in volume of fibres are filled with products of leaching. An increase in the temperature of heat treatment from 3500C to 7500C lead to a decrease in the volume of micropores in glass fibres (medium 8%) and reduce frangibility of fibres.

ELECTRODES WITH HIGH ENERGY CAPACITY AND ELECTROLYTES FOR POWER SOURCES

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It is necessary to improve the cycling properties and energy capacity for metal hydride and lithium power sources. 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.

Further development of the method of combinatorial screening for battery electrode materials has been carried out. 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. The method has been developed and tested basing on spinel $LiMn_2O_4$ as a standard insertion electrode material.

The development of a new method in preparation of $LiFePO_4$/C composite using fully liquid mixing of precursor from solutions including sucrose as a source of carbon for enhanced electronic conductivity has been carried out. The method gives a material having good redox capacity in range 110-130 mAh/g in lithium cells. The 2nd impregnation with sucrose/carbon provides even better percolation and gives a $LiFePO_4$ of almost theoretical capacity 155-160 mAh/g even at a quite high cycling rate. The method allows an easy and fast preparation of $LiFePO_4$ and can be used in combinatorial studies of $LiFe_{1-x}M_xPO_4$ (M = Co, Mn, Ni) solid solutions. Solid solutions of $Li_{1-x}Zr_xFePO_4$ have been studied using the combinatorial method. The studies have not confirmed any advantage of using Zr- doping reported before (S.-Y. Chung et al. Nature Materials, 1 (2002) 123). The electrode performance has remained unchanged.

Additionally a teaching work has been done: 1) ac impedance training (workshops and seminars of ca. 10 h) for students postgraduate students; 2) ac impedance training in Summer School “Electrochemistry Methods” held at University of Southampton in July

2004 (workshops of ca. 10 h); 3) assisting and consulting postgraduate students at University of Southampton.

INTEGRATION OF ELECTROLYTIC HYDROGEN INTO THE HYDROGEN STORAGE DEVICES

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Catalysis and spillover are two basic factors characterizing the hydrogen sorption kinetics in metal hydrides and composite systems. Both the catalysis and electrochemical performance of metal hydride electrodes is strongly influenced by the initial particle size of the alloy powder, by the type and the amount of the conductive additive and also by the thickness of the electrode. Studies of catalytic properties of hydrogen injection phenomena in tungsten trioxide WO_3 were initiated with two aims: WO_3 as an inorganic media for hydrogen storage, and WO_3 as hydrogen sensor material. Test experiments on hydrogen spillover effect by using glass substrate, thin films of Pd and WO_3 (using thin film coating facilities at ISSP UL) gave confidence that WO_3 could be used as an indicator of hydrogen presence in metal hydrides only if electronic contact is ensured. Electrical and optical investigations of interfaces Pd/WO_3; MH/WO_3; $SiO_2/WO_3/Pd$ are started to demonstrate the hydrogen spillover phenomena from catalyst (Pd) to inorganic substrate with or without ionic conductor between.

Search for another metal and-or alloy with catalytic properties similar to Pd metal (able to split H_2 molecule and facilitate spillover of atomic hydrogen onto non-metallic surfaces) is initiated. The first material to be test will be Raney Nickel. Electrodes were prepared from Ni substrate and filled with different catalysts and fillers to prove the hydrogen absorption in an electrode at potentials below or close to HER potential. Current-potential and impedance characteristics will be used to characterize the electrodes.

It is of fundamental importance to investigate whether the abnormally large hydrogen absorption in small clusters arises due to size, preponderance of surface atoms, or the charged state of the cluster, or the presence of special catalysts. Studies of structural, H_2 gas sorption-desorption kinetics and electrochemical properties of new composites obtained by ball milling and based on hydrogen- spillover effect and consisting from hydride forming alloy, glass and conductive filler material – carbon are initiated.

RESEARCH OF CHEMICAL GAS SENSORS: SELECTIVITY AND RESPONSE/RECOVERY TIMES

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Gas sensors are designed to provide optimum performance for each individual gas, but typically there are number of shortcuts and limitations as a result of compromises between needs and possibilities. Sensor rise and fall times are affected by many factors,

including age, chemisorption, cumulative exposure to target gas and interfering gases, and maintenance.

The recovery time for chemical gas sensors based on resistivity changes is longer than the response one. That means, that the adsorption of the gas molecules on the surface of sensor layer (semiconducting metal oxide, chalcogenide or another material) can be a strong chemisorption process. It can lead to the formation of the covalent chemical bonds, namely strong p-bonds in which the holes captured by adsorbed molecules participates.
Our idea is to used different surface activation methods to destroy chemisorbed gas layer and reach faster recovery of sensor. First method we used was an activation of the surface of gas sensing layer with light using different light sources. Commercial TGS 822 sensor was used as sample in experiments. In this case SnO_2 semiconductor with thin catalyst layer is the gas sensitive material and only short wavelength light showed impact on sensor recovery time. Another method was designed for closed chambers of sensors and/or sensor arrays, using two additional electrodes for spark ignition. There were two effects during spark ignition in sensor chamber when recovery process is activated (only in atmosphere containing air) – light produced can desorb captured gas molecules, and ozone generated can destroy volatile compounds in the chamber (left after exposition of sensor to the test gas).

PONG – PERSONAL ODOUR NUISANCE GUARDIAN

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All human senses except for olfaction have its technological counterparts. This is a great disadvantage as most of the information in nature is exchanged by means of chemical signals. Nowadays only human-based odour measurement method is defined in European Standard EN 13725:2003 on olfactometry. Odour measurements performed with humans are expensive, time-consuming and don't inspire trust in the gross society. The idea of this project is to develop a sensor device that simulates human being in his responses to odours. This is a very ambitious task from conceptual and technological point of view. So far, no system or a device has been proposed, which is able to correctly detect and identify odorous components online in ambient air. Concentrations are generally very low, and odorants are often chemically reactive compounds. This far, human odour perception has not successfully been transcribed by analytical instruments. The application potential of such an invention is enormous. Proposed artificial odour recognition system would be an alternative to human measurements, as described in the EN 13725:2003. Self-adjusting and self-learning, multi-component, hierarchical, instrumental odour recognition system for air quality assessment will be developed to control the odour nuisance in human society. The project target will be to develop a compact, mobile measurement system/analyzer based on new generation of sensors (self-organising nano-structures) with pre-concentration module (combined cryogenic and adsorption/desorption technologies). A very ambitious task, which must be solved in this project is to identify transformation between patterns of the detection system and human responses to odour (malodour or fragrance). Panel studies in laboratory and sensory field assessments of odour annoyance will provide the necessary data to combine instrumental measurements with human perception results.

This proposal was submitted to EC 6FW Call FP6-2003-NEST-B-1 as instrument: STREP/STIP with Proposal ID number: 012212 (submission deadline: April 14, 2004; participants: Finland, Denmark, Poland, Lithuania, Latvia; Coordinator J. Kleperis (Latvia)). Unfortunately proposal didn't reach necessary points during evaluaton.

LEAD-FREE SOLDERING QUALITY LABORATORY-CURRENT RESOURCES AND REQUIREMENTS

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With EC WEEE directive now mandating a phase out of lead in electronics soldering by July 2006 and Japan's efforts to do the same even sooner, lead-free is rapidly taking on momentum around the world. In order to help the local small and medium enterprises to change the technologies and solve associated problems, In FP6 project "GreenRoSE" foreseen to set up soldering quality laboratory. To take into consideration the great expenses, at the beginning the laboratory will be located in Tele and Radio Research institute (ITR, Poland) and Institute of Solid State Physics (ISSP,Latvia) using equipment of both institutes and may be equipment of other organizations. During transition time to lead- free soldering there is supported by project "GreenRoSE". In the later time the laboratory activities depend on needs of industry such services. If it will be necessary, the laboratory may be becomes as branch laboratory.

Now the main aim is to be aware the solving tasks, available equipment, the choosing of standards and learning. In process there is envisaged an informative and training support from ES partners.

APPLICATION OF OZONE AND ENVIRONMENTAL MONITORING METHODS IN GRAIN DRYING

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Recently ozone is proposed as a replacement for chemical fungicides, including methyl bromide on grains, fresh fruits and vegetables in post-harvest processing. Ozone O_3 can be generated by electrical discharges in air and is currently used in the medical industry to disinfect against microorganisms and viruses, as a means of reducing odor, and for removing taste, color, and environmental pollutants in industrial applications. The attractive aspect of ozone is that it decomposes rapidly (half-life of ozone is only 20 min) to molecular oxygen without leaving a residue. Electrical generation of ozone eliminates the handling, storage, and disposal problems of conventionally used post-harvest pesticides. This attribute makes ozone an attractive candidate for controlling insects and fungi in stored grain; however, few studies have been published on its efficiency as an insecticide.

Ozone's influence on the germination power of grains only started and no results are available yet.

In this report we will inform about preliminary results from the project "Ozone application in agriculture" supported by Latvian Ministry of Education and Science (Market oriented science capacious project part) and Agricultural Farm "Mazkalnini" from Tervete region (Latvia). During implementation the first stage of the project, the barn with grain storage–drying facility in the Farm "Mazkalnini" was equip with computerized monitoring of moisture, temperature and ozone concentrations in an air. Four sensor arrays were locate in three different regions of storage-drying facility: in the inlet of air prepared for drying (by mixing outside air with preheated and dried in an oven heated with wood) – one array; on the top of corn-bin (there were four bins with capacity around 80 tons and the thickness of grain layers from 2 to 3 meters) – two arrays; in the border between outside and inner side of barn where laborers reside - one array.

First measurements were made without supply of an ozone to test the sensor arrays and collect reliable information about temperatures and moistures in storage – drying facility in different weather conditions. Results were collected during 4 months in an autumn 2004. Temperature and humidity monitoring results are highly informative and can help to organize storage–drying process most economic and reliable.

AIR POLLUTANTS (Cl_2, NO, P_2O_5) REGISTRATION USING OZONE AS TESTING REAGENT

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It is well known, that many gases can react with ozone, but it is new idea – to use ozone to register some extremely small concentrations of some air pollutants. Small ozone generator was made, which generates ozone. Atmospheric air and ozone mixture was gathered in the bottle. If, for example, the air pollutant is chlorine, it quickly disintegrates ozone regarding next reaction chain:

$$\mathbf{Cl_2} + O_3 = 2ClO + O$$
$$O + O_3 = 2O_2$$
$$2ClO = O_2 + \mathbf{Cl_2}$$

This reaction repeats many billions times. In fact chlorine (polluting substance) is working as a catalyst. It means, that one chlorine molecule can interact with billions ozone molecules and destroy them. That is why large change of ozone concentration depends from small chlorine concentrations.

That is why sensitivity of this method is much better, then many other methods. Ozone sensor measure residual ozone quantity, and this sensor is made in our laboratory. The same catalyst properties has also NO, P_2O_5 , and may be some other dangerous air pollutants. So, we can register also them, using this method.

TRAFFIC CAUSED POLLUTION AND NOISE PROBLEMS: INVENTORY, DIRECT MEASUREMENTS AND MODELLING

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Riga, the capital of the Republic of Latvia, is not only the centre of industry, business, entertainment and tourism, but also the home for 794500 inhabitants (1/3 from all inhabitants in Latvia). Number of inhabitants in Riga is reducing slowly, caused by negative birth rate, immigration and moving people to countryside around city. Nevertheless, the number of traffic in the streets of Riga is increasing from year to year by 8-12%. The most important and famous place in Riga is the Old Town (oldest houses from 16^{th} century), which in 1998 was joined by UNESCO to the heritage of the world culture. Now the Old Town is the place in Riga most crowded by tourists and polluted by cars.

An air quality management system AIRVIRO is used for an inventory of air pollution sources in Riga and their related dispersion calculations (from 1994). DOAS equipment is used for air quality monitoring as on the background level, as well as on the street level in Riga. Inventory results show that traffic on the streets of Riga is responsible for 80% of all NO_x, 78% of all CO and 68% of all VOC emissions in Riga. Calculated dispersion concentrations coincide quit well with directly measured values primarily on main streets with intense traffic.

Latvia is going to associate with European Union in near future, and now is adopting also air quality quid lines accordingly EU legislation. For year 2010 it will be necessary to ensure the annual concentrations of NO_2 and benzene no more as 40 and 5 $\mu g/m^3$ accordingly, but for Riga it will be problems, as it is shown by our dispersion calculations for year 2010. Some suggestions are given how to prevent it.

MODELING OF ENERGY EFFICIENCY OF BUILDING CONSTRUCTIONS AND THEIR U-VALUE DETERMINATION BEFORE INSTALLATION AND POST-EVALUATION OF THERMAL PERFORMANCE OF ENVELOPES

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Because of the occurrence of considerable heat exchange with the external environment in the envelope of buildings, the total energy consumption of a building depends on the thermal performance of the facade, floor and roof. Residential and public houses are the major thermal energy consumers. It is estimated that building space heating consumes some 65% of the total delivered heat by centralised district heating plants. The using of the thermal insulation for the building envelope is an enormous potential for energy savings. One of most important task is increasing of thermal resistance values for various building constructions. Therefore, the measurement method of U-value in the field is required for post-evaluation of thermal performance of envelopes. There have been several attempts at the in-situ measurement of U-value. According to the result of the

experiment there were considerable divergences, particularly in heavy weight walls such as concrete, between the measured U-value and the real value. By analysis, it was shown that this error was caused by lateral heat loss in the wall, which accounted for about 50 % of the supplied heat flow. A simple Excel program is developed for calculation heat loses through the building envelope and its separate building elements. It calculates the saved heat energy depending on the construction of thermal isolation layer on the outside walls.

ACADEMIC KNOWLEDGE STATISTICAL DIAGNOSTIC OF FIRST TERM STUDENTS AT UNIVERSITY

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The statistical diagnostic potential of an academic knowledge of first term students has been considered on the basis upon the experience gained during several years at an university by lecturing several courses on the use of IT in law within the framework of the study programme of Public Law. The course discusses the use of computer technologies in obtaining the information and the further processing and analysis of the collected data. The courses lectured have covered 1^{st}-4^{th} term regular and extra-mural students allowing to observe the independence and purposefulness of students as regards the given tasks, namely, their skills of learning. Students commence their studies being at very different levels of the general training, including also skills of using computer technologies. The observations during several years have shown that these differences are not reducing. The data of the Entrance Board of the university concerned regarding 2000 – 2002 on the 1^{st} term regular and extra-mural students have been analyzed in the paper. 6 populations of regular and extra-mural students within a period of three years have been analyzed. The average level of knowledge according to the secondary education certificate differs for about 4 grades between the first and the last student of the population in the list of the matriculated students both for the regular and extra-mural studies. To overcome the 4-grade gaps in the academic knowledge, for example, within one academic group highly effective didactic instruments are necessary in order to ensure successful mastering of the new material within the envisaged time schedule and amount. Moreover, the more successful students must not be bored but those less successful must not lag behind hopelessly. Practice has shown that the electronic study materials allow to balance the class process. A gap of about 2 grades has been observed between the populations of regular and extra-mural students.

Scientific publications
Published in 2004

1. L. Grinberga, J. Kleperis. Toward Hydrogen Energy in Latvia". Scientific Proceedings of Riga technical University "Power and Electrical Engineering", series 4, vol. 12, 2004, p. 50-56.
2. L.Grinberga, Preliminary results on new composite materials for hydrogen evolution/storage; NORSTORE conference, Stavern, Norway http://www.norstore.ife.no/workshops/2004_Stavern/Presentations/03_04_Grinberga.pdf,.

3. L. Grinberga, J. Kleperis, The perspectives of Hydrogen energy in Latvia. Will be published in January 2005: Proceedings of the Local Conference: "Energetics and Environment in Baltics", University of Latvia, Riga, August 12, 2004; (in Latvian, 11 pages).
4. J. Kleperis, L. Grinberga, G. Vaivars "Hydrogen evolution and absorption researches in Latvia" Presentations Materials of JRC-IE training workshop on "Mapping European knowledge on Hydrogen Storage" Petten, The Netherlands, 28-29th of October 2004: http://www.jrc.nl/
5. V. Linkov, J. Shang, G. Vaivars, G. Gericke and L. Petrik. Zirconium phosphate nanoparticles / PEEK composite membranes for DMFC. In: Fuel Cells Science & Technology 2004. 6-7 October 2004, Hilton Munich Park Hotel, Germany. P2.60.
6. G. Vaivars, N.W. Maxakato, T. Mokrani, L. Petrik, J. Klavins, G. Gericke and V. Linkov. Zirconium Phosphate Based Inorganic Direct Methanol Fuel Cell// Materials Science (Medziagotyra) 10, 2 (2004) 162-165.
7. G. Vaivars, T. Mokrani, N. Hendricks and V. Linkov. Application of the Zirconium Phosphate Based Inorganic Membranes in Fuel Cells// Journal of Solid State Electrochemistry, 8, 11 (2004) 882-885.
8. G. Vaivars. Materials and Process Design for Direct Methanol Fuel Cells. In: Materials in Manufacturing Conference, 14-15 October 2004. UCT. 2004. P.60-61.
9. P. Fornasini, G. Dalba, R. Grisenti, J. Purans, A. Sanson, A. Vaccari, F. Rocca, EXAFS studies of lattice dynamics and thermal expansion, Phys. Stat. Solidi (c) 1 (2004) 3085–3088.
10. J.Gaidelene, A.Kuzmin and J.Purans, Oxygen K-edge x-ray absorption near-edge structure in crystalline and amorphous molybdenum trioxides, J. Phys.: Condens. Matter 16 (2004) 6619–6625.
11. 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. Methods Phys. Res. A 531 (2004) 321-326.
12. A.Kuzmin, J. Purans and G. Moreau, Full multiple scattering analysis of x-ray absorption near edge structure at the Eu L3-edge in EuO, J. Alloys and Compounds 374 (2004) 89-92.
13. G. Heisbourg, N. Dacheux, S. Hubert, J. Purans, Kinetic and thermodynamic studies of the dissolution of thoria-urania solid solutions, Journal of Nuclear Materials 335 (2004) 5-13.
14. J. Purans, J. Gaidelene, A. Kuzmin and C. Guéry, XAFS Study of Hydrogen Intercalation in Polycrystalline ReO3, in Proc. 6th International Meeting on Electrochromism I.M.E. – 6, Brno (Czech Republic), August 29th to September 2nd, 2004.
15. I.Steinberga, J. Kleperis, Urban Air Pollution: Input from Car Parking Places. In the book: Urban Transport. Ed. C.A.Brebbia, WIT Press, Southampton, Boston, UK, 2004, p. 231-239.

16. J. Kleperis "Pārskats par vides trokšņa problēmām Rīgā". Grāmatā: V. Imers, D.Šatrovska, J. Kleperis "Eiropas Savienības politika vides trokšņa samazināšanā un tās ieviešana Latvijā", grāmata, sagatavotājs: Baltijas Vides Forums, iespiest "Gandrs",, Rīga, 2004., lpp. 21-27.
17. J.Kleperis, Ozons un tā ietekme uz cilvēku veselību. Publikācija žurnālā „DOCTUS", 2004. gada jūnija numurs, 6 lpp.
18. G. Kizane, J. Tiliks, A. Vitinš, J. Rudzitis. Tritium localisation and release from the ceramic pebbles of breeder. – Journal of Nuclear Materials. August 2004. Vols. 329-333. Part 2. Pp. 1287-1290.
19. G. Ķizāne, J. Tīliks, A. Vītiņš, E. Kolodinska. The effect of magnetic field and high temperature on the properties of blanket ceramics. – In book: Proceedings of the 11th International Workshop on Ceramic Breeder Blanket Interactions, December 15-17, 2003, Tokyo, Japan. JAERI-Conf 2004-012. / Ed. Mikio Enoeda. Japan Atomic Energy Research Institute. July 2004. - Pp. 120-129.

Accepted for publication in 2004

1. E. Avendano, 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 (2005) (in press).
2. 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 (2005) (in press).
3. P. Fornasini, S. a Beccara, G. Dalba, R. Grisenti, J. Purans, A. Sanson, F. Rocca, D. Diop, EXAFS and local thermal expansion, Physica Scripta (2005) (in press).
4. J. Gaidelene, A. Kuzmin, J. Purans and C. Guéry, Influence of hydrogen intercalation on the local structure around Re ions in perovskite-type ReO3, Phys. stat. sol. (c) (2005) (in press).
5. A.Kuzmin, R. Kalendarev, J. Purans, J.P. Itie, F. Baudelet, A. Congeduti and P. Munsch, EXAFS study of pressure-induced phase transition in SrWO4, Physica Scripta (2005) (in press).
6. A.Kuzmin, J. Purans and R. Kalendarev, Ab initio calculations of the Ni K-edge XANES in NicMg1-cO solid solutions, Phys. stat. sol. (c) (2005) (in press).
7. J. Purans, G. Heisbourg, N. Dacheux, Ph. Moisy and S. Hubert, XAFS study of local structure with picometer accuracy: Th1-xUxO2 and Th1-xPuxO2 solid solutions, Physica Scripta (2005) (in press).
8. J. Purans, B. Fourest, C. Cannes, V. Sladkov, F. David, L. Venault, M. Lecomte, Structural Investigation of Pd(II) in concentrated nitric and perchloric acid solutions by XAFS, J. Phys.Chem. B (2005) (in press).
9. V. Vorohobovs, J. Kleperis. Negative Resistance and Temperature Stabilisation of Small Objects. Iesniegts „Transport and Telecommunication".

Lectures on Conferences

20th Scientific conference of Institute of Solid State Physics of University of Latvia, Riga, 2004

1. L. Grinberga, Influence of structure and composition on hydrogen evaluation on the electrodes of different materials;.
2. Vladimirs Vorohobovs, Jānis Kleperis. Mazu objektu temperatūras stabilizācijas problēmas un risinājumi.
3. Jūlija Hodakovska, Jānis Kleperis. Gāzu molekulu "nospiedumu" veidošana plānās metālu kārtiņās.
4. U.Kanders, J.Kļaviņš, N.Zeltiņš, K.Bormanis, Modeling of energy efficiency of building constructions and their U-value determination before installation and post-evaluation of thermal performance of envelopes.
5. U.Kanders, J.Kļaviņš, U.Kanders, J.Kļaviņš, Academic knowledge statistical diagnostic of first term students at university, 20th Scientific Conference of Institute of solid state physics UL, Riga, February 16-18, 2004.
6. Ē. Pentjušs1, A.Lūsis, K. StabiņšC Sprieguma lineārās izvērses pielietojums akumulātoru kapacitātes un pretestības noteikšanai

15th International Conference on Defects in Insulating Materials,Riga (Latvia) July 11-16, 2004.
J. Purans, A. Kuzmin, R. Kalendarev, J.Gaidelene.

6th International Meeting on Electrochromism IME–6, Brno (Czech Republic), Aug.29- Sept.2, 2004.

1. J. Purans, A. Kuzmin, J.Gaidelene: XAFS study of hydrogen intercalation in polycritaline ReO_3.
2. J.Gabrusenoks: Dynamical properties of the WO_3 lattice

COST D18 "Lanthanide Chemistry for Diagnosis and Therapy" Annual Workshop, A Coruña (Spain), Sept. 23-25, 2004.
J. Purans, A. Kuzmin. X-spectrscopy of lanthanides.

EMINENT Workshop, Riga Technical University, April 23-24, 2004
1. L. Grinberga, J. Kleperis. Hydrogen Energy perspectives, and Report on, Journal "Enerģijas Pasaule" (The World of Energy)

International Symposium on Metal Hydrogen Systems, Fundamental and Applications - MH2004, Crakow Poland, September 6-9, 2004
L. Grinberga, J. Kleperis "Advanced media for hydrogen storage".

Starptautiska konference "EcoBAlt 2004", Rīga, 6.-7. maijs, 2004.g

1. S. Blumberga, A. Vīksna, J. Kleperis, Gaisa kvalitāte un PM10 koncentrācijas Rīgā 2003. gadā. (Air quality and PM10 concentrations in Riga on 2003).

2. J. Kleperis, A. Plāte. Smaku problēmas un to pārraudzības aktivitātes latvijā. Odour problems and management activities in Latvia.
3. J. Kleperis, E. Zavickis. Air quality index – example from Riga.

First NORSTORE conference, Stavern, June 2-5, 2004, Norway
L.Grinberga "Preliminary results on new composite materials for hydrogen evolution/storage".

Conference: "Energetics and Environment in Baltics", University of Latvia, Riga, August 12, 2004.
J. Kleperis "The perspectives of Hydrogen energy in Latvia".

Conference "Energy Systems and Environment", Riga Technical University, Riga, Latvia, Oct. 14-16, 2004.
Liga Grinberg "Toward Hydrogen Energy in Latvia".

JRC-IE training workshop on "Mapping European knowledge on Hydrogen Storage", Petten, The Netherlands, Oct.28-29, 2004.
J. Kleperis "Hydrogen evolution and absorption researches in Latvia".

International Conference "Urban Transport 2004", Dresden, May 19-21, 2004.
J. Kleperis "Urban Air Pollution: Input from Car Parking Places".

Battery and Fuel Cell Materials Symposium of International Battery Materials Association, Graz, Austria, 18-22 April, 2004.
1. G. Vitins, A.D. Spong and J.R. Owen. "Combinatorial discovery of electrode materials"
2. A.D. Spong, G.Vitins and J.R. Owen. "Combinatorial screening of lithium battery materials"

Engineering R&D 2004, Peninsula, May 28, 2004.
1. T. Mokrani, G. Vaivars, Ji Shan and V. Linkov. Engineering Aspects of Low Temperature Fuel Cells.
2. T. Mokrani, G. Vaivars, Ji Shan and V. Linkov. Development of an Inorganic Direct Methanol Fuel Cell.

Fuel Cells Science and Technology 2004, October 6-7, 2004, Munich, Germany
V. Linkov, J. Shan, G. Vaivars, G. Gericke and L. Petrik. Zirconium phosphate nanoparticles / PEEK composite membranes for DMFC.

Advanced Membrane Technology II. May 23-28, 2004. Kloster Irsee/Swabian Conference Center, May 26, 2004, Germany:
V. Linkov, G. Vaivars, B.J.Bladergroen, J. Shan and G. Gericke. New composite membranes for DMFC.

DIDACTIC SYSTEM LABORATORY

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

Research Area and Main Problems

Research field of the Laboratory is related to

- investigation of possibilities to use "client-server" and "virtual laboratory" technology to create new methods of e-education;
- development, application and education on cluster computing.

Scientific Staff

1. Prof.,Dr.phys. J.Kuzmin
2. Dr.phys. 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.
6. LU PPF "Introduction to Cluster Computing" – lectures, Dr. A.Kuzmin.

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 (Prof.. A.Geske, lect. L.Kuzmina)
2. Latvian schools

Italy

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

Main Results

VIRTUAL PHYSICS LABORATORY

J.Kuzmin, A. Kuzmin

In year 2004 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 2004 are described briefly below.

- WebCT technology in a e-education applications.

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

System WebCT is elaborated outside Latvia and aimed to computerization of educational process in universities and schools. Latvian university use this system from 2003. WebCT has many positive features, but there are a lot of deficiencies. Main is absence of means to implementation programmed dialog with student during learning course material. Another WebCT minus is rather complicated technology of creating typical didactic structures.

Source material for System "AMATA" can be just graphical files (.jpg / .gif /.bmp) and explanatory texts. These elements System transforms to course in html format. Explanatory texts can contain questions, students answer analysis procedures, demonstrations (as javascript files), tasks and other didactics elements of course.

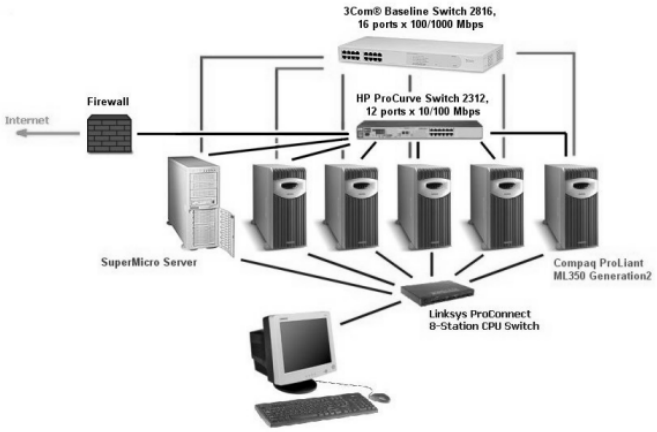
System "AMATA" supplements WebCT with some built in didactic functions:

- AND/OR/NOT operations with keywords.
- Student answer processing before analysis.
- Structuring of course material.
- Course advanced elements generation.

System "AMATA" was used to prepare WebCT courses "Programming in PASCAL", "HTML programming elements" and "JavaScript programming" for LU students education. Approbation of these courses will start in 2005.

- Further Developments of Latvian SuperCluster system

The LASC system was significantly upgraded at the beginning of 2004. The new front-end node, having two Pentium 4 XEON 3.066GHz CPUs, 5 GB RAM and the RAID-disk subsystem was installed. The second network, based on Gigabit Ethernet technology, was added for parallel computations tasks, and a new firewall system was installed for cluster protection. As a result, the total computation resources available to the users were significantly improved. At present, the theoretical peak power of the cluster is about 19 GFlops, the total physical memory is 25 GB, and the total disk storage is 1.8 TB. The detailed information on the cluster configuration, its resources, and different useful documentation/links are available at the LASC website (http://www.cfi.lu.lv/lasc/). The website provides also with real-time status monitoring of the LASC activity.



Basic concept of the parametric execution system "SPIDER" is shown in Figure 5. "SPIDER" is based on the SPMD (Single Program Multiple Data) programming paradigm, and its main goal is to give users the ability to execute a large number of sequential jobs over a large number of computers, in particular organized in a cluster. "SPIDER" can be installed on any homogeneous or heterogeneous cluster, running Linux RedHat 7.x operating system and interconnected via TCP/IP based network with SSH support. The use of secure shell interface for communications between nodes makes it possible to use "SPIDER" not only in a cluster environment but also over public networks such as Internet.

At present, the "SPIDER" system is successfully used on LASC for two types of problems. The first one was previously described in [9] and is related to ab initio calculations of x-ray absorption spectra (XAS) from nanoparticles. In this case, the shell script runs first a special code for nanoparticle construction, then the XAS for each atom in the nanoparticle is independently calculated by the FEFF code [10] in parallel way using the "SPIDER" scheduler, and finally another special code calculates the total XAS for the whole nanoparticle as an average of signals for each atom [9].

Another problem addressed on LASC using "SPIDER" is related to a visualisation of simulation results using the rendering software POV-Ray™ [11], a tool for producing high-quality static and dynamic computer graphics. POV-Ray™ [11] is copyrighted freeware and exists for many operating systems as Linux/UNIX, Windows and Macintosh. It is well suitable for artistic, scientific and business purposes, allowing to create stunning three-dimensional graphics. The main problem with using POV-Ray™ on standard single-CPU computers is a long time required by rendering algorithm already for the single scene. Obviously, the time will be even longer for movies creation. However, rendering operation can be easily parallelised. In the case of single static pictures, the picture can be divided into non-overlapping parts, which can be rendered in parallel. In the case of movies, each frame can be rendered independently. The speed of rendering process scales nearly linear with the number of processors, that makes the use of cluster very efficient. The "SPIDER" system allows currently to run sequential version of POV-Ray™ to render in parallel both static and dynamic scenes. The future use of this approach will include direct visualisation of (Reverse-)Monte Carlo or Molecular Dynamics simulations results.

The experience gained during development and installation of the LASC system was used for preparation of the new lecture course ”Introduction to Cluster Computing” at LU PPF.

Scientific Publications

Published in 2004

1. Yu. Kuzmin, *Virtualization of Science and Education*, in *Proc. 2st Int. Conf. “Information Technologies and Management”, April 15-16, 2004*, (Information System Institute, Riga, Latvia, 2005).
2. A. Kuzmin, *Latvian SuperCluster - LASC: Recent Developments*, in *Proc. 2st Int. Conf. “Information Technologies and Management”, April 15-16, 2004*, (Information System Institute, Riga, Latvia, 2005).
3. L.Kuzmina, J.Kuzmins, *Virtuālā klātbūtne mācībās. Sistēmā SOLO*, LU Zin. Raksti, 2005.

Participation in Conferences

1. Yu. Kuzmin, 2nd International Conference on “Information Technologies and Management”, Riga (Latvia), April 15-16, 2004.
2. A.Kuzmin, LU ISSP 20. Scientific Conference, Riga (Latvia), February 16-18, 2004.
3. A.Kuzmin, 2nd International Conference on “Information Technologies and Management”, Riga (Latvia), April 15-16, 2004.
4. L.Kuzmina, J.Kuzmins, 62 Latvian University Conference, Riga, February 2004.

NONLINEAR PROCESSES IN SOLIDS

Head of Division *Dr. hab. 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 emphasis on pattern formation and catalytic surface reactions, as well as on the atomic and electronic structure of advanced materials, with emphasis on calculations of defective 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 (2 weeks).
2. Prof. Dr. R.A. Evarestov, St. Petersburg University, Russia (3 weeks).

Our scientific visits abroad

1. Dr. hab. E. Kotomin, Max Planck Institute for Solid State Physics, Stuttgart, Germany (9 months), University of Osnabrück, Germany (2 weeks), Northwestern University, USA (1 week), University of Pennsylvania, USA (1 week)
2. Dr. hab. V. Kuzovkov, Braunschweig University of Technology, Germany (3 months)
3. Dr. Yu. Zhukovskii, Max Planck Institute for Solid State Physics, Stuttgart, Germany (1 month), University of Osnabrück, Germany (1 month), St. Petersburg University, Russia (1 month)
4. Dr. A. Popov, European Molecular Biology Laboratory, Grenoble, France (11 months)
5. Dr. R. Eglitis, University of Osnabrück, Germany (11 months)
6. Dr. G. Zvejnieks, JET-EFDA/CSU, Great Britain (1 month)
7. Dr. S. Piskunov, University of Osnabrück, Germany (3 months)
8. V. Kashcheyevs, Tel Aviv University, Israel (11 months)
9. D. Gryaznov, Max Planck Institute, Stuttgart, Germany (11 months)

International Cooperation

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) Max Planck Institut (MPI) für Festkörperforschung, Stuttgart (Prof. J. Maier) Max Planck Institut (MPI) für Plasmaphysik, Garching (Prof. H. Zohm) Braunschweig University of Technology (Prof. W. von Niessen) Gesellschaft für Schwerionenforschung, Darmstadt (Prof. K. Schwartz)
Israel	School of Physics and Astronomy, Tel Aviv University (Prof. A. Aharony) Ben Gurion University of the Negev (BGU), Ber Sheeva (Prof. D. Fuks)
Latvia	Institute of Solid State Physics (ISSP) (Prof. J. Purans) Transport and Telecommunication Institute (TTI) (Prof. Yu.N. Shunin)
The Netherlands	Eindhoven University of Tehnology (TUE) (Prof. A.P.J. Jansen)
Russia	St. Petersburg University (SpbU) (Prof. R.A. Evarestov)
Spain	University of Barcelona (UB) (Prof. F. Illas)
Sweden	Uppsala University (Prof. K. Hermansson)
UK	King's College London (Prof. L. Kantorovich) University College London (Prof. A.M. Stoneham)
USA	California Institute of Technology (CalTech), Pasadena (Dr. E. Heifets)

Main Results

LARGE-SCALE SIMULATIONS OF SURFACE REACTIONS

V.N. Kuzovkov,
W. von Niessen (*Braunschweig University of Technology, Germany*),
A.P.J. Jansen and R. Salazar (*Eindhoven University of Tehnology, the Netherlands*).

In collaboration with *Eindhoven University of Technology, the Netherlands* we presented a tool for scaling laws relating the typical space and time scales obtained in microscopic Monte Carlo simulations to both experimental system sizes and relevant diffusion coefficients. One of the most interesting features of surface reactions is that in many cases pattern formation, structures with some well--defined length scale, sometimes with symmetries and temporal behavior, such as oscillations, traveling waves, spirals, Turing patterns, are observed. A usual approach to a study this pattern formation is reaction—diffusion (RD) equations, which simulate the dynamic behavior of chemical reactions on

surfaces. However, these partial differential equations give only approximate solutions and gave in several cases completely wrong results, because they are based on the local mean field approximation, meaning well--stirred reactants at the microscopic level, ignoring all local correlations between reactants, as well as fluctuations and lateral interactions among adsorbates. The RD equations operate with the coverages which are macroscopic continuum variables and thus neglect the discrete structure of solids, and do not describe the actual chemical process underlying the pattern formation. An exact method to solve the *master equation* for such systems is the *Monte Carlo* (MC) method. To compare MC simulations with experimental pattern formation, it is necessary to fill the gap between the length scale of the individual particles and the diffusion length. This would be a very large and slow simulation, due to the huge number of particles involved and the fast diffusion rates which means that most of the simulation time is spend for diffusion of particles instead of chemical reactions. Although only the MC simulations provide solutions to the exact master equations for the surface reactions, they are not suitable for efficient parallelization, due to a random selection of lattice sites. However, there is another important approach for simulating the discrete events on the lattices, the Cellular Automata (CA). We have studied, under which conditions the CA could reproduce adequately MC simulations of chemical reactions on surfaces. We found that the main requirement is the use of large diffusion coefficients. We performed large-time and large-size computer simulations for chemical reactions on surfaces. By using large parallel simulations, it is possible to derive scaling laws which allow us to extrapolate results to even larger system sizes and larger diffusion coefficients, thus permitting a direct comparison with real experiments.

In collaboration with *Braunschweig University, Germany* we studied forced oscillations in a self-oscillating surface reaction model. The harmonic resonance, subharmonic and superharmonic entrainment, quasiperiodic and chaotic behavior are well known to occur in nonlinear self-oscillating systems which are subject to a periodic forcing. Harmonic resonance occurs if the periodic forcing signal has a frequency very similar to that in the undisturbed system and results in an amplification of the oscillations. In this case the so-called *phase locking* occurs, i.e. the system oscillates with the response frequency with a constant phase difference to the external signal. A microscopic lattice gas model for the catalytic $CO+O_2$ reaction on Pt(110) subject to external periodic forcing is studied by means of cellular automaton simulations. Harmonic resonance, subharmonic and superharmonic entrainment, quasiperiodic as well as chaotic behavior are among the observed phenomena in this model when the gas phase concentration of CO as an external control parameter is periodically varied and interacts with the self-oscillating reaction system**.**

DISTINGUISHING DETERMINISTIC&NOISE COMPONENTS IN ELM TIME SERIES

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

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.

It was first observed at ASDEX Tokamak in 1982 that externally heated plasmas can suddenly reach an operating regime of improved confinement. The regimes of low and high confinement are referred to as L-mode and H-mode, respectively. The transition from L-mode to H-mode is normally accompanied by appearance of recurrent magnetohydrodynamic instabilities known as *edge localized modes* (ELMs). These manifest themselves as short bursts of energy and particles as outer layer of plasma is suddenly pealed off and then flows along the magnetic field lines to the divertor plates.

We proposed a new approach to analysis of ELM time-series. This is based on the use of the auto-regresive moving average (ARMA) model. It is demonstrated that the chaos discovered earlier in some ELM time-series by detecting unstable periodic orbits (UPOs) might be fictitious - the result of uncritical processing of experimental data, or of erroneous interpretation of the results of the analysis.

QUANTUM THEORY OF TRANSPORT PHENOMENA IN MESOSCOPIC SYSTEMS

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

In collaboration with Tel Aviv University (Profs. A. Aharony and O. Entin-Wohlman), we have performed theoretical analysis of charge transfer by surface acoustic waves (SAWs). Electronic transport generated by SAW is a particular manifestation of adiabatic quantum pumping effect with potential applications in metrology (current and capacitance standards) and quantum computations (solid state implementation of a flying qubit).

A typical experimental setup consists of a few-micrometer long quasi-one-dimensional constriction in a high-mobility two-dimensional electron gas. Surface acoustic waves of several GHz frequency are launched in the longitudinal direction resulting in a finite dc current component along the constriction. We have suggested a simple one-dimensional model that includes the effect of an electrostatic barrier controlled by the external gate and a piezoelectric potential generated by the running SAW. The acoustoelectic current is calculated within the adiabatic approximation. The model qualitatively reproduces all experimentally observed features of the acoustoelectic current: plateau structure in the gate voltage and SAW amplitude dependencies that correspond to the transfer of an integer number of electronic per period; great sensitivity of the accuracy of the plateaus to the phase of a secondary counter-propagating SAW; effects of the longitudinal voltage bias. Application of our recently developed resonance approximation explains the formation of

integer steps as a sequential capturing of several electrons in a moving quantum dot formed by the SAW potential.

At low temperatures (milli-kelvin range) correlation effects in closed nanoscale strctures get pronounced and the approximation of non-correlated electrons becomes inapplicable. We are working at the extension of our formalism which includes the most important correlation effects (such a formation of the Kondo anomaly at the Fermi level) at a semi-quantitative level. We have recently obtained an exact solution of a non-linear system of truncated equations of motion for a single localized level embedded into an arbitrary external network in the presence of spin-polarizing external field.

DEFECTS AND POLAR SURFACES OF ADVANCED PEROVSKITES

E.A. Kotomin, Yu.F. Zhukovskii, R.I. Eglitis, and S. Piskunov,
G. Borstel (*University of Osnabrück, Germany*),
R.A. Evarestov (*St. Petersburg University, Russia*),
F. Illas, N. Lopez, and J. Carrasco (*University of Barcelona*, *Spain*)
E. Heifets (*California Institute of Technology, Pasadena, USA*),
D. Fuks (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
K. Hermansson (*Uppsala University, Sweden*)
and J. Maier (*MPI, Stuttgart, Germany*)

Ab initio quantum chemical calculations have been performed for a number of advanced ABO_3 materials 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), Density Functional Theory (DFT) and their hybrids (B3PW, B3LYP). 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. 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, University of Barcelona*, *Spain,* and *Uppsala University, Sweden* we have studied *F* centers (O vacancies) in $SrTiO_3$ perovskite and demonstrated that their properties are much closer to defects in partly

covalent SiO_2 rather traditional *F*-centers in ionic oxides (MgO and Al_2O_3). For first principles calculations on the defective structures of cubic $SrTiO_3$ we have used both CRYSTAL and VASP codes. Due to existence of different kinds of bonds in $SrTiO_3$ one can observe a competition between the tendency to trap the electrons associated with the missing oxygen in vacancy (*F* center) or to localize them on the Ti *3d* orbitals. The creation of a neutral O vacancy results in the new electronic state below the conduction band, which is consistent with experimental estimate indicated small ionization energy for the oxygen vacancy. The formation energy of the *F* center with respect to oxygen atoms depends on the size of supercell and was found to vary from 8.94 eV to 7.65 eV for supercell sizes containing from 40 to 240 atoms. The formation of oxygen vacancies is accompanied by a large relaxation of the first and second nearest neighbours. The localization of the electrons on titanium ions is consistent with photoemission studies on the surface of $SrTiO_3$, which indicate the formation of Ti^{3+} ions when surface defects are created by Ar^+-ion bombardment.

Progress in solid oxide fuel cells needs new materials for cathodes. One of promising materials is $LaMnO_3$ perovskite doped with Sr. Of principal 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 stabilization of 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

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

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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 and VASP codes is used also to understand better the nature of conductivity in the AgCl(111)/α-Al_2O_3(0001) interface.

In collaboration with *Osnabrück University, Germany, University College London, UK,* and *Ben Gurion University Ber Sheeva, 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 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 *Osnabrück University, Germany,* we have performed *ab initio* calculations for copper adsorption on a regular, defect-free TiO_2- and BaO- terminated (001) surfaces of a cubic $BaTiO_3$, using *a posteriori* HF-CC method as implemented into the *CRYSTAL-03* computer code. To clarify the nature of the interfacial bonding, we use slab models of the Cu/$BaTiO_3$(001) interfaces with different one-side substrate coverages, varied from 1/8 monolayer (ML) up to 1/2 ML, over both TiO_2- and BaO-terminated surfaces. TiO_2 termination has been found to be energetically more favorable for the adsorption of copper atoms. In agreement with previous experimental and theoretical data, our calculations indicate essential contribution of atomic polarization into the interaction between Cu atoms and surface O^{2-} ions. An increase of substrate coverage by copper simultaneously reduces the (*per* adatom) binding energy and enhances the interatomic interactions inside growing metallic film.

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.

Scientific publications

Published in 2004

1. E. Heifets, W.A. Goddard III, E.A. Kotomin, R.I. Eglitis, and G. Borstel, *Ab initio* calculations of the $SrTiO_3$ (110) polar surfaces. - Phys. Rev. B, 2004, 69, 035408 (p. 1-7).
2. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, Resonance approximation and charge loading/unloading in adiabatic quantum pumping. - Phys. Rev. B., 2004, 69, 195301 (p. 1-9).
3. R. Salazar, A.P.J. Jansen, and V.N. Kuzovkov, Synchronization of surface reactions *via* Turing-like structures. – Phys. Rev. E, 2004, 69, 031604 (p. 1-4).
4. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, and S. Dorfman, First principles simulations of the regular Cu/MgO(001) interface. – Surf. Sci., 2004, 566-568, p. 122-129.
5. E.A. Kotomin, E. Heifets, S. Dorfman, A. Gordon, and D. Fuks, Atomistic calculations of perovskite polar surface structures. – Surf. Sci., 2004, 566-568, p. 231-235.

6. V.N. Kuzovkov, V. Kashcheyevs, and W. von Niessen, Reply to Comment on 'Exact analytic solution for the generalized Lyapunov exponent of the two-dimensional Anderson localization'. - J. Phys.: Cond. Matter, 2004, 16, p. 1683-1685.

7. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, S. Dorfman, A.M. Stoneham, and G. Borstel, Adhesion trends and growth mode of ultra-thin copper films on MgO. – J. Phys.: Cond. Matter, 2004, 16, p. 4881-4896.

8. G. Zvejnieks, V.N. Kuzovkov, O. Dumbrajs, A.W. Degeling, W. Suttrop. H. Urano, and H. Zohm, Autoregressive moving average model for analyzing edge localized mode time series on Axially Symmetric Divertor Experiment (ASDEX) Upgrade tokamak - Phys. Plasmas, 2004, 11, p. 5658-5667.

9. O. Kortlüke, V.N. Kuzovkov, and W. von Niessen, Forced oscillations in a self-oscillating surface reaction model. - Phys. Chem. & Chem. Phys., 2004, 6, p. 1227-1229.

10. L. Grigorjeva, D.K. Millers, V. Pankratov, R.T. Williams, R.I. Eglitis, E.A. Kotomin, and G. Borstel, Experimental and theoretical studies of polaron optical properties in $KNbO_3$ perovskite. - Solid State Commun., 2004, 129, p. 691-696.

11. A.V. Sidorenko, A.J.J. Bos, P. Dorenbos, C.W.E. van Eijk, P.A. Rodnyi, I.V. Berezovskaya, V.P. Dotsenko, and A.I. Popov, Storage properties of Ce^{3+} doped haloborate phosphors enriched with 10B isotope. - J. Appl. Phys., 2004, 95, p. 7898-7902.

12. S. Piskunov, E. Heifets, R.I. Eglitis, and G. Borstel, Bulk properties of $SrTiO_3$, $BaTiO_3$ and $PbTiO_3$ perovskites: an *ab initio* HF/DFT study. – Comput. Mater. Sci., 2004, 29, p. 165-178.

13. R.I. Eglitis, E.A. Kotomin, and G. Borstel, Computer modeling of point defects in ABO_3 perovskites and MgO. - Comput. Mater. Sci., 2004, 30, p. 376-382.

14. Yu.F. Zhukovskii, E.A. Kotomin, and G. Borstel, Adsorption of single Ag and Cu atoms on regular and defective MgO(001) substrates: an *ab initio* study. - Vacuum, 2004, 74, p. 235-240.

15. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, Quantized charge pumping by surface acoustic waves in ballistic quasi-1D channels. - Euro. Phys. J. B, 2004, 39, p. 385-396.

16. A.W. Degeling, J.B. Lister, Y.R. Martin, and G. Zvejnieks, Were the chaotic ELMs in TCV the result of an ARMA process? - Plasma Phys. Control. Fusion, 2004, 46, p. L15-L21.

17. R.I. Eglitis, E.A. Kotomin, and G. Borstel, Large-scale computer modelling of point defects, polarons, and perovskite solid solutions. - Defect & Diffusion Forum, 2004, 226-228, p. 169-180.

18. R.I. Eglitis, S. Piskunov, E. Heifets, E.A. Kotomin, and G. Borstel, *Ab initio* study of the $SrTiO_3$, $BaTiO_3$, and $PbTiO_3$ (001) surfaces. - Ceram. Intern. (Proc. 2nd Int. Conf. ICMAT, Singapore, 2003), 2004, 30, p. 1989-1992.

19. 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. - Appl. Surf. Sci. (Proc. Spring EMRS, Strasbourg, 2003), 2004, 226, p. 298-305.

20. R.A. Evarestov, E.A. Kotomin, D. Fuks, J. Felsteiner, and J. Maier, Ab initio calculations of the $LaMnO_3$ surface properties. - Appl. Surf. Sci. (Proc. Int. Meeting on Applied Physics, Badajos, 2003), 2004, 238, p. 457-463.
21. E. Heifets, R.A. Evarestov, E.A. Kotomin, S. Dorfman, and J. Maier, Atomistic modelling of polar $LaMnO_3$ surfaces. - Sensors & Actuators B (Proc. Spring EMRS, Strasbourg, 2003), 2004, 100, p. 81-87.
22. D. Fuks, S. Dorfman, I. Bakaleinikov, A. Gordon, and E.A. Kotomin, The electronic structure of perovskite manganates. - Solid State Ionics (Proc. Spring EMRS, Strasbourg, 2004), 2004, 173, p. 107-111.
23. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, and S. Dorfman, A comparative study of Ag and Cu adhesion on MgO(001) surface. - Superlattices and Microstructures (Proc. Spring EMRS, Strasbourg, 2004), 2004, 36, p. 63-72.
24. V.S. Vikhnin, S. Kapphan, and R.I. Eglitis, Localized polaronic exiton and active impurity problems in incipient and relaxor ferroelectrics. - Ferroelectrics (Proc. 3rd Int. Seminar on Relaxor Ferroelectrics, ISRF-III, Dubna, 2000), 2004, 299, p. 11-20.
25. V.S. Vikhnin, R.I. Eglitis, and G. Borstel, Polaronic exitons in ferroelectric oxides: phemenological and microscopic theory, and manifestation of polaron exiton phase. - Ferroelectrics (Proc. 3rd Int. Seminar on Relaxor Ferroelectrics, ISRF-III, Dubna, 2000), 2004, p. 21-33.
26. O. Sychev, Yu.F. Zhukovskii, E.A. Kotomin, and G. Borstel, *Ab initio* calculations of copper nanostructures on MgO substrate. - Solid State Phenomena (Proc. Fall EMRS, Warsaw, 2003), 2004, 99-100, p. 219-222.
27. V.N. Kuzovkov, E.A. Kotomin, and G. Zvejnieks, Modelling of pattern formations in thin metallic film growth on crystalline substrates. - Comput. Model. New Technol. (Latvia), 2004, 8, p. 7-19.
28. J.R. Kalnin, How to overcome instructional learning. – Proc. 2. Int. Conf. "Information Technologies and Management" (IT&M, Riga, 2004), 2004, p. 21-25.
29. Yu.F. Zhukovskii, O. Sychev, E.A. Kotomin, G. Borstel, and Yu.N. Shunin, DFT modelling of transition metal adhesion on the MgO(001) surface. – Proc. 2. Int. Conf. "Information Technologies and Management" (IT&M, Riga, 2004), 2004, p. 60-75.
30. Yu.A. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, and Yu.N. Shunin, Diffusion of silver ions on the $AgCl(111)/\alpha\text{-}Al_2O_3(0001)$ interface: first principles simulation. – Proc. 2. Int. Conf. "Information Technologies and Management" (IT&M, Riga, 2004), 2004, p. 76-83.
31. S. Piskunov, E.A. Kotomin, E. Heifets, and Yu.N. Shunin, The electronic structure of $SrTiO_3$, $BaTiO_3$, and $PbTiO_3$ perovskite (001) surfaces: *ab initio* DFT/B3PW calculations. – Proc. 2. Int. Conf. "Information Technologies and Management" (IT&M, Riga, 2004), 2004, p. 84-109.

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Presentations at Conferences

I. 20th ISSP Conference (Riga, Latvia, February, 2004).

1. G. Zvejnieks and V. Kuzovkov, "Distinguishing deterministic and noise components in ELM time series". Abstracts: p. 37.
2. Yu.F. Zhukovskii and E.A. Kotomin. "Influence of defects on the adhesion of transition metals on non-polar MgO(001) surface: comparative theoretical analysis". Abstracts: p. 47.
3. S. Piskunov, R.I. Eglitis, and E.A. Kotomin, "Use of hybrid density functional theory for *ab initio* calculations of defective perovskite crystals". Abstracts: p. 48.
4. J.R. Kalnin, "Determination of the transport coefficients and averaging procedure". Abstracts: p. 96.
5. D. Bocharov and V. Kashcheyevs, "Quantum computation and ion traps". Abstracts: p. 106.

II. The 2nd International Conference "Information Technologies and Management", IT&M'04 (Riga, Latvia, April, 2004).

1. Yu.F. Zhukovskii, O. Sychev, E.A. Kotomin, G. Borstel, and Yu.N. Shunin, "DFT modelling of transition metal adhesion on the MgO(001) surface". Abstracts: p. 21-22.
2. Yu.A. Mastrikov, Yu.F. Zhukovskii, E.A. Kotomin, and Yu.N. Shunin, "Diffusion of silver ions on the AgCl(111)/α-Al2O3(0001) interface: first principles simulation". Abstracts: p. 23-24.
3. S. Piskunov, E.A. Kotomin, E. Heifets, and Yu.N. Shunin, "The electronic structure of $SrTiO_3$, $BaTiO_3$, and $PbTiO_3$ perovskite (001) surfaces: ab initio DFT/B3PW calculations". Abstracts: p. 25-26.
4. J.R. Kalnin, "How to overcome instructional learning". Abstracts: p. 62-63.

III. Spring European Materials Research Society (E-MRS) Meeting (Strasbourg, France, May, 2004).

1. S. Dorfman, S. Piskunov, E.A. Kotomin, and D. Fuks, „*Ab initio* calculations of the atomic and electronic structure of BaSrTiO3 (BST) solid solutions". Abstracts: D-II.4.
2. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, and S. Dorfman, "*Ab initio* study of the growth mode for thin Cu films on oxide substrate". Abstracts: G-XI.01.
3. Yu.F. Zhukovskii, E.A. Kotomin, Yu. Mastrikov, and J. Maier, "*Ab initio* simulations on AgCl(111) surface and AgCl(111)/α-Al2O3(0001) interface". Abstracts: H/P.26.
4. D. Fuks, S. Dorfman, I. Bakaleinikov, A. Gordon, and E.A. Kotomin, „The electronic structure of perovskite manganates". Abstracts: K/P.17.
5. Yu.F. Zhukovskii, E.A. Kotomin, D. Fuks, and S. Dorfman, "A comparative study of Ag and Cu adhesion on MgO(001) surface". Abstracts: T-VIII.03.

IV. 12th International Conference of Solid Surfaces, ICSS-12 (Venice, Italy, June, 2004)

1. D. Fuks, S. Dorfman, Yu.F. Zhukovskii, E.A. Kotomin, and A.M. Stoneham, "Theory of the growth mode for a thin metallic film on an insulating substrate". Abstracts: SS3-ThM10.

V. 2nd Seeheim Conference on Magnetism (Seeheim, Germany, June, 2004).

1. K. Küpper, J. Balasz, M. Kadiroglu, G. Borstel, R.I. Eglitis, H. Hesse, K.C. Prince, A. Takacs, T. Crainic, M. Matteucci, D. Wett, R. Szargan, A. Winiarski, E.Z. Burzo, and M. Neumann, "Electronic and magnetic properties of Sr_2FeMoO_6". Abstracts: p. 27.

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VI. The 15th International Conference on Defects in Insulating Materials, ICDIM'04 (Riga, Latvia, July, 2004)

1. R.I. Eglitis, E.A. Kotomin, and G. Borstel, "Large scale computer modeling of point defects in ABO_3 perovskites". Abstracts: p. 4.
2. V.S. Vikhnin, S.E. Kapphan, and R.I. Eglitis, "Charge transfer vibronic excitons: from idea to experiment, theory and applications". Abstracts: p. 4.
3. F. Illas, N. Lopez, J. Carrasco, E.A. Kotomin, Yu.F. Zhukovskii, S. Piskunov, J. Maier, and K. Hermansson, "First principles simulations of *F* center in $SrTiO_3$ perovskite". Abstracts: p. 51.
4. Yu.F. Zhukovskii and E.A. Kotomin, "Transition metal adsorption on defective MgO(001) surface: *ab initio* study". Abstracts: p. 70.

VII. 6th International Conference on Diffusion in Materials, DIMAT'04 (Cracow, Poland, July, 2004)

1. D. Gryaznov, J. Fleig, and J. Maier. "Numerical study of grain boundary diffusion in nanocrystalline materials". Abstracts: O-22.

VIII. 9th European Conference on Organised Films (Valladolid, Spain, July, 2004).

1. E.M. Fernandez, R.I. Eglitis, G. Borstel, and L.C. Balbas, "Adsorption and dissociation of water on non-ideal surfaces of alumina: a first principles study". Abstracts: p. 110.

IX. 32nd Course of the International School of Solid State Physics "Radiation Effects in Solids" (Erice, Italy, July, 2004)

1. 23. A.I. Popov, "Radiation induced defects in halides and oxides", Abstracts: p. 39.
2. E.A. Kotomin, "Radiation induced defects in halides and oxides: Theoretical Approach". Abstracts: p. 40.
3. E.A. Kotomin, "Modeling of colloid formation in halides and oxides". Abstracts: p. 41.
4. A.I. Popov, "Photo-stimulated storage phosphors: physics and applications radiation imaging". Abstracts: p. 57.
5. G. Zvejnieks, "Monte Carlo computer simulations of radiation defect accumulation kinetics and surface diffusion controlled self-organized reactions", Abstracts: p. 63.

X. Theory of Fusion Plasmas Conference, (Varenna, Italy, August, 2004)

1. G. Zvejnieks, V.N. Kuzovkov, O. Dumbrajs, A. W. Degeling, W. Suttrop, H. Uran, and H. Zohm, "Distinguishing the deterministic and noise components in the ASDEX upgrade ELM time series". Abstracts: P-7.

XI. Euro-Summer School on Condensed Matter Theory "Quantum Coherence, Correlations, and Mesoscopics" (Windsor, UK, August, 2004)

1. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, "Resonant transmission and quantized charge transfer in adiabatic quantum pumping". Abstracts: P1.11.

XII. Nano and Giga Challenges Microelectronics Symposium and Summer School Research and Development Opportunities (Cracow, Poland, September 13-17, 2004)

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1. S. Piskunov, E.A. Kotomin, and E. Heifets, "The electronic and atomic structure of $SrTiO_3$, $BaTiO_3$, and $PbTiO_3$ (001) surfaces: Ab initio DFT/HF hybrid calculations". Abstracts: p. 194.
2. S. Piskunov, S. Dorfman, D. Fuks, and E.A. Kotomin, "$Ba_xSr_{1-x}TiO_3$ perovskite solid solutions studied by means of ab initio electronic structure calculations and thermodynamics". Abstracts: p. 195.
3. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin, O. Sychev, and G. Borstel, "DFT modeling of copper adhesion on regular $BaTiO_3$(001) surfaces". Abstracts: p. 196.

XIII. International conference "Electronic structure: principles and Applications", ESPA'04 (Valladolid, Spain, September, 2004).

1. G. Borstel and R.I. Eglitis, "Large scale computer modelling of point defects in perovskite crystals". Abstracts: L6.
2. E.A. Kotomin and E. Heifets, "First principles calculations of the atomic and electronic structure of ABO_3 perovskite surfaces". Abstracts: L7.
3. E.M. Fernandez, R.I. Eglitis, G. Borstel, and L.C. Balbas, "Adsorption and dissociation of water on non-ideal surfaces of alumina: a first principles study". Abstracts: P63.

XVI. Fall Materials Research Society (MRS) Meeting (Boston, MA, USA, November, 2004).

1. E. Heifets, E.A. Kotomin, R.A. Evarestov, and J. Maier, "The *ab initio* atomic and electronic structure calculations for ABO_3 perovskite polar surfaces". Abstracts: p. 129.
2. E.A. Kotomin , F. Illas , N. Lopez , J. Carrasco , Yu.F. Zhukovskii, Yu. Mastrikov, and J. Maier, "First-principles calculations of *F*-centers in $SrTiO_3$ perovskites". Abstracts: p. 138.

XV. The 50th Annual Meeting of the Israel Physical Society (Haifa, Israel, December, 2004).

1. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, "Adiabatic quantum pumping and charge quantization due to resonant transmission". Abstracts: p. 129.

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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 holography 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 RTD of high sensitive photoresists in the visible region for holography and lithoghraphy for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed. R&D of Bragg grating structures for optical communication systems in planar waveguides based on amorphous chalcogenide semiconductor thin films were performed. The methods for fabrication of subwavelength-gratings and surface-relief features with nanometer scale have been developed.

Scientific Staff

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

PhD Students

1. I.Kuzmina
2. O.Balcers

Students

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Technical Staff

1. J.Gurovs
2. D.Popele
3. U.Poriņš

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).
3. Dr. J.Teteris, Institute of Optics of the Technical University Berlin, Germany (10 days).

Visitors from abroad

Dr. R.Petruskevicius, Institute of Physics, Vilnius, Lithuania (10 days).

Cooperation

Latvia

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

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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).

Germany

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

Lithuania

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

Main Results

HOLOGRAPHIC RECORDING IN AMORPHOUS As_2S_3 FILMS BY A 633 nm He-Ne LASER

A.Ozols, Dm. Saharovs , M.Reinfelde

Hologram recording in As_2S_3 films is usually made by an Ar^+ laser (λ=488.0 or 514.5 nm). It is based on photoinduced structural changes (PSC) involving As-As bond transformations. We report on the experimental studies of holographic grating (with periods Λ=0.55-20 μm) recording by either unfocused (recording light intensity I=0.58-0.78 W/cm^2) or focused (I=68-125 W/cm^2) He-Ne laser (λ=632.8 nm≈633 nm) beams in 5.4 μm thick a–As_2S_3 films sputtered on a glass substrates. Focused recording was much more effiecient (the maximal diffraction efficiency (DE))η_{max}=12.1%) than unfocused one (η_{max} =0.11%). The DE versus Λ dependence also differs. Periods Λ=0.7μm were optimal for unfocused recording whereas Λ=5-20 μm for the focused one. The recording was practically stable for, at least, several months. No photoinduced changes in absorption spectra (measured by Specord M40 spectrometer in 400-900 nm range) or periodic film thickness changes (by NT-MDT type AFM) were found. Thus 633 nm recording was purely phase one. The annealing of films decreased the recording efficiency by one order of magnitude. The recording mechanism is not clear but, most probably, it is based on another type of PSC involving photoinduced bond switching of sulfur atoms and their diffusion [1]. In the case of focused beams the recording seems to be thermally stimulated. The advantages of the 633 nm recording: 1) expensive Ar^+ laser is not needed; 2) reflection holograms of higher quality can be recorded because of much higher homogeneity.

[1] V.K.Tikhomirov, K.Asatryan, T.V.Galstian, R.Vallee, A.B.Seddon. Phil. Mag. Lett., 2003, vol.83, No2, pp.117-124.

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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.

ASYMMETRIC RELIEF REFLECTION GRATINGS IN As-S-Se THIN FILMS

Ilona Kuzmina and Janis Teteris

Thin films of amorphous chalcogenide semiconductors can be applied both as a medium for direct phase recording and as photoresists where recording is formed by surface modulation. The recording of Bragg gratings and application of them to obtain asymmetric relief on surface were studied. Relief gratings with asymmetric triangular profile possess high spectral selectivity and property to concentrate the diffracted light into a specific one order therefore those are widespread used in spectroscopic devices. Diffraction efficiency is maximum for definite wavelength defined by the blazing angle. To obtain such gratings we used recording scheme of Bragg gratings where laser beems fell perpendicular onto the sample from opposite sides but in this case the sample was turned in respect of beems of incidence and formed angle with them. The maximum diffraction efficiency (DE_{max}) of gratings due to high refractive index of films theoretically is expected in UV spectral range. Amorphous As-S-Se films were used as a media and He-Ne laser was used as a source of light for recording. The optimal thickness of thin films for DE_{max} of Bragg gratings was found. The influence of recording, chemical treatment and reconstruction conditions on the diffraction efficiency of relief gratings was investigated. Asymmetric relief gratings that are sensitive to polarization of light and have one diffraction order with DE_{max} at fixed angle of incidence were obtained.

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HOLOGRAPHIC RECORDING OF SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

Mara Reinfelde and Janis Teteris

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

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

The recording of the subwavelength gratings with a period of 0.15 μm – 1 μm was performed by holographic method. The fringe period for two intersecting light beams in a media with high refractive index n can be expressed as $\Lambda=\lambda_0/2\ n\ \sin\theta$, where λ_0 is the wavelength of laser light in vacuum, n is refractive index of the resist and θ is the half-angle between the laser beams inside the resist. The right angle prisms with n= 1.8 – 2.6 were used to increase the value of θ. The grating period and profile after chemical etching was measured by AFM. The transmission, reflection and polarization properties of the obtained gratings were studied.

APPLICATION OF AMORPHOUS CHALCOGENIDE THIN FILMS IN OPTICAL RECORDING TECHNOLOGIES

J.Teteris

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

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

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IMMERSION HOLOGRAPHIC RECORDING IN AMORPHOUS CHALCOGENIDE THIN FILMS

J.Teteris and M.Reinfelde

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

[1]. Teteris, J. and Reinfelde, M., 2004, *J. 0pt.A:Pure Appl.Opt.* **6**, S151-S154.

Scientific Publications
Published in 2004

1. J. Teteris and M.Reinfelde, S*ubwavelength-period gratings in amorphous chalcogenide thin films.* J. Opt. A: Pure and Applied Optics **6,** pp. S151-S154, 2004.
2. A.Ozols and M.Reinfelde, *Polarization holograms and diffraction anisotropy in amorphous chalcogenides.* J. Opt. A: Pure and Applied Optics **6,** pp. S134-S141, 2004.
3. M.Reinfelde, J.Teteris and I.Kuzmina, *Amorphous chalcogenide thin films as a media for holographic recording,* Proc. SPIE, **5566,** pp. 243-249, 2004.
4. I.Kuzmina and J.Teteris, *Bragg and asymmetric relief reflection gratings in As-S-Se thin films,* Latv. Journ. Phys. Techn. Sc. **5,** 3- 11, 2004.
5. J.Poriņš, A.Ozols, J.Eimuss and Ģ.Ivanovs. *Nonlinear effects in telecommunication fibers.* Sakaru pasaule (Communications World), 2004, No1 (33), pp.90.-91.(in Latvian).
6. J. Porins, A.Ozols, G.Ivanovs and J.Eimuss. *Nonlinear optical losses in telecommunication fibres.* Latvian Journal of Physics and Technical Sciences, 2004, No4, pp. 48 – 57.
7. A.Ozols and M.Reinfelde. *Anisotropy of light diffraction by holographic gratings in a-As-S-Se films.* Scientific Proc. of RTU. Series 1: Material Science and Applied Chemistry, 2003, vol.6, pp. 126-132.

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In Press

1. A.Ozols, V.Kampars, M.Reinfelde, V.Kokars. *Effect of chromophore groups on the holographic characteristics of azobenzene oligomers*. Scientific Proc. of RTU: Material Science and Applied Chemistry.
2. A.Ozols, M.Reinfelde. *Angular selectivity of thin gratings*. Proc. SPIE.
3. A.Ozols, M.Reinfelde, V.Kampars, V.Kokars. *Structure optimization of azobenzene oligomers for holography*, Physica Status Solidi (c).
4. J.Teteris. *Application of amorphous chalcogenide thin films in optical recording technologies.* Proc. SPIE.
5. M.Reinfelde and J.Teteris. *Holographic recording of subwavelength structures in amorphous chalcogenide thin films.* Proc. SPIE.
6. I.Kuzmina and J.Teteris. *Bragg and asymmetric relief reflection gratings in As-S-Se thin films.* Proc. SPIE.
8. J.Teteris and M.Reinfelde. *Application of amorphous chalcogenide thin films in optical recording technologies.* Physics and Chemistry of Glasses.

Lectures on Conferences

20th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, February 16-18, 2004

1. A.Ozols, M.Reinfelde, V.Kampars, V.Kokars. *Effect of chromophore groups on the holographic recording in azobenzene oligomers*. Abstracts, p.9.
2. J.Teteris. *Application of amorphous chalcogenide semiconductors in optical technology.* Abstracts, p.8.
3. M.Reinfelde and J.Teteris. *Subwavelength-period grating in amorphous chalcogenide semiconductors.* Abstracts, p.10.
4. O.Balcers and J.Teteris. *Amorphous chalcogenide based optical chemical sensors.* Abstracts, p.101.
5. I.Kuzmina and J.Teteris. *Asymmetric relief gratings in As-S-Se thin films.* Abstracts, p.11.

4th Int. Conf. on Amorphous and Microcrystalline Semiconductors, July 5-7, 2004, Sant-Peterburg, Russia

1. I.Kuzmina and J.Teteris. *Bragg and asymmetric relief reflection gratings in As-S-Se thin films.*
2. M.Reinfelde, J.Teteris and I.Kuzmina. *Polarisation properties of holographic gratings in amorphous chalcogenide films.*

The 4th Int. Conf. on Advanced Materials and Devices, AOMD-4, Tartu, Estonia, July 6-9, 2004

1. A.Ozols, M.Reinfelde. *Angular selectivity of thin gratings*. Abstracts, p.21.
2. J.Teteris. *Application of amorphous chalcogenide thin films in optical recording technologies.* Abstracts, p.20.
3. I.Kuzmina and J.Teteris. *Asymmetric relief reflection gratings in As-S-Se thin films.* Abstracts, p.43.
4. M.Reinfelde and J.Teteris. *Holographic recording of subwavelength structures in amorphous chalcogenide thin films.* Abstracts, p.43.

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The 15th Int.Conf. on Defects in Insulating Materials, ICDIM – 2004, July 11-16, 2004, Riga, Latvia

1. A.Ozols, M. Reinfelde. *Optimization of azobenzene oligomers for holography.* Abstracts, p.130.

2. I.Kuzmina, J.Teteris and M.Reinfelde. *Application of amorphous chalcogenide thin films in optical recording technologies.* Abstracts, p.132.

The Innovative Mass Storage Technologies Workshop, IMST`04, September 28-29, 2004, Aachen, Germany

1. J.Teteris. *Solid immersion holographic recording in amorphous thin films.* Abstracts, P.D06.

The 45th Scientific Conference of Riga Technical University, Riga, Latvia, October 11-15, 2004

1. A.Ozols, V.Kampars, M.Reinfelde, V.Kokars. *Effect of chromophore groups on the holographic characteristics of azobenzene oligomers*. Abstracts.

The 14th International Symposium on Non-Oxide and Novel Optical Glasses, ISNOGXIV, November 7-12, 2004, Florida, USA

1. J.Teteris. *Application of amorphous chalcogenide thin films in optical recording technologies.* Abstracts. p.64.

Master Thesis

1. Dm. Saharovs, *Holographic information recording in amorphous As_2S_3 films in the red part of spectrum,* 2004.
2. A. Groza, Influence of light polarization on optical recording in amorphous chalcogenide thin films, 2004.

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WIDE BAND GAP MATERIALS

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

Research Area and Main Problems

Rapid development of technology requires continuous elaboration of new materials, which could accumulate huge information, operate better and faster in the same time reducing their dimensions as small as possible. Wide band gap materials based on III, IV and V group elements including AlN, BN and diamond are promising for various applications with optoelectronics and dosimetry among them. Besides the bulk materials, produced by various methods recently different types of nanomaterials have been also sintered. The properties of each material largely depend on defects presented in it and forming their energy levels within the energy band gap. Therefore, the spectral investigation of a material can give essential information about defects existing in it.

During the last decade the laboratory of Wide band gap materials is working on investigation of spectral characteristics and light-induced energy accumulation in bulk materials: AlN ceramics, c-BN ceramics, c-BN single crystals, h-BN, natural and synthetic diamonds as well as in h-BN nanotubes and AlN nanotips. Part of investigations was performed together with the collaboration partners from abroad. The following studies are performed: photoluminescence and its excitation, optically stimulated luminescence and its characteristics, thermally stimulated luminescence and some dosimetric characteristics. The results obtained contain information about lighi-induced processes in material including luminescence mechanisms, processes of energy accumulation and release and sometimes it is as possible to reveal defect structure. Applicability of the material in UV light dosimetry is also evaluated.

Scientific Staff:	**Ph. D. Students:**	**Students:**
1. Dr. Hab.Phys, Assoc. Prof. B.Berzina	1. J.Sils	1. R.Krutohvostov
2. Dr. L.Trinkler		2. A.Auzina

Visitors from abroad

1. Dr. M.Benabdesselam. University of Nice-Sophia Antipolis,Nice,France (1 weak).
2. Dr. R Tomashunas. Vilnius University, Lithuania (1 month).

Scientific Visits Abroad

1. J.Sils. Ludvigs Maximillian University Munich, Germany (11 month).
2. L.Trinkler . University of Nice-Sophia Antipolis, Nice, France (10 days).
3. B.Berzina. University of Nice-Sophia Antipolis, Nice, France (10 days).
4. R.Krutohvostov. University of Nice-Sophia Antipolis, Nice, France (1 month).
5. B.Berzina. Institute of Physics and Semiconductorrs, Belarus Academy of Sciences, Minsk, Belarus (3 days).
6. B.Berzina. University of Lviv, Lviv, Ukrain (3 days).

Collaborations

Latvia

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

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

USA
Wake Forest University, Department of Physics, Winston-Salem (Prof. R.T. Williams)
Wake Forest University, Nanotechnologies, Winston-Salem (Prof. D. Carroll).

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

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

Lithuania
Vilnius University, Vilnius, (Prof. R. Tomashunas).

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.

OPTICAL PROPERTIES OF NATURAL AND SYNTHETIC DIAMONDS

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

Two types of diamonds are studied. One of them is synthetic CVD diamond and the other ones are the natural diamond. The properties of photoluminescence (PL), optically stimulated luminescence (OSL) and thermoluminescence (TL) were studied.

In the case of natural diamond it was observed that both the PL spectrum and OSL/TL emission spectra consist of well-known blue (450 nm) and green (510 nm) bands named as A luminescence related to luminescence centers containing different types of nitrogen-related defects. Excitation spectra are similar for both two PL bands forming a weak broad band at ~280 nm (240-360 nm region), but the main and more intensive excitation band is situated at the long wavelength edge of the fundamental absorption spectrum. 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.

In the case of synthetic CVD diamond the observed luminescence properties differ from those of natural diamond. In CVD diamond the PL consists of 430 nm band whereas the OSL and TL spectra show a wide 500 nm band. The excitation spectra of PL, OSL and TL are approximately similar to those observed for natural diamond. Light-induced processes being different for natural and synthetic diamonds were discussed and luminescence mechanisms have been offered.

Analysis of dosemetric characteristics of natural and synthetic diamonds was done which are promising for material application in UV light dosimetry especially within the UVC spectral region. From the OSL excitation spectra it follows that spectral sensitivity of diamond falls into the UVC range, whereas the OSL and TL luminescence spectra are located within the visible light region, thus suitable for usual detection. For optical stimulation the stimulation spectra fall into a broad visible/near infrared region implying that the stored signal is subject to the optical bleaching in ambient light conditions. Dosimetric TL peaks of diamond materials are located in the 280-330 ^{0}C range, suitable for detection. No thermal fading of the stored OSL and TL signal at room temperature was observed.

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.

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Scientific Publications
Published in 2004

1. L. Trinkler, B. Berzina, M.Benabdesselam, P.Iacconi, K. Atobe, L. Bøtter-Jensen. *Radiation induced luminescence processes in c-BN.* Radiation measurements, 38 (2004) 615-618.

2. B. Berzina, L. Trinkler, R. Krutohvostov, R. T. Williams, D. L. Carroll, R. Czerw, and E. Shishonok. *Photoluminescence excitation spectroscopy in boron nitride nanotubes compared to microcrystalline h-BN and c-BN.* phys. stat. sol. (c) **2**, No1, (2005) 318-321.

3. L.Trinkler, B.Berzina, S.C. Shi, L.C.Chen, M.Benabdesselam and P.Iacconi. *UV light induced luminescence processes in AlN nanotips and ceramics.* phys. stat. sol. (c) **2**, No1, (2005) 334-338.

Accepted for publication 2004

1. M.Benabdesselam, P.Iacconi, L.Trinkler, B.Berzina. *Pot*ential application of some wide band gap materils for UV dosimetry. Submitted to phys. stat. sol. (c). (accepted)
2. M. Benabdesselam, P.Iacconi, L.Trinkler, B.Berzina, J.E.Butler. *Optical bleaching, TSL and OSL features of CVD diamond*. Submitted to Radiat. Prot. Dosim. (accepted)

Lectures on Conferences

Workshop Defects and Impurities in Crystalline Boron Nitride Compounds, (Diepenbeek-Haselt, Belgium, February 20-21, 2004)

1. B.Berzina, L.Trinkler, R. T. Williams, D. L. Carroll, and R .Krutohvostov. *Luminescence of c-BN ceramics and BN nanotube / h-BN mixture.* (invited report).

The 15th International Conference on Defects in Insulating Materials ICDIM (Riga, Latvia, July 11-16, 2004)

1. B.Berzina, L.Trinkler, R. T. Williams, D. L. Carroll, R.Czerw, R.Krutohvostov and A.Auzina. *Luminescence of BN Nanotube/h-BN Powder Mixture*, (oral report). (Book of Abstracts, p. 46)
2. L.Trinkler, B.Berzina, S.C.Shi, L.C.Chen, M.Benabdesselam, and P.Iacconi. *UV Light Induced Luminescence Processes in AlN Nanotips and Ceramics,* (poster). (Book of Abstracts, p. 68).
3. M.Benabdesselam, P.Iacconi, L.Trinkler, B.Berzina. *Potential Application of Some Wide Band Gap Materials for UV Dosimetry*, (poster).(book of Abstracts, p 142).

15th European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, Nitrides & Silicon Carbide, (Riva Del Garda, Trentino, Italy, September 12-17, 2004)

1. L.Trinkler, B.Berzina, M.Benabdesselam, P.Iacconi. *UV Light Induced Luminescence Processes in Natural and CVD Diamonds*, (poster). (Book of Abstracts, 15.6.5.)

14th International Conference of Solid State Dosimetry (Yale University, USA, June 27-Jule 2, 2004)

1. M.Benabdesselam, P.Iacconi, L.Trinkler, B.Berzina,J.Butler. *Optical Bleaching, TSL and OSL Features of CVD Diamond*, (poster).

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

1. I,Megnis, B.Berzina, L. Trinkler, and E. Palcxevskis. *Spectral Characterization of AlN Nanopowders.* (Book of Abstracts, p.66).
2. L.Trinkler, B.Berzina, Shi Shih Chen, M.Benabdesselam, P.Iacconi. *Processes of Intrinsic and Impurity-Related Luminescence in AlN Ceramics and Nanotips.* (Book of abstracts, p. 80).
3. B.Berzina, L.Trinkler, R.Krutohnostov, R.T.Williams, and D.L.Carroll. *Spectral Characteristics of Some Boron Nitride Nanomaterials.* (Book of Abstracts, p. 81).
4. A.Auziņa, L.Trinkler. B.Berzina, M.Benabdesselam, and P.Iacconi. *Spectral Characteristics of Some Synthetic Diamonds.* (Book of Abstracts, p.82).

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LABORATORY OF OPTICAL MATERIALS

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

Research Area and Main Problems

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

Research in laboratory is focused on following problems:

- investigation of advanced optical materials and designs of vision appliances – tinted, high refractive glasses, antireflective coatings, multifocal and progressive, and contact lenses;

- effect of aberrations in eye structures and appliances on retinal image formation and on the psychophysically detected human visual response;

- design of the model eye with externally controllable light scattering (electrooptic PLZT ceramics, polymer dispersed liquid crystals PDLC);

- effect of stimuli blurring and decrease of contrast and colour contrast on the stereo threshold;

- designs of software to display visual stimuli on computer screen for studies of monocular vision perception, suppression and rivalry mechanisms of binocular vision;

- digital visual stimuli image processing determinant for analyse of the human visual response (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. Prof. I.Lācis
2. Prof. M.Ozolinsh
3. Dr. J.Dzenis
4. Dr. V.Grabovskis
5. Dr. G. Krūmiņa

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

Graduate Students
1. B.Sc. S. Fomins
2. B.Sc. I.Ļeonovs

Visitors from abroad
Prof. J.M.Bueno, Murcia University , Spain (4 weeks)
Prof. R. van Ee, Utrecht University (1 week)

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Scientific visits

M. Ozolinsh – Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand 10.04.-16.04.2004.
M.Ozolinsh – University of Murcia, Optics Laboratory 14.09.- 20.09.2004.
G.Krumina – Delft University 1.11.-10.11.2004.
G.Ikaunieks – Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand 10.04.-16.04.2004.

Partners abroad

Italy	Florence University , Italy, (Prof. S. Villani)
	Universita` di Roma "Tor Vergata" (Prof. I. Davoli)
Sweden	Lund University (Prof. S.Svanberg)
	Department of Clinical Science of Karolinska Institute (Dr. H. Richter)
	Chalmers TH, Sweden (Prof. L.Komitov)
Norway	Buskerud Høgskolan, Institutt for optometri (Prof. J.R.Bruenich).
England	Bradford University (Prof. D.Whittaker)
	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	**I**nstitut fur Arbeitsphysiologie an der Universität Dortmund
The Netherlands	Utrecht University (Prof. R. van Ee)
France	Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand (Dr.M.Colomb)
Russia	Saint-Petersburg Electrotechnical University

MAIN RESULTS

SIMULATION WITH (OF) DIFFERENT QUALITY STIMULI ON STEREOTHRESHOLD

G.Krumina*, M.Ozolinsh, I.Lacis*, V.A.Lyakhovetskii*****
***University of Latvia, Department of Optometry and Vision Science, Latvia**
*** Inst. of Solid State Physics, Riga*
****Saint-Petersburg Electrotechnical University, Saint-Petersburg, Russia*

The purpose of this study is to investigate the correlation between stereothreshold and quality of monocular stimuli to induced unequal images on the retina. The stereothreshold was estimated and compared using three methods to induce artificial conditions of amblyopia, cataract and uncorrected anisometropia and to compare results with real these conditions data.

Defocusation method with optical lenses was used for induced uncorrected myopic and hyperopic anisometropia and anisometropic amblyopia. For artificial cataract we used PLZT and PLDC plates that simulated very good real conditions of cataract. The third method is monitor direct stimuli for which we that could change blurring degree and contrast level induced amblyopia and cataract. The stereo sense was stimulated with light filters or liquid crystal (LC) shutters. In all conditions one eye saw constant clear stimuli, but second eye had different quality stimuli.

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The stereothreshold using colour filters was two times greater as using LC shutters. The stereothreshold value of induced cataract with PLZT and PLDC plates increased very quickly, if difference between both eyes visual acuity were 0.4 and more, to compare the same conditions in defocusation and monitor stimuli method.

The cataract influence more stereothreshold as the same conditions of uncorrected anisometropia or anisometropic amblyopia if eyes had unequal visual acuities.

SCATTERING EFFECTS IN VISION BY POLYMER DISPERSED LIQUID CRYSTALS

M. Ozolinsh*, J. M. Bueno, E. Berrio**, P. Artal**, A. Kozachenko*****
**Department of Optometry and Vision Science, University of Latvia*
***Laboratorio de Óptica, Universidad de Murcia, Spain*
****Dept. Liquid Crystal Physics, Chalmers University of Technology, Göteborg, Sweden*

Polymer dispersed liquid crystal (PDLC) is an optically scattering material with the scattering level depending on the applied voltage. We used a plate with a 10-μm thick layer of PDLC to measure the effects of the light scattering on the visual performance. With an artificial eye including the PDLC device, objective measurements of the point-spread function (PSF) were performed. The results show that the peak and skirts of PSF decrease and increase in accordance with the scattering level; this simulates well the manifestation of the ocular cataract. Note that the degree of depolarization in the central part of the PSF increases with the scattering level. With the device placed in the front of an eye and scattering level changed, subjective measurements of visual functions were carried out. As in the case of PLZT ceramics studied previously, light scattering depends on the wavelength, and the vision impairment was more remarkable for blue visual stimuli. A noticeable reduction of the visual performance (measured by means of visual acuity, contrast sensitivity, maximum fusion angle of stereodiparity, and stereoacuity) was observed, when slightly increasing scattering. The device under consideration proved to be a useful tool for studying scattering effects in vision.

VISUAL SEARCH OF COLOURED STIMULI IN UNFAVOURABLE VIEWING CONDITIONS

M. Ozolinsh*, G. Ikaunieks, J.R. Bruenich*****
** Inst. of Solid State Physics, Riga*
***Department of Optometry and Vision Science,University of Latvia;*
****Institutt for optometri, Høgskolen i Buskerud, Norway*
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Visual perception of different road signs and marks as well achromatic as colour contrast stimuli is diminished in unfavourable viewing conditions (fog, glare of oncoming vehicle lights, presence of eye cataract). In most cases contrast sensitivity, visual acuity, visual search time depends also on stimuli colour. The purpose of our studies was to determine mesopic visual perception capability of stimuli related to those used as traffic and road marks.

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We have measured visual acuity using greyscale and different colour contrast Landolt C optotypes exposed on computer screen. Experiments were performed indoors simulating artificial cataract (likely similar also to foggy weather conditions) with special PDLC polymer dispersed liquid crystal eye occluders. Applying an alternate low voltage to the occluder allowed to obtain simultaneous changes of light scattering and diminishing of visibility. Besides the contrast sensitivity for colour contrast (measured in ***L*a*b**** coordinates) Gabor gratings was investigated for white(grey)-red white-green, white-red, white-yellow stimuli, thus subtracting primary or complimentary colours comparing with same brightness achromatic gratings. Visual search was performed using technique similar to quoted in papers[1], looking for search stimuli in environment of different colour distractors.

We have also performed psychophysical perception threshold measurements of green-white and blue-white stimuli similar to road information boards and parallel electrophysiological detection of visual evoked potential (VEP) for different level of induced light scattering at different level of side illumination.

The highest degree of diminishing of colour contrast stimuli perception due to induced light scattering was detected for white-yellow (subtraction of blue) Landolt C and Gabor gratings and white-green information stimuli.

[1] Hurden A., Moorhead I.R., Ward P., Taylor J.A.F., Goodman T., Squire T.J., Walkey H.C. and Barbur J.L. (2002). A model for visual performance at mesopic light levels. Phase II: Final report and recommendations. Cambridge, UK: Scientific Generics Ltd.; Walkey H.C., Harlow J.A., and Barbur J.L. Mesopic visual search performance can be predicted using a new mesopic contrast metric. Vision in Vehicles 10 , Derby University Press Press, 2004.

ASSESSMENT OF OCULAR STEREOVISION PREVALENCE AND EYE DOMINANCE STABILITY

M. Ozolinsh*, K. Anisko, G.Krumina****
** Inst. of Solid State Physics, Riga*
***Department of Optometry and Vision Science, University of Latvia, Riga, Latvia*

Present paper reports on development of equipment for studies of the eye dominance and ocular stereo prevalence using black-white and color stereostimuli. Two methods of stereostimuli separation are used for experiments: color filter goggles and phase separation with liquid crystal shutter goggles. The eye stereo prevalence stability is studied at step-by-step artificial deterioration of the retinal image quality, particularly in the dominant eye. Presented stimuli have been blurred using spatial Gaussian filtering and using controllable light scattering induced by polymer dispersed liquid crystal cells placed in front of the dominant eye. Stimuli blurring and light scattering reveal a different influence on the eye ocular prevalence alterations – blurring caused more smooth changes of the prevalence toward the nonblurred stimuli eye, inducing of moderate scattering revealed large influence differences for different color stimuli on eye prevalence, however at sufficient high scattering level the nonstable switching from one eye prevalence to other eye prevalence took place.

HUMAN VISION COLOR CONTRAST SENSITIVITY TESTS

Maris Ozolinsh*, Sergejs Fomins, and Michéle Colomb*****
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***Dept. of Optometry, University of Latvia, Latvia*
****Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand , France*
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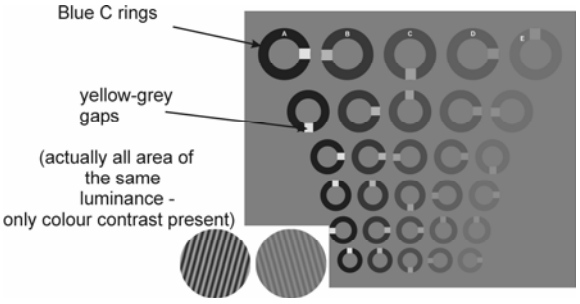
Coloured stimuli for human vision acuity and colour contrast sensitivity tests using advanced digital printing and digital photoprocessing are developed for quantitative evaluation of patients vision colour deficiency.

Advanced techniques of stimuli colour detection and digital colour printing allow to develop tests for human vision colour vision quantitative evaluation. We have used "Ocean Optics" spectrometer with 4 cm integrating sphere to measure colour gamut and homogeneity of different kind of digital print (ink jet, laser print) and KODAK and FUJI digital photoprocessing facilities in order to develop letter type: Snellen, Landolt, Pelli-Robson charts, and different colour contrast and spatial frequency Gabor gratings to measure isoluminant colour stimuli visual acuity and contrast sensitivity. Stimuli colour vectors in ***CIE xyz*** colour space were chosen as along the confusion lines of protanopes, deuteranopes and tritanopes as well allowing to evaluate the contrast sensitivity of some typical opponent colours in adverse viewing situations (fog, rain, +glare, presence of sunglasses) of essential everydays' stimuli: red-yellow, yellow-green, white-blue – examples of the traffic lights and panels. Alternating size and colour contrast optotypes and gratings were presented on achromatic background with luminance equal to saturated blue colour (corresponding to digital RGB [0,0,255]). Steps of colour contrast for stimuli along confusion lines were chosen corresponding to equal distances between colours in the ***La*b**** colour space (steps with equal $[\Delta Q]^2 = [\Delta L]^2 + [\Delta a^*]^2 + \Delta[b^*]^2$) . The best stimuli colour uniformity and spatial resolution were derived for photoprocessing samples. We have designed different size letter charts and contrast sensitivity charts related to achromatic ***Vistech Consultants*** contrast sensitivity chart. Charts were successfully applied to diagnose vision for patients with colour deficiency. Approbation of tests for other visual pathologies (cataract, *etc*.) and for simulated adverse weather conditions is in progress.



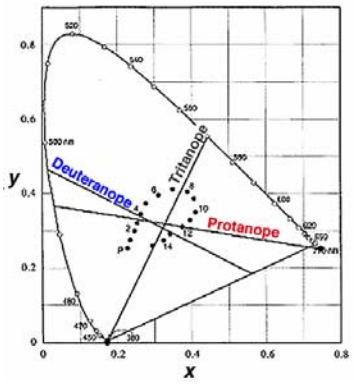


Figure. Colour visual acuity charts – Landolt C (and Gabor gratings for colour contrast sensitivity). Colours are arranged along confusion lines in CIE xyz colour space

Assessment of ocular

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STEREOVISION PREVALENCE AND EYE DOMINANCE STABILITY

M. Ozolinsh*, K. Anisko, G.Krumina****
** Inst. of Solid State Physics, Riga*
***Department of Optometry and Vision Science, University of Latvia, Riga, Latvia*

Present paper reports on development of equipment for studies of the eye dominance and ocular stereo prevalence using black-white and color stereostimuli. Two methods of stereostimuli separation are used for experiments: color filter goggles and phase separation with liquid crystal shutter goggles. The eye stereo prevalence stability is studied at step-by-step artificial deterioration of the retinal image quality, particularly in the dominant eye. Presented stimuli have been blurred using spatial Gaussian filtering and using controllable light scattering induced by polymer dispersed liquid crystal cells placed in front of the dominant eye. Stimuli blurring and light scattering reveal a different influence on the eye ocular prevalence alterations – blurring caused more smooth changes of the prevalence toward the nonblurred stimuli eye, inducing of moderate scattering revealed large influence differences for different color stimuli on eye prevalence, however at sufficient high scattering level the nonstable switching from one eye prevalence to other eye prevalence took place.

COLOUR STIMULI PERCEPTION IN ADVERSE VIEWING CONDITIONS

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***Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand, France*
****Department of Optometry and Vision Science, University of Latvia*

Studies are devoted to vision perception in adverse viewing conditions of stimuli with varying colour and luminance contrast considering: the difference of different colour stimuli transfer through light scattering environment (and in case of eye pathologies also in the eye); variance in retinal images blur and contrast; and physiological variation in structure and distribution density of three retinal S, M and L cone photoreceptor systems.

Parallel to the basic knowledge the topic is of great interest in applied vision research, particularly for safe driving in adverse weather, in mesoscopic conditions, presence of glare etc.We have measured visual acuity using greyscale and different colour contrast Landolt C optotypes exposed on computer screen. Experiments were performed indoors simulating artificial cataract (likely similar also to foggy weather conditions) with special PDLC polymer dispersed liquid crystal eye occluders. Applying an alternate low voltage to the occluder allowed to obtain simultaneous changes of light scattering and diminishing of visibility. Other measurements were carried out in artificial fog chamber producing different fog conditions within viewing distance of 6-10 m.

Besides mentioned before the contrast sensitivity for colour contrast (measured in ***L*a*b**** coordinates) Gabor gratings was investigated for white(grey)-red white-green, white-red comparing with same brightness achromatic gratings. Applying of white-yellow stimuli allowed to change the stimuli blue channel content (subtracting the blue primary within the yellow details) most scattered in fog.

The highest degree of diminishing of colour contrast stimuli perception due to induced light scattering was detected for white-yellow (subtraction of blue) Landolt C and Gabor gratings and white-green information stimuli.

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Scientific publications
Published in 2004

1. G. Krumina, M. Ozolinsh, V.A. Lyakhovetskii, "Stereovision by visual stimulus of different quality." In": "Ocu*lar Biomechanics*," Helmholtz Research Institute for Eye Diseases, Moscow, 282-89 (2004).
2. M. Ozolinsh and G. Papelba, "Eye Cataract Simulation Using Polymer Dispersed Liquid Crystal Scattering Obstacles," *Ferroelectrics* V.304, 207–212 (2004).
3. J.M.Bueno, E.Berrio, M. Ozolinsh, and P. Artal," Degree of polarization as an objective method of estimating eye scattering", *J. Opt. Soc. Am.* A/Vol. **21**, pp.1316-21 (2004).
4. M. Ozolinsh, S. Fomins, and M.Colomb, "Optotypes for human color contrast sensitivity tests," In: *Proc. OSAV'2004, Int. Topical Meeting on Optical Sensing and Artificial Vision*, Saint Petersburg, Russia, p.18-21 (2004).

Accepted for publication in 2004

1. M. Ozolinsh, S. Fomins, and M.Colomb, "Human Color Vision Acuity and Contrast Sensitivity Tests," *OSA J.Opt.Techn.*
2. M. Ozolinsh, K. Anisko, G. Ikaunieks and G. Krumina, "Assessment of ocular stereovision prevalence and eye dominance stability," *Proc. SPIE*.

Reports in conferences

1. G. Krumina, M. Ozolinsh, V.A. Lyakhovetskii, "Stereovision by visual stimulus of different quality." ***The 4th Conf. "Ocular Biomechanics-2004"***, Moscow, 2004.
2. G, Krumina, M. Ozolinsh, and I. Lacis, "Induced monocular blur and stereo threshold changes". ***ECVP-2004***, Budapest, 2004.
3. M. Ozolinsh, G. Ikaunieks, and J.R. Bruenich, "Visual search of coloured stimuli in unfavourable viewing conditions ." ***The 3rd International Conference on Traffic & Transport Psychology***, Nottingham, p.43, 2004.
4. M. Ozolinsh, M.Colomb, and G. Ikaunieks, "Colour stimuli perception in adverse viewing conditions." Abstr**.** ***The II EOS Topical Meeting on Physiological Optics***, Granada, p.25, 2004.
5. G. Krumina, I. Lacis, and M. Ozolinsh, "The influence of external effects on stereothreshold." Abstr. ***The II EOS Topical Meeting on Physiological Optics***, Granada, p.56, 2004.
6. J.M. Bueno, E. Berrio, M. Ozolinsh, P. Artal, "Impact of Ocular Scattering on Visual Performance." Abstr. ***The II EOS Topical Meeting on Physiological Optics***, Granada, p.24, 2004.
7. G. Krumina, M. Ozolinsh, I. Lācis, V. Lyakhovetskii, "Stereovision Estimation in Conditions of Blurring Simulation '" Abstr. ***The 3rd Int.Conf. "Advanced Optical Materials and Devices AOMD-3"***, Tartu, July 2004, p.47.
8. M. Ozolinsh, K. Anisko, G.Krumina, "Assessment of ocular stereovision prevalence and eye dominance stability,"Abstr**.** ***The 3rd Int.Conf. "Advanced Optical Materials and Devices AOMD-3"***, Tartu, July 2004, p.28.
9. M. Ozolinsh and G. Ikaunieks, "Vision in Unfavourable Viewing Conditions," Abstr. ***The 3rd Int.Conf. "Advanced Optical Materials and Devices AOMD-3"***, Tartu, July 2004, p.28.
10. M. Ozolinsh, J.M. Bueno, E. Berrio, P.Artal, and A. Kozachenko, "Scattering Effects in Vision by Polymer Dispersed Liquid Crystals," Abstr. ***The 3rd Int.Conf. "Advanced Optical Materials and Devices AOMD-3"***, Tartu, July 2004, p.48.

`

11. M. Ozolinsh, G. Ikaunieks, J.M. Bueno, E. Berrio, A. Kozachenko, and G. Andersson, Human Eye Photoreceptor Acuity at Different Colour Contrast Stimuli." Proc. ***«Basic Problems of Optics»***, ***Topical Meeting on Optoinformatics***, St.Petersburg, 2004, p.33-35.
12. M. Ozolinsh, S. Fomins, and M. Colomb, "Optotypes for Human Color Contrast Sensitivity Tests." Proc. ***Conference OSAV-2204 Optical Sensing and Artificial Vision***. St.Petersburg, 2004, p.129.

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SURFACE PHYSICS

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

Research Area and Main Problems

- photo-, thermo- and atmosphere-induced modifications of structure, optical and mechanical properties of fullerite C_{60} studied by microindentation, dislocation mobility and AFM methods.
- structural modifications and hardening effect in ionic crystals under irradiation with fast (MeV-GeV) ions (Au, Pb, Bi, S, and Ni); effect of ion species, energy loss and fluence on radiation damage and hardening.
- adhesion and related phenomena on metal/metal and metal/oxide interfaces..

Scientific staff

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

Technical staff

4.A.Petersons

Students

5. L.Gailīte
6. G.Bakradze

Visitors from abroad

Prof. K.Schwartz, Darmstadt, Germany (1 week)

Scientific Visits Abroad

1. Dr.F.Muktepavela, Krakow, Poland (1 week).
2. Dr.F.Muktepavela, St.Petersburg, Kaluga, Russia (1 week).
3. Dr.I.Manika, Darmstadt, Germany (2 weeks).

Cooperation

Latvia

1. Institute of Physical Energetics, Latvian Academy of Sciences (Dr.J.Kalnacs)
2. Riga Technical University (Prof.V.Mironovs)
3. Daugavpils Pedagogical University (Dr.R.Pokulis, E.Tamanis)

Germany

GSI, Darmstadt (Prof.K.Schwartz).

Israel

Technion, Haifa (Dr.S.Stolyarova).

PHANTOMS -IST Nanoelectronic network (Dr.J.Maniks)

Main Results

PHOTO-INDUCED TRANSFORMATIONS IN FULLERITE C_{60} SINGLE CRYSTALS AND POLYCRYSTALLINE FILMS

I.Manika[1], J.Maniks[1], R.Pokulis[2]
[1]Institute of Solid State Physics, University of Latvia
[2] Daugavpils Pedagogical University

The polymerization of fullerite (99.9 % C_{60}) under light irradiation has been investigated by indentation hardness, dislocation mobility, and AFM methods. The conditions of photopolymerization are elucidated. It has been found that the photopolymerization is observed in the face-centered-cubic phase of fullerite in the temperature range of 260-400K. The photopolymerization occurs under the UV and visible light irradiation in the fundamental absorption region and around the fundamental band edge at photon energies exceeding the threshold of 1,5-1.6eV, which is related to photogeneration of excitons in fullerite. The efficiency of polymerization increases with decreasing the wavelength. The polymerized phase is localized in the near-surface layer of 1-3 μm, which thickness corresponds to the light penetration depth.

Two phototransformed phases, which differ by the hardness and thermal stability, are found to appear: (a) well-known all-carbon polymer composed of fullerene dimers (C_{120}) and (b) the hard modification of the photopolymer (HV=0,65 -1 GPa). The photoinduced polymerization of fullerite is explained by the phototochemical 2+2 cycloaddition reaction, in which depending on temperature and air exposure, all-carbon fullerene dimers (C_{120}) or $C_{120}O$ dimers are created. The C_{60} molecules in a $C_{120}O$ dimer possibly are connected by an oxygen bridge and a single carbon bond. The hard photopolymerized phase is formed in the oxygen-contaminated subsurface layer of 0.5-1 μm at temperatures ranging from 290 to 340 K. This phase is thermally less stable and transforms to well-known all-carbon photopolymer under heating at 310-320K.

It has been found, that the major role in the photopolymerization under irradiation with UV light at $\lambda \leq 150$ nm in air atmosphere plays the photogeneration of ozone and its reaction with fullerite.

The effect of post-irradiation hardening, which manifests as increase in hardness during the storage of light-irradiated fullerite crystals in dark, has been observed. The effect is explained by continuation of polymerization under residual stress.

HARDENING AND LONG-RANGE STRESS EFFECTS IN LIF CAUSED BY HIGH-FLUENCE IRRADIATIONS WITH ENERGETIC BI, NI, KR AND S IONS

J. Maniks, I. Manika
Institute of Solid State Physics, University of Latvia

The limits of the ion-induced hardening, and the effects of internal and long-range stresses in LiF crystals irradiated with Bi, Ni, Kr, and S ions, having a specific energy of 10 MeV/u, are studied. A considerable hardness increase, bending of the crystals, formation of dislocations in distant non-irradiated parts of the crystals, and initiation of fracturing under the high-fluence irradiation (up to 10^{13} cm^{-2}) are observed. It is shown that the irradiation with heavy ions (Bi) gives rise to dislocations and work hardening mainly in the region adjacent to the

irradiated one while in the case of lighter ions (Ni and S), which create highly non-uniform depth distribution of radiation defects, the stress gradients are created and dislocations are formed also inside the irradiated zone. The heavy ions, which cause severe track core damage, generally induce a higher stress.

In cooperation with GSI, Darmstadt, Germany.

ADHESION, MICROHARDNESS AND RADIATION RESISTANCE OF NANOSTRUCTURED ALN AND ALN/TIN TRIBOLOGICAL COATINGS

F.Muktepavela, V.Skvortsova
Institute of Solid State Physics, University of Latvia

The coatings were deposited by plasma reactive sputtering on Al_2O_3, WC (tungsten carbide), Si and stainless steel substrates. It was found that the nanostructured multilayer AlN/TiN films have better adhesion, fracture toughness and wear resistance if compared with those for AlN and TiN single layer coatings. Such behaviour may be related to higher strength and plasticity of nanostructured coatings, which are favourable for comparatively intense relaxation processes on the interfaces. The γ-irradiation caused the hardening of coatings by about 30%, which is ascribed to creation of point defects. No destruction or debonding of AlN films on Al_2O_3 and WC substrates under γ-irradiation at doses up to 10^6 Gy was found to occur. This assumption agrees also with the change of optical properties. For AlN/Si system the destruction of the Si substrate under irradiation was observed due to generation of high internal and interfacial stresses.

POWDER Fe-Cu COMPOSITES OBTAINED BY MAGNETIC-IMPULSE COMPACTION AND INFILTRATION

F.Muktepavela[1], V.Mironovs[2]
[1]*Institute of Solid State Physics, University of Latvia*
[2] *Riga Technical University*

Magnetic-impulse method based on interaction of strong pulse electromagnetic fields with metal work piece is widely used for compacting of powder materials. Generally the magnetic-impulse compaction (MIC) and subsequent sintering of powders is performed using a container (shell) of highly conductive metal (copper, aluminum, or copper alloys). After compaction the shell is usually removed as a waste product. This study reports on the properties of Fe-Cu powder composites obtained by MIC with the use of the metallic (cooper) shell as infiltration medium at the final stage of sintering. The magnetic-impulse compacted, preliminary sintered and Cu-infiltrated Fe powder material exhibits improved properties (density γ =8000 kg/m^3, porosity Θ = 2%, hardness HV_{10} = 1,7GPa, tensile strength σ_B = 0,5 GPa, elongation δ = 8%) compared with those for materials obtained by MIC but without infiltration.

Scientific publications
Published in 2004

1. J.Maniks, I.Manika, J.Kalnacs. *Photo-induced polymerization and stress effects in fullerite C_{60}.* Fullerenes, Nanotubes and Carbon Nanostructures, 2004, vol.12, No.1/2, pp.269-273.
2. J.Maniks, I.Manika, J.Kalnacs. *Photo-induced modifications of the structure and microhardness of fullerite C_{60},* Hydrogen Materials Science and Chemistry of Carbon Nanomaterials, Ed.T.N.Veziroglu, Kluver Academic Publishers, 2004, pp.167-176.
3. I.Manika, J.Maniks, L.Gailite, K.Kundzins. *Effects of ion fluence and energy loss on hardening of LiF irradiated with energetic ^{58}Ni ions.* Latvian Journal of Physics and Technical Sciences, 2004, No.1, pp.37-46.
4. I. Manika , J. Maniks. *Depth profiles of hardening in lithium fluoride irradiated with swift ^{58}Ni ions.* Phys.Stat.Sol.(a), 2004, vol.201, No9, pp.2042-2052.
5. I.Manika, J.Kalnacs, *Long range hardening effect in ion-implanted molybdenum.* Engineering Materials &Tribology, Materials of the XII International Baltic conference, Riga, Latvia, September 23-24, 2004, pp.116-119.
6. F.Muktepavela, I.Manika, V. Skvortsova. *Adhesion and radiation stability of AlN and AlN/TiN thin coatings on metallic and non-metallic substrates.* Engineering Materials &Tribology, Materials of the XII International Baltic conference, Riga, Latvia, September 23-24, 2004, pp.175-178.
7. V.Mironovs, D.Serdjuk, F.Muktepavela. *Profiles of the wastes of stamping products.* Engineering Materials &Tribology, Materials of the XII International Baltic conference, ,Riga, Latvia, September 23-24, 2004, pp.46-50.
8. V.Mironovs, D.Serdjuk, F.Muktepavela. *Perforated steel profiles on the base of industrial wastes.* Proc.3-rd Int. Conf. "Materials and Coatings for Extreme Performances", Katciveli, Crimea, Ukraine, 16-20 September 2004, pp.559-565.
9. V.Mironovs, D.Serdjuk, F.Muktepavela. *Steel profiles from the perforated bands*. Proc. 4-th Int. DAAM Conf. Industrial Engineering, Tallin, Estonia (ed.J.Papstel), Tallin University of Technology, April 29-30, 2004, pp.138-140.
10. V.Mironovs. F.Muktepavela. *Powder Iron-Copper Composites obtained by magnetic impulse compaction and infiltration.* In: Powder Metallurgy&Composite Materials (NASB), Minsk, 2004, pp.119-124.

Accepted for publication 2004

1. I.Manika, J.Maniks, K.Schwartz, C.Trautmann and M.Toulemonde. *Energy loss and fluence dependency of swift- ion- induced hardening in LiF*. Phys.Stat.Sol.(c), 2005, vol.2, No.1, pp.434-437.
2. I.Manika, J.Maniks, P.Kulis, L.Gailite. *Hardening in LiF induced by energetic Ni ions and recovery of structure and properties under annealing*, Phys.Stat.Sol.(c), 2005, vol.2, No.1, pp.430-433.
3. F.Muktepavela, G.Bakradze, E.Tamanis, S.Stolyarova, N.Zaporina. *Influence of Mechanoactivation and Mechanical Properties of Metal/Oxide Interfaces.* Phys.Stat.Sol.(c), 2005, vol.2, No.1, pp.339-342.
4. I.Manika, J.Maniks, P.Kulis, L.Gailite. *Hardening in LiF induced by fast Kr and Ni ions and recovery of structure and properties under annealing*, SPIE Proceedings.

5. I.Manika, J.Maniks, K.Schwartz, C.Trautmann. *Hardening and long-range stress effects in LiF caused by high-fluence irradiations with energetic Bi, Ni, Kr and S ions*. SPIE Proceedings.
6. F.Muktepavela. The role of Diffusion in Superplasticity and Brittleness of Fine-grained Binary Eutectics. Defects and Diffusion Forum.

Lectures on Conferences

20th Scientific Conference of Institute of Solid State Physics,
University of Latvia, Riga, February 16 - 18, 2004

1. L.Gailite, I.Manika, J.Maniks. *Formation of dislocations in LiF crystals under irradiation with energetic ^{209}Bi, ^{58}Ni and ^{36}S ions*. Abstracts, p.55.
2. J.Maniks, I.Manika. *Obtaining of nanostructured materials by high-energy (MeV-GeV) ion irradiation*. Abstracts, p.65.

15-th Int. Conference on Defects in Insulating Materials (ICDIM-2004)
July 11-16, Riga, Latvia

1. I.Manika, J.Maniks, K.Schwartz, C.Trautmann and M.Toulemonde. *Energy loss and fluence dependency of swift- ion- induced hardening in LiF*, Abstracts p.81.
2. I.Manika, J.Maniks, P.Kulis, L.Gailite. *Hardening in LiF induced by energetic Ni ions and recovery of structure and properties under annealing*. Abstracts p.81.
3. F.Muktepavela, N.Zaporina, S.Stolyarova. *Influence of Mechanoactivation and Mechanical Properties of Metal/Oxide Interfaces*. Abstracts p.69.

4th International Conference on Advanced Optical Materials and Devices (AOMD),
Tartu, Estonia, July 6-9, 2004

1. Manika, J.Maniks, K.Schwartz, C.Trautmann. *Hardening and long-range stress effects in LiF caused by high-fluence irradiations with energetic Bi, Ni, Kr and S ions*. Abstracts p.17.
2. I.Manika, J.Maniks, P.Kulis, L.Gailite. *Hardening in LiF induced by fast Kr and Ni ions and recovery of structure and properties under annealing*. Abstracts p.40.

VI Int.Conference on Diffusion in Materials, Krakov, Poland, July 18-23, 2004

1. F.Muktepavela. *The Role of Diffusion in Superplasticity and Brittleness of Fine-grained Binary Eutectics.*

XII International Baltic Conference "Engineering & Tribology", Riga, Latvia,
September 23-24, 2004

1. I.Manika, J.Kalnacs. *Long range hardening effect in ion-implanted molybdenum*.
2. F.Muktepavela, I.Manika, V.Skvortsova. *Adhesion and radiation stability of AlN and AlN/TiN thin coatings on metallic and non-metallic substrates*.

XLII Междунар. Конф. Актуальные проблемы прочности. Калуга, Россияб
26-29 мая 2004

1. Ф.Муктепавела, Я.Маникс. *Деформационно - индуцированные состояния хрупкости и сверхпластичности межфазных границ мелкодисперсных эвтектик*. Материалы конф., стр.76

Doctoral Thesis

1. R.Pokulis. *Structural changes in fullerite C_{60} induced by light-irradiation and ambient oxygen*, Riga, 2004.

Bachelor Thesis

1. L.Gailite. Formation of dislocations in LiF crystals under irradiation with high- energy ions, Riga, 2004.

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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 radioactivity and nuclear materials in Latvia
- application of the nuclear spectral methods to solve the technological processes
- 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
- physical, structural and magnetic properties of solid state fine particles.

International projects

1. EC FP5 TARI Project (2001-2004) "Magnons in diluted antiferromagnetic materials (MIDAM)".
2. EC FP6 TARI Project (2004-2005) "Effect of dilution on infra-red absorption in antiferromagnetic materials (EDAAM)"

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. sc. A.Pavlenko
18. Mag. sc. A.Abramenkova

Technical Staff

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

Students

1. Bach. sc. A. Andrejevs
2. Bak. sc. A. Dzalbs
3. I. Motmillere

Visitors from abroad

Prof. T. von Egidy, Technische Universitaet Muenchen (3 days).

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Scientific visits abroad

Dr. hab. A.Afanasjev Notre Dame University, Notre Dame,USA (10 month).
Dr. hab. J. Berzins European Commisssion Euratom, Brussels,Belgium (10 days).
Dr. hab. J. Berzins European Commisssion Euratom, Luxembourg (5 days).
Bach.sc. A.Dzalbs International Nuclear Physics Conference INCP2004. Gőteborg, Sweden, June 27- July 2, 2004.
Dr. D.Riekstina, International Symposium, Bulgaria, Albena (1 week)
Dr. hab. N. Mironova-Ulmane, 20.01.2004-2.02.2004, Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Frascati, Italy
Dr. A.Kuzmin, 20.01.2004-2.02.2004, Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Frascati, Italy
Dr. hab. N.Mironova-Ulmane, Institute of Physics Tartu Estonia (1week +1 week)
Dr. hab. N.Mironova-Ulmane, Ural Technical University, Ekaterinburg, Russia (1 week)
Dr. A. Petrov, University of Roma (3 days).
Dr. A.Petrov , Technische Universitaet Wien, Austria (3 days).

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. Institute of Wood Chemistry (Dr. hab. G. Dobele, Dr.hab. G. Telesheva, Dr.hab.T.Dizbit)
7. Riga Technical University, Faculty of Material Science and Applied Chemistry (Prof. J.Dehtjar,).

USA

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

Brasil

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

Lithuania

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

Canada

1. Department of Astronomy and Physics, Saint Mary's University, Halifax (Mg.A.Aleksejevs)
2. Department of Physics, Acadia University, Wolfville (Mg.S.Barkanova)

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Czech Republik
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).

Italy
1. Laboratori Nazionali di Frascati, Istituto Nazionale di Fisica Nucleare, Frascati (M.Cestelli Guidi, A. Marcelli)
2. Dipartimento di Scienze Geologiche, Universitá Roma Tre, Rome (M. Piccinini)
3. INFM and Dipartimento di Fisica, Università di Trento, Povo (Trento)(G.Mariotto)
4. INFM and Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (Cosenza) (E.Cazzanelli)

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

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

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

Russia
1. Ural State University, Ekaterinburg (Prof. A. Nikiforov).
2. Ural Technical University, Ekaterinburg (Prof. B.Shulgin)

Austria
1. Ruder Boskovic Institute, Zagreb (Prof. S.Music).
Atomic Institute of Austrian Universities, Vienna (Prof. H.Weber).

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

Main Results

THE NUCLEUS 194IR STUDIED WITH TRANSFER AND NEUTRON CAPTURE REACTIONS

H.-F.Wirth, G.Graw, R.Hertenberger[1], M.Balodis, J.Bērziņš, N.Krāmere[2], J.Jolie[3], T.von Egidy[4]

Structure of ^{194}Ir is investigated via (n,γ), (n,e-), (d,p) and (d,α) reaction spectroscopy. These different methods of measurement have led to a more developed level scheme. In 2004, we already have 60 levels. New levels are established mainly below 750 keV with spin values from 0 to 5 with their depopulation. One should note that only 15 levels are with a positive parity.

We try to employ several models for interpretation. Since the shape of the nuclei with Z about 177 and mass numbers higher than 190 is not well defined, both geometric and algebraic models help to understand the structure from different viewpoints.

The simplest geometric model with clear physical principles is axially-symmetric prolate model using Nilsson configurations for a weakly deformed nucleus (deformation parameter delta is about 0.10 to 0.12). Nilsson orbits used for interpretation are proton orbits $3/2^+[402]$, $1/2^+[400]$ and $11/2^-[505]$, as well as neutron orbits $3/2^-[512]$, $1/2^-[510]$ and $11/2^+[615]$.

For a number of band heads, appropriate superimposed rotational levels have been proposed. Although one does not expect exact rotational energy relations of the type I(I+1), a search for rotational bands can be justified. For levels being interpreted in framwework of this model, rotational parameter A is variating from about 10 to 20 keV (e.g., the ground state rotational band 0 keV 1^-, 84 keV 2^-, 184 keV 3^-), up to 30-40 keV (e.g., positive parity bands with band heads 147 keV 4+, 270 keV 3^+, 518 keV 2^+). The 518 keV 2^+ 722 keV 3+ band can be interpreted as a gamma-vibrational band connected to the 147 keV 4^+, 561 keV 5^+ rotational band.

Probably, we can use triaxiality already tested for several odd iridium nuclei. Rather detailed is the ^{193}Ir study using this model approach. We do not know serious studies of this kind for odd-odd nuclei. In ^{194}Ir, it is comparatively simple to identify “triaxial” structures within positive parity levels. Axially-symmetric approach does not explain the band 270 keV 3^+, 519 keV 4^+, and triaxial approach can help.

Several attempts to use the IBFFM algebraic model have happened for ^{194}Ir. In calculations using this model are presented. New level scheme data can be compared with these “old” calculations, since this model does not mean detailed fit to experimental results.

There are recent supersymmetry calculations. In the conference version of the (d,α) reaction results, an attempt is made to compare the ^{194}Ir and ^{196}Au level structure.

Differences with the ^{192}Ir level structure would be of interest. Evidently, a smaller deformation is expected for ^{194}Ir if we limit ourselves to a rather approximate axially symmetric prolate version. These differences should be shortly discussed in the ^{194}Ir journal publication being in preparation.

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3. Universitaet Koeln, Germany
4. Technische Universitaet Muenchen, Germany

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NUCLEAR STRUCTURE OF ^{127}Te STUDIED WITH (n,γ) AND (d,p) REACTIONS AND INTERPRETED WITH IBFM AND QPM

J. Honzátko[*], V. Bondarenko[**], I. Tomandl[*], T. von Egidy[***], H.-F. Wirth[***], D. Bucurescu[$], V. Yu. Ponomarev[+$$], N. Marginean[$], R. Hertenberger[++], G. Graw[++], Y.~Eisermann[++], L. Rubaček[#]

The γ-ray and particle spectroscopy with high energy resolution in combination with polarized deuteron beams allowed the observation of almost 154 levels up to 4 MeV. Spin-parities and single particle strengths were assigned to the most of the observed states by using the DWBA and CCBA analyses. The almost complete experimental set of level energies, secondary γ-ray branches and spectroscopic strengths has been interpreted in terms of IBFM-1 and QPM model calculations. Both the models give a generally good description of the observable features below 2 MeV excitation energies. Only satisfactory description of strength functions and of the degree of fragmentation of the particle-type states was obtained at higher energies with the IBFM-1 due to the boson space cut-off effect. In this respect the QPM ensures much wider model space where its dimension varies between 500-700 configurations. A reasonably good description of the summed 3/2- and 7/2- strengths was obtained with the QPM. Strong correlation in their behavior at A≈130 could be recognized through the coupling interference of $2d_{3/2}$ and $3s_{1/2}$ quasiparticles to the 3- type phonons and with the
coupling of 2+ types phonons to the $3p_{3/2}$ and $2f_{7/2}$ quasiparticles. The transfer study reveals a series of states with 'anomalous' angular and asymmetry distributions. This could be accounted for by inelastic multi-step mechanisms. It was demonstrated that conclusions on single particle spectroscopic factors especially for the high-lying states depend crucially on the choice of proper coupled channels. Another source of uncertainties are the restricted knowledge of real form factors for the inelastic scattering interaction, the relative importance of different multipolarities in inelastic routes and to a small degree the DWBA optics that could lead to large deviations of measured distributions for individual states.

LOW-SPIN MIXED PARTICLE-HOLE STRUCTURES IN ^{185}W

V. Bondarenko[**], J. Honzátko[*], I. Tomandl[*], T. von Egidy[***], H.-F. Wirth[***], A.M. Sukhovoj[$$], L.I. Simonova[**], J. Bērziņš[**], P. Alexa[##], R. Hertenberger[++], G. Graw[++], Y.~Eisermann[++]

A comprehensive level scheme of ^{185}W has been established using one-nucleon transfer reactions supplemented by thermal neutron capture results. Polarized deuteron beams provided the spin-parity determination for almost all levels observed below 3 MeV. Also an essentially complete set of 1/2-, 3/2- states has been obtained in this energy region. A large number of observed levels can be interpreted in terms of rotational bands associated with Nilsson configurations. That reflects the validity of the axially symmetric deformation in this transitional nucleus. Low-spin levels below 1 MeV are assigned to rather pure quadrupole and octupole vibrations coupled to the quasiparticle states closest to the Fermi level. Other old and newly established states around 1 MeV offer an example of structures with mixed one-quasiparticle and vibrational components. The established band structures slightly above this region indicate a progressively greater degree of mixing. A number of angular and asymmetry

distributions can not be fitted with DWBA calculations because they would require additional multi steps to the simple one-step direct transfer mechanism. These 'anomalous' shapes mostly appear in transitions to moderately high rotational band members. This leads in some cases to worse agreement with simple Nilsson model predictions.
An obvious fact of significant fragmentation of one-quasiparticle strength and their quantitative evaluation is provided predominantly from the (d,t) and (d,p) DWBA analysis. It is in particular interesting, that both particle- and hole-type configurations are almost equally contributed into the observed band structures although some hints for the preference of this effect in the negative-parity system continue to be more obvious. This statement would be of importance for the theoretical interpretation since its presence might indicate that the extra exchange by vibrational phonons across the Fermi surface has an enormous effect of breakdown of the individual properties of Nilsson states. The observation of (d,p) hole states might indicate that inner shells are only partially occupied. This empirical feature can be partly understood as a clear experimental evidence of the importance of configurational $\Delta N=2$ mixing that embraces $N=5, 7$ together with $N=4, 6$ orbits. Finally, the significance of configurational mixing and compression of the spectra in a transitional nucleus such as ^{185}W are a straightforward indication of the loss of quadrupole deformation at the peak of the hexadecapole deformation.

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THEORETICAL INVESTIGATION OF FINITE NUCLEI WITHIN MICROSCOPIC THEORIES

A.V.Afanasjev

Self-consistency effects in superheavy nuclei were studied using the relativistic mean field theory. Our results show that these effects are important in the definition of shell structure and thus the localization of the island of enhanced stability. They also show that previous suggestions within the framework of phenomenological models, that $Z=114$, $N=184$ is the doubly magic superheavy nucleus, are highly questionable. The study of the effects of proton-neutron pairing in rotating $N \cong Z$ 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 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. A large overview article devoted to this topic has been submitted to Physical Review C.
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

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continued. They involve a number of important physical questions such as rotational properties of nuclei in actinide region ^{250}Fm and ^{253}No, 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/hyperdeformed bands around ^{108}Cd, the rotational properties of nuclei at the neutron-drip line (study within the framework of the CRMF theory), the importance of the role of nuclear magnetism 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.
Nuclear astrophysics studies were concentrated on the investigation of the pycnonuclear reactions in the crust of white dwarf and neutron stars. The article devoted to ^{12}C+^{12}C reaction has been submitted to Physical Review C. Investigation of the dependence of pycnonuclear fusion reactions on the properties of neutron-rich nuclei is in progress. In particular, we are interested to see how the rates are changed when reacting nuclei are very neutron rich and close to the neutron drip line.

On the invitation of the Editors of Physics Reports we wrote a review article discussing the theoretical developments of the relativistic Hartree+Bogoliubov theory and its applications to nuclei under extreme conditions.

A DIMENSION FORMULA FOR REDUCED PLETHYSMS

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

In nuclear theory, the physical models, based on symmetries described by group theory – Interacting Boson Models, Restricted Dynamics Models, etc., make intensive use of chains of subgroups of the general linear group GL(n). The nuclear states in these models are associated with the basis states of irreducible representations (IR) of corresponding groups. Thus, there is a need to find branching rules of IR's of group G into IR's of its subgroup H.

A powerful method for finding such branching rules is provided by plethysm techniques, basing on combining Schur functions. For small values of degrees of Schur functions, one can compute plethysms quite easily. Though, the evaluation of plethysms fast becomes impossible even for the most powerful computers in the case of medium and large values of these degrees, necessary in applications for medium and heavy nuclei.

However, since groups G and H as subgroups of GL(n), have finite ranks, there is no need to compute complete plethysms. It is enough to evaluate only the reduced plethysms – the part of plethysms, containing only Schur functions with up to a given number of rows.

In the case of complete plethysms, there is a well known dimension formula, allowing to control the correctness of resulting plethysms. However, there is no analogous formula in literature in the case of reduced plethysms. We have derived such dimension formula for reduced plethysms, basing on the Interacting Boson Model formalism and using step by step process [A1].

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QUARK-GLUON VERTEX FUNCTION IN DYSON-SCHWINGER AND BETHE-SALPETER EQUATIONS OF QUANTUM CHROMODYNAMICS

A.Dzalbs

The Dyson-Schwinger approach to QCD is developing rapidly during several past years, and recent detailed investigations of quark-gluon vertex and scattering kernel are already done in terms of form factors of corresponding Green's functions. In our work, we investigate the evolution of form factors of quark-gluon vertex function, employing the vertex equation which is deduced from the complete resummation of dressed gluon ladders. Our use of dressed gluon propagator, beyond gluon dressing by Dirac delta function, allows us to evaluate the impact of infrared finite part on already known three form factors (considering them as functions of two momenta, instead of simplifications done by other authors) of quark-gluon vertex as well as to put the well-grounded constraints on remaining nine form factors, the most of which belong to the transverse part of the vortex and, therefore, one can apply for them the Ward-Takahashi identities. Additionally, we test the theoretically feasible case of infrared vanishing gluon dressing or gluon dressing without infrared enhancement. The obtained quark-gluon vertex is used for the construction of a gap equation as well as for the building of a quark-antiquark scattering kernel for Bethe-Salpeter equation. The phenomenological implications – quark constituent masses and mass spectrum of quark-antiquark bound states – are drawn [B2,B3].

RADIOLOGICAL IMPACT ASSESSMENT OF THE SHUT-DOWN SALASPILS NUCLEAR REACTOR

D. Riekstina, J. Berzins, O. Veveris, J. Alksnis, V. Feldbergs

The aim of the present work was to gain an overview about the background level of radioactivity and gamma radiation in the 3x3 km area around the Salaspils (Latvia) nuclear reactor after its shutting down. The ultimate design of the project was to assess the impact environmental background level during its 37 years long working time. For this purpose we have carried out:

1) The determination of radioactivity in soils;
2) the determination of radioactivity in groundwater;
3) the measurement of gamma-ray background in the checkpoints.

The total number of checkpoints of soils was 113. The groundwater was taken from 34 places. The minimal detectable activity of the gamma-spectrometric analysis was from 0.3 up to 1 Bq/kg.

Cs-137 and natural radionuclides Th-232, U-238, K-40 were detected in soils. The concentration of Cs-137 varies in the range 0.3-227 Bq/kg or 20-1940 Bq/m^2. It was established that the concentration of Cs-137 in neighbouring checkpoints could differ significantly. It could be explained by the type of soil and the collection place (coniferous or leafy forest, grassland, plough land etc.). In all water samples the concentration of Cs-137 was lower than the minimal detectable activity. The determined radionuclide concentration in all samples is in agreement with the average level in Latvia.

In the control zone the average gamma background was 50 nSv/h ±15% and the maximum value-100 nSv/h. All results of detected gamma background show that they do not differ from the natural background, and correlations with a placement of the nuclear reactor were not observed.

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LEACHABILITY OF RADIONUCLIDES IN SYSTEM CEMENT COMPOUND-WATER

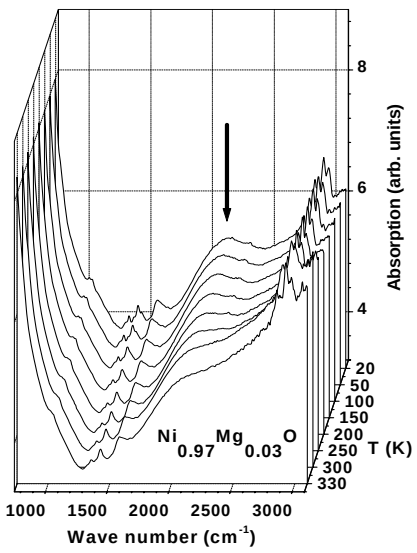
D. Riekstina, O. Veveris, G. Abramenkova

The developments of radioactive by-products in the nuclear reactors, caused by their work, form the so-called radioactive waste. Part of these wastes is in the water phase. In order to bury this type of radioactive waste in the specialized storages, it is necessary to transform them into solid form. One way to do this is cementing. The basic requirement is: the particular cement compound should guarantee the long-term capture of radionuclides and isolation of them from the environment even if it comes into contact with water. To compare the results we have chosen the leachability index of radionuclides as one of the features of cement compound. One experiment was carried out within 90 days. For qualitative and quantitative estimation of radionuclides, we have used the high-resolution gamma-spectrometer with Ge-Li detector and liquid scintillation spectrometry. In the present work the authors discuss influence of various factors to leaching of radionuclides from cement compound: temperature, water pH, homogeneity, water/cement relationship, various additives in cement, and others. The experimentally obtained results are demonstrated and discussed by authors.

INFLUENCE OF DIAMAGNETIC IMPURITIES ON MID-IR ABSORPTION IN ANTIFERROMAGNETIC INSULATOR NiO

N. Mironova-Ulmane, A. Kuzmin,
M. Cestelli Guidi*, M. Piccinini*,, A. Marcelli***

The magnetic properties of antiferromagnetic nickel oxide NiO can be strongly influenced by admixture of non-magnetic ions. For example, $Ni_cMg_{1-c}O$ solid solutions represent a nice example of diluted antiferromagnetic system, whose magnetic properties vary from antiferromagnetic-like behaviour for c=1 to diamagnetic-like behaviour for c=0.



In this work, we present the influence of diamagnetic magnesium impurities on the absorption band at ~2000 cm^{-1} in polycrystalline $Ni_cMg_{1-c}O$ ($c \geq 0.6$) solid solutions. We found that both intensity and position of the band show strong composition and temperature dependence, which can be attributed to the joint excitation of one optical phonon and two magnons at the Brillouin zone-boundary. The estimated two magnon energy ~1525 cm^{-1} for c=0.97 is in good agreement with our previous findings by the Raman spectroscopy.

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INFLUENCE OF RADIATION DEFECTS ON EXCITON-MAGNON INTERACTIONS IN NICKEL OXIDE

N.Mironova-Ulmane, V. Skvortsova, A. Kuzmin, I. Sildos*

Influence of radiation defects on the optical absorption spectrum of nickel oxide (NiO) was studied at the temperature 6 K in the near infra-red energy range 7750-8300 cm^{-1}, corresponding to the magnetic-dipole transition $^3A_{2g}(F) \rightarrow {}^3T_{2g}(F)$ at nickel sites. NiO single-crystals, grown by the method of chemical transport reactions on MgO(100) substrates, were irradiated by the neutron fluences up to $5x10^{18}$ cm^{-2}. Two sharp lines were observed at the low-energy side of the band: the peak at 7805 cm^{-1} is assigned to the pure exciton transition, whereas the peak at 7845 cm^{-1} to the exciton-magnon excitation, which occurs at the Brillouin zone-centre (BZC). An increase of the defects concentration at higher fluences results in a lowering of the magnon satellite peak intensity. The long-wavelength BZC magnon absorption is sensitive to the long-range magnetic ordering, which becomes destroyed in the presence of radiation defects. Therefore, the observed decrease of the peak intensity is attributed to a decrease of the spin-spin correlation length due to inhomogenious broadening.

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

MAGNETIC IONS EXCHANGE INTERACTIONS IN NIO-MGO SOLID SOLUTIONS

N.Mironova-Ulmane, V. Skvortsova, A. Kuzmin, U. Ulmanis, I. Sildos*, G.Mariotto, E.Cazzanelli*****

In this work we reviewed recent experimental data and their interpretation for $Ni_cMg_{1-c}O$ solid solutions with an emphasis on the exchange interactions between Ni^{2+} ions. We show that different experimental methods provide with complementary information and allow deeper understanding of $Ni_cMg_{1-c}O$ system. It was found that a dilution of nickel oxide with magnesium ions affects strongly atomic structure and optical, magnetic and vibrational properties. Opposite to conventional point of view, the local symmetry at Ni^{2+} ions sites lowers upon dilution due to magnetic interactions between neighbouring nickel ions. The magnetic interactions can be accessed through the study of optical and Raman spectroscopy, since both one-magnon and two-magnon excitations contribute strongly to optical and Raman spectra. We found that one-magnon energy dependence on composition shows unexpected trend which can be explained by strong decrease of the spin-spin correlation length upon dilution, however further studies are required to understand this behaviour.

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** In cooperation with INFM and Dipartimento di Fisica, Università di Trento, Povo (Trento), Italy
*** In cooperation with INFM and Dipartimento di Fisica, Università della Calabria, Arcavacata di Rende (Cosenza), Italy

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CRITICAL INDEXES FOR MAGNETIC PHASE TRANSITION IN Ni FINE PARTICLES

A.Petrov[1], I.Kudrenickis[1], M.Maiorov[2]
[1]Institute of Solid State Physics, University of Latvia
[2]Institute of Physics, University of Latvia

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 β and γ { $M_s \sim |-\varepsilon|^{\beta}$, $\chi \sim |-\varepsilon|^{-\gamma}$, 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 γ 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.

Scientific Publications

1. V. Bondarenko, J. Honzatko, I. Tomandl, T. von Egidy, H.-F. Wirth, A. M. Sukhovoj, L.Simonova, P. Alexa, J. Berzins, R. Hertenberg, Y. Eisermann, G. Graw, Low-spin mixed particle-hole structure in ^{185}W, submitted in Nucl. Phys. A.
2. H.-F. Wirt, R. Hertenberg, M. Balodis, J. Berzins, N. Kramere, J. Jolie, T. von Egidy, The nucleus ^{194}Ir studied with transfer and neutron capture reactions, submitted in Nucl. Phys. A.
3. J. Honzátko , V. Bondarenko , I. Tomandl, T. von Egidy, H.-F. Wirth, D. Bucurescu, V. Yu. Ponomarev, N. Marginean, R. Hertenberger, G. Graw, Y. Eisermann, L. Rubaček, Nuclear structure of ^{127}Te studied with (n,γ) and (d,p) reactions and interpreted with IBFM and QPM, Nucl. Phys. A in print.
4. N.S.Kelsall,… A.V.Afanasjev, S.Frauendorf, I.Ragnarsson et al.,High-spin structure of N ~ Z nuclei around the A= 72 region, Eur.Phys. Journ. A 60 (2004) 131-132.
5. A.V.Afanasjev and S.Frauendorf, Neutron-proton pairing in rotating N=Z nuclei: dominance of the isovector component, Nuclear Physics A 746 (2004) 575-578.
6. L.R.Gasques, A.V.Afanasjev,M.Beard, L.C.Chamon, P.Ring and M.Wiescher, Pycnonuclear reaction rate between neutron-rich nuclei, Nuclear Physics A, in press.
7. A.V.Afanasjev and S.Frauendorf,Description of rotating N=Z nuclei in terms of isovector pairing, submitted to Physics Review C,
8. J.E.Bastin, R.-D.Herzberg, N.Amzal, A.V.Afanasjev et al. In-Beam Gamma-ray and conversion-electron study of ^{250}Fm, submitted to Physical Review C.
9. A.V.Afanasjev and S.Frauendorf, Central depression in nuclear density and its consequences for the shell structure of superheavy nuclei, Physics Review C, in press.
10. P.Reiter,T.L.Khoo,I.Ahmad,A.V.Afanasjev, Structure of the Odd-A, Shell-stabilized Nucleus ^{253}No, submitted to Physical Review Letters.
11. L.R.Gasques, A.V.Afanasjev, M.Beard, M.Wiescher, P.Ring, L.C.Chamon, and E.F.Aguilera, ^{12}C+^{12}C reaction in stars, to be submitted to Physical Review C.

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12. A.J.Boston, C.J.Chiara, M.Devlin, D.B.Fossan, K.Starosta, A.V.Afanasjev and I.Ragnarsson, Collective dipole bands in ^{110,112}Te: stability against magnetic rotation, submitted to Journal of Physics G.
13. D.Vretenar, A.V.Afanasjev, G.A.Lalazissis, and P.Ring, Relativistic Hartree-Bogoliubov Theory: Static and Dynamic Aspects of Exotic Nuclear Structure, Physics Reports, p. 1-160, in press.
14. A.V.Afanasjev and S.Frauendorf, Self-consistency effects in superheavy nuclei, American Institute of Physics, Proceeding series, in press.
15. J.A.Castilho Alcaras, J.Tambergs, T.Krasta, J.Ruža, O.Katkevičius. A Dymension Formula for Reduced Plethysms. submitted to Journ. of Math. Phys. 2004 (7 pages).
16. A.Aleksejevs, S.Barkanova, T.Krasta, J.Tambergs. Study of Neutron Properties in Quark Potential Model Approach. submitted to Physica Scripta 2004 (34 pages).
17. I. Taure, D. Riekstina, O. Veveris: Neutron activation analysis. *(*Accepted for publication in Letters of Latvian University).
18. N. Mironova-Ulmane, A. Kuzmin, M. Cestelli Guidi, M. Piccinini and A. Marcelli, Influence of diamagnetic impurities on mid-IR absorption in antiferromagnetic insulator NiO, Phys. stat. sol. (c) (2005) (in press).
19. E. Cazzanelli, A. Kuzmin, G. Mariotto and N. Mironova-Ulmane, One-magnon Raman scattering in $Ni_cMg_{1-c}O$ solid solutions, Phys. stat. sol. (c) (2005) (in press).
20. N. Mironova-Ulmane, V. Skvortsova, A. Kuzmin and I. Sildos, Influence of radiation defects on exciton-magnon interactions in nickel oxide, Proc. SPIE (2005) (in press).
21. N. Mironova-Ulmane, V. Skvortsova, A. Kuzmin, U. Ulmanis, I. Sildos, E. Cazzanelli, G. Mariotto, Magnetic ions exchange interactions in NiO-MgO solid solutions, Fiz. Tver. Tela (2005) (in press).21. F.Muktepavela, I.Manika, V.Skvortsova. Adhesion and radiation stability of AlN and AlN/TiN thin coatings on metallic and non-metallic substrate. Engineering materials & Tribology * 2004. Materials of the XII International Baltic Conference, September 23-24, Riga Latvia, p.175-178.
22. J.Ruža. On the EPR paradox. In: Proceedings of International conference „Quantum Theory: Reconsideration of Foundations – 2" (Ed. A.Yu.Khrennikov), Växjö, Sweden, 2003 (Växjö University Press, 2004), p.479-485.
23. J.Tambergs. Problems of Dialogue between Quantum Mechanics and Theology. In: „Zvaigžņotā Debess (The Starry Sky)", Autumn 2004 (No.185), p.3-10 and Winter 2004/2005 (No.186), p.3-10 (in Latvian).

2 4. J.Tambergs. The Biblical and Scientifical World View on the Beginning of Universe and Mankind. In the book: „In the beginning God II. The sermons of contemporary Latvian Lutheran parsons on Old Testament." Compiled by Yu.Rubenis. (Publishing house „Zvaigzne ABC", Rīga), p.326-333 (in Latvian).

25. J.Tambergs. Participation in the discussion „Frontiers of science. Physics (Zinātnes robežas. Fizika)". „Terra", November-December, 2004, p.10-13.

J.Tambergs.

Lectures on Conferences

20th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Rīga, February 16-18, 2004

1. I.Tomandl, J. Honzatko, V. Bondarenko, J. Berzins, K-isomer studies in tungsten isotopes, p. 31.

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2. J.Berzins, D. Riekstina, O. Veveris, Environmental radiation monitoring of soil and ground water using gamma spectrometrical methods, p. 32.
3. M. Balodis, A change of nuclear deformation in the mass number region near 150 and 190.
4. A.Aleksejevs, S.Barkanova, T.Krasta, J.Tambergs. Study of Neutron Properties in Quark Potential Model. p.28
5. A.Dzalbs. Quark-Gluon Vertex Function of Dyson-Schwinger Equations in QCD. p.29.
6. V. Skvorcova. $Mn_cMg_{1-c}O$ Radiation defects thermal stabilitaty, p.60.
7. A.Petrov,I.Kudrenickis,M.Maiorov.Critical indexes for magnetic phase transition in Nifine particles.- Abstracts of the annual Conference of Solid State Institute, Riga, 2004, Latvia, p.87

XII Feofilov symposium on spectroscopy of crystals activated by rare earts and transition metal ions

1. N. Mironova - Ulmane, V. Skvortsova, A. Kuzmin,U. Ulmanis, I. Sildos. Magnetic ions exchange interaction in NiO-MgO. Ekaterenburg- Zarechnyi. Russia, September22-25, 2004, p.30.

ICDIM 2004, July 12-16, Riga,Latvia. p.86.

1.V. Skvortsova, N. Mironova-Ulmane, U. Ulmanis . Complex defects formation in $Mn_cMg_{1-c}O$ and $Ni_cMg_{1-c}O$ single solid solution.

2**.** N. Mironova-Ulmane, A. Kuzmin, M. Cestelli Guidi, M. Piccinini and A. Marcelli, Influence of diamagnetic impurities on mid-IR absorption in antiferromagnetic insulator NiO.

4th International Conference on Advanced Optical Materials and Devices (AOMD-4)

1. N. Mironova-Ulmane, V. Skvortsova, A. Kuzmin and I. Sildos, Influence of radiation defects on exciton-magnon interactions in nickel oxide, , 5-10 July, 2004, Tartu, Estonia p.16.

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.

International Nuclear Physics Conference INCP2004, Gőteborg, Sweden, June 27 – July 2, 2004. Book of Abstracts.

1. A.Dzalbs. Quark-gluon vertex function in Dyson-Schwinger and Bethe-Salpeter equations of Quantum Chromodynamics. p.269.

International Conference "EcoBalt 2004", Riga, May 6-7, 2004

1. D. Riekstina, O. Veveris, G. Abramenkova, Leachability of radionuclides in system cement compound-water, p.23.

International Symposium INSINUME 2004 "Radioprotection of the Environment Albena, Bulgaria 27-30 September, 2004

1. D. Riekstina, J. Berzins, O. Veveris, J.Alksnis, V. Felsbergs, Radiological impact assessment of the shut-down Salaspils nuclear reactor, p.49.

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Workshop: "Experiences in Combating Illicit Trafficking of Nuclear and Radioactive Materials" in Vilnius, Lithuania on 29 - 30 September 2004

1. J. Berzins, A. Skujina “Management of accidents in Latvia”

Lectures at Universities, Institutes …

Dr. hab. 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

Luther Academy of the Latvian Lutheran Church

3. Science and religion

Dr. J. Ruza

Riga Technical University: General physics.

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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, photonics 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, optically induced switching effect and second harmonic generation 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. Prof.. L.Brehmer, Potsdam University, Potsdam, Germany (1 week)
2. Prof.J.M.Nunzi, Angers University, Angers, France (1 week)
3. Dr.habil. M.Bouvet, P.M.Curie University, Paris, France (1 week)
4. Ph.D.student W.Chen, Angers University, Angers, France (2 weeks)

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. 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)

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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

DETECTION OF BLUE LIGHT BY SELF-ASSEMBLED MONOLAYER OF DIPOLAR MOLECULES

O.Neilands, N.Kirichenko, I.Muzikante, E.Fonavs, L.Gerca, S.Jursenas, R.Valiokas, R.Karpicz, L.Valkunas

Dipolar donor-acceptor molecules show pronounced changes in the dipole moment upon photoexcitation, resulting in transformation of their optical and electrical properties. A monolayer of 4'-(3H-1,2,5-dithiazepan-5-yl)benzylidene indan-1,3-dione (DMABI-2S), possessing high electric dipole moment is self-assembled (SAM) on Au layer. Analysis of the IR vibrational and fluorescence spectra of SAMs supports the conclusion about the specific tight packing of the molecules in the SAM structure. The changes of the surface potential on irradiation with blue-light is measured by Kelvin probe technique. The reversible changes of surface potential of the order several tenths of milivolts is induced by irradiation of the sample. The relationship between absorption spectra and spectral dependence of the surface potential is observed. Such SAM structures can be applied for design of molecular sensors and 2D recognition devices.
In cooperation with Institute of Physical Energetics, LAS (Latvia), Riga Technical University (Latvia), IMSAR, Vilnius University (Lithuania), Institute of Technology, Linköpings University (Sweden), Institute of Physics (Lithuania) and Faculty of Physics, Vilnius University, (Lithuania).

STUDIES OF HOST-GUEST THIN FILMS OF CORONA POLED BETAINE TYPE POLAR MOLECULES BY KELVIN PROBE TECHNIQUE AND ATOMIC FORCE MICROSCOPY

R.Dobulans, D.Cepite, E.Fonavs, I.Muzikante, A.Tokmakov, D.Erts, B.Polakov

Corona poled host-guest films with PMMA as host and N-(indan-1,3-dion-2-yl)pyridinium betaine as guests show a considerable increase of the surface potential. The increase of surface roughness and formation of grains of the corona poled films are shown.

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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) and Institute of Chemical Physics, University of Latvia.

ALL-OPTICAL POLING OF DMABI MOLECULES IN A POLYMER MATRIX

A.Vembris, A.Apostoluk, M.Rutkis, A.Tokmakov, I.Muzikante, S.Dabos-Seignon, J.-M.Nunzi

Many organic compounds have nonlinear optical properties due to the orientation of the molecules in a polymer matrix. In this work, all-optical poling and second harmonic generation in a composition consisting of 1 mass% of 2-4′-dimethylamino-benzylidene-1,3-indandione (DMABI) compound in poly(methyl methacrylate) (PMMA) matrix were studied. Thin films were prepared by solvent casting. The 1.064-μm fundamental and 532-nm second harmonic wavelengths of a Nd:YAG laser were used. It is shown that DMABI molecules can be oriented by the method of all-optical poling, and that the process is related to the photoinduced switching between two equally stable states of the molecule.
A DMABI molecule can be oriented in the syndioatactic PMMA polymer by the method of all-optical poling. It is shown that the process is not related to the trans–cis isomerization but presumably with the photoinduced switching between two equally stable states of the molecule. The confirmation has been received from a smaller second order nonlinear susceptibility and a larger orientation relaxation time as compared with the DR1–MMA system. DMABI can be considered as a new-type non-azo molecule exhibiting all-optical poling via photoinduced orientation.

In cooperation with Institute of Physical Energetics, LAS (Latvia) and Laboratoire des Propriétés Optiques des Matériaux et Applications, Université d'Angers (France)

PHOTOINDUCED PHENOMENA IN ORGANISED POLAR ORGANIC FILMS

I.Muzikante, E.Fonavs, B.Stiller, L.Brehmer

Organic materials have received considerable attention because of their large dipole moments and optical nonlinearities. The switching is important for optoelectronic effects including second harmonic generation. Organic materials for photonic applications contain chromophore dipoles consisting of acceptor and donor groups bridged by a delocalized π-electron system. Both calculations and experimental data show a reversible highly dipolar photoinduced intramolecular charge transfer in betaine type molecules accompanied by change of the sign and the value of the dipole moment.
Arrangement of polar molecules in films is studied both by atom force microscopy and surface potential measurements. To understand photoresponse of these materials, their

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spectroscopic and electrical properties are studied. The morphology and photoinduced surface potential switching of the self-assembled monolayers and polymer films are investigated.
Corona poled host-guest films with PMMA as host and N-(indan-1,3-dion-2-yl)pyridinium betaine, N-(5-nitroindan-1,3-dion-2-yl)pyridinium betaine and N-[4'-(5-t-Bu-indan-1,3-dion-2-yl)phenyl]-pyridinium betaine as guests and corona poled polymer films with chemically attached N-(indan-1,3-dion-2-yl)pyridinium betaine were investigated.
Reversible switching of the surface potential of polymer films with incorporated or chemically attached betaine molecules are observed at irradiation in the 360-400nm spectral region, where intramolecular charge transfer in betaine molecule takes place. The experimentally observed changes of the surface potential on irradiation is considerably higher in corona poled regions of the films. The experimentally obtained response to irradiation lasts several minutes. The best response of the surface potential is observed polymer film with chemically attached betaine group.
Photoinduced change of the surface potential of poled polymer films observed in UV and visible spectral region has the maximum close to the PIET absorption band of IPB molecules giving rise to a change of dipole moment of the IPB group and depends on orientation of the latter. Due to photogeneration of charge carriers the maximums of surface potential of poled and un-poled IPB oligomer films may arise at longer wavelengths at 450nm.

In cooperation Riga Technical University (Latvia), Institute of Physical Energetics, LAS (Latvia) and Potsdam University, Potsdam (Germany).

OPTICAL AND ELECTRICAL PROPERTIES OF ORIENTED THIN FILMS OF OLIGOMER CONTAINING BETAINE TYPE MOIETY IN SIDE CHAIN

I.Muzikante, E.Fonavs, A.Tokmakov, D.Cepite, B.Stiller, L.Brehmer, O.Neilands

Non-linear optical and electrical properties of polymer films obtained by dipole orientation of active units are reported. Novel polar oligomer with N-(indan-1,3-dion-2-yl)pyridinium betaine (IPB) as side group is studied. Orientation of polar groups in oligomer thin films causes an increase of the photo-induced change of surface potential at irradiation in the region of photo-induced electron transfer (PIET) where the IPB group exhibits a reversible change of the value and sign of dipole moment. At longer wavelengths the value of the surface potential of oligomer may be determined by transport of photo-generated charge carriers.
Photo-induced change of the surface potential of poled IPB oligomer thin films observed in UV and visible spectral region has the maximum close to the PIET absorption band giving rise to a change of dipole moment of the IPB group and depends on orientation of the latter.

Due to photo-generation of charge carriers the maximums of surface potential of poled and un-poled IPB oligomer films may arise at longer wavelengths at 450nm. In the case of poled IPB oligomer films additional increase of the surface potential is observed at above 500nm is observed.

In cooperation Riga Technical University(Latvia), Institute of Physical Energetics, LAS (Latvia) and Potsdam University, Potsdam (Germany).

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THIN FILMS OF PHTHALOCYANINE DERIVATIVES FOR OZONE AND AMMONIA SENSING

M.Bouvet, I.Muzikante, E.Fonavs, A.Tokmakov, R.Dobulans

Vacuum-evaporated thin films of phthalocyanine derivatives were studied for their gas sensing properties. The electrical properties of phthalocyanines can be influenced by adsorption of oxidizing or reducing gases. Applicability for gas sensors is determined, mainly, by response, stability and reproducibility of physical properties of materials when exposed to gases. Most of the studies concerning phthalocyanine-based gas sensors are devoted to the detection of NO_2. Our interest concerns ozone (O_3), which is a fairly good oxidizing agent present in the atmosphere, and ammonia (NH_3), which is a reducing species. The conductivity measurements of thin films of nickel phthalocyanine (NiPc) and fluorinated phthalocyanine (F_8PcCu) were carried out. The effects of gases were also studied by changes of surface potential measured by the Kelvin probe technique. Surface potential (ΔVS) increases under ozone for NiPc but decreases in the case of F_8PcCu. This response is correlated to the nature of majority charge carriers, of p-type in NiPc and of n-type in F_8PcCu. For the latter, conductivity decreases under O_3 and increases under NH_3.

In cooperation with Institute of Physical Energetics, LAS (Latvia) and Université Pierre et Marie Curie, Paris (France).

Scientific publications

Published in 2004

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*, 2004, Vol. 212, pp. 421-426.
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,* Vol.144, Eds. M.Shur, A.Zukauskas, Kluwer Academic Publishers, pp.261-269, 2004.

Accepted for publication 2004

1. I.Muzikante, E.Fonavs, L.Gerca, B.Stiller, L.Brehmer, E.Markava, D.Gustina, Optically induced switching of dicyclohexylamino substituted azobenzene derivatives in thin ordered films, *SPIE Procedings*, 2004
2. A.Vembris, A.Apostoluk, M.Rutkis, A.Tokmakov, I.Muzikante, S.Dabos-Seignon, J-M.Nunzi, All optical poling study the DMABI molecule in a polymer matrix, *SPIE Proceedings*, 2004
3. I.Muzikante, E.Fonavs, B.Stiller, L.Brehmer, Photoinduced phenomena in organised polar organic films, *Advances in Colloid and Interface Science*, 2004

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4. I.Muzikante, E.Fonavs, A.Tokmakov, D.Cepite, B.Stiller, L.Brehmer, O.Neilands, Optical and electrical properties of oriented thin films of oligomer containing betaine type moiety in side chain, *Physica status solidi* (b), 2004

Lectures on Conferences

Latvijas universitātes Cietvielu fizikas institūta 19.zinātniskā konference, Rīga, Latvija, 2004.gada 16.-18.februāris

20th Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, Latvia February 16-18, 2004

1. D.Cepīte, A.Klimkāns, I.Muzikante, B.Stiller, L.Brehmer, *DMABI ditiola atvasinājuma monoslāņU uz Au(111) virsmas izpēte un modelēšana, Monolayers of dithiol derivative of dmabi on au(111): characterization and simulation,* Abstracts, p.70.
2. R.Dobulans, E.Fonavs, I.Muzikante, A.Tokmakovs, Bouvet, *Niķeļa un fluorētā vara ftalocianīna plāno kārtiņu elektriskās īpašības ozona un amonjaka vidē, Investigation of electrical properties of metal phthalocyanines in the presence of ozone and amonia*, Abstracts, p.75.
3. A.Vembris, A.Tokmakovs, I.Muzikante, A.Apostoluk, J.M.Nunzi*, DMABI molekulu vispārējā optiskā orientēšana un nelineāro optisko īpašību pētījumi polimēra matricā, All optical poling and studies of nonlinear optical properties of DMABI molecules in polymer matrix*, Abstracts, p.72.
4. A.Tokmakovs, A.Vembris, L.Gerca, I.Muzikante, E.Laizāne, E.Markava, D.Gustiņa, *Fotoizomerizācijas procesi azobenzola atvasinājumi plānās kārtiņās, Photoisomerization process in thinfilms of aazobenzene derivatives,* Abstracts, p.74.

School on Polymers and Composites for Microelectronics and Robotics, Wierzba/Wejsuny, Great Mazurian Lakes, Poland, May 10 – 13, 2004

1. A.Tokmakovs, A.Vembris, L.Gerca, E.Laizāne, I.Muzikante, E.Markava, D.Gustiņa, *Photoisomerization process in thin films of azobenzene derivatives*, Abstracts, pp.80.
2. A.Vembris, M.Rutkis, A.Tokmakov, I.Muzikante, A.Apostoluk, J.M.Nunzi, *All optical poling and studies of nonlinear optical properties of DMABI molecules in polymer matrix*, Abstracts, p.79

4th International Conference on Advanced Optical Materials and Devices AOMD-4, Tartu, Estonia, July 6-9, 2004

1. I.Muzikante, E.Fonavs, L.Gerca, S.Jursenas, R.Valiokas, R.Karpicz, L.Valkunas, *Optical and photoelectrical properties of self-assembled monolayers of dipolar molecules*, Abstracts, p.50.
2. D.Cepite, A.Klimkāns, I.Muzikante, B.Stiller, L.Brehmer, *Monolayers of dithiol derivative of DMABI on Au(111): characterization and simulation*, Abstracts, p.49.
3. I.Muzikante, E.Fonavs, L.Gerca, B.Stiller, L.Brehmer, E.Markava, D.Gustina, *Optically induced switching of dicyclohexylamino substituted azobenzene derivatives in thin ordered films*, Abstracts, p.30.
4. A.Vembris, M.Rutkis, A.Tokmakov, I.Muzikante, A.Apostoluk, J-M. Nunzi, *All optical poling and studies of nonlinear optical properties of DMABI molecules in polymer matrix*, Abstracts, p.51.

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5. A.Tokmakov, L.Gerca, A.Vembris, E.Fonavs, I.Muzikante, B.Stiller, L.Brehmer, E.Markava, D.Gustina, *Influence of UV-VIS light on physical properties of thin films of azobenzene derivatives*, Abstracts, p.51.

European Conference on Organised Films ECOF-2004, Valladolid, Spain, July 22-25, 2004

1. I.Muzikante, E.Fonavs, A.Tokmakovs, L.Gerca, A.Vembris, B.Stiller, L.Brehmer, E.Markava, D.Gustina, Photoinduced switching effects in monolayers of photoisomerizable chromophores, Book of Abstracts, pp. 104.
2. I.Muzikante, E.Fonavs, A.Tokmakovs, D.Cepite, A.Vembris, B.Stiller, L.Brehmer, A.Apostoluk, J.-M.Nunzi, O.Neilands, Optical and electrical properties of oriented thin films of oligomer containing betaine type moiety in side chain, , Book of Abstracts, pp. 120.

Linear and Nonlinear Optics of Organic Materials IV, Part of SPIE's International Symposium on Optical Science and Technology, SPIE's 49th Annual Meeting, Colorado Conention Center, Denver, USA, August 2-3, 2004

W.Chan, A.Apolostuk, S.Dabos-Seignon, J.-M.Nunzi, A.Vembris, I.Muzikante, E.Fonavs, A.Quatela, M.Casalboni, *Stability and polarity studies of all optically poled polymers*, Abstracts.

3rd International Conference on Prophyrins and Phthalocyanines, Louisiana, USA, July 11-16, 2004

M.Bouvet, I.Muzikante, E.Fonavs, A.Tokmakov, R.Dobulans, *Thin films of phthalocyanine derivatives for ozone and ammonia sensing*, J.Porhyrins and Phtalocyanines, Vol.8, No.4-6, 2004, pp.616

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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.

Scientifical Staff

1. Dr. A.Kristins
2. Dr. Hab. A.Zelenkovs

Technical Staff

1. I.Guza
2. D.Gusevs
3. I.Gvardina
4. J.Melderis
5. J.Tibergs
6. J.Veinbergs
7. S.Zelenkovs
8. A.Grablevskis

Cooperation

Latvia

1. Joint-stock company *Latvenergo*
2. *Kokarde* Ltd
3. Latvia Technology Park

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4. Riga Technical University
5. *Trafik* Ltd
6. IB *Biakss*
7. *GROG* Ltd
8. *DataPro* Ltd
9. *Apollo AS* Ltd

12.*AlarmLat* Ltd
13.*Mikoniks* Ltd
14.*Energoremonts*
Rīga Ltd

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
13. SIA "Nienhaus & Lotz Lettland" etc.

Lectures on Conferences

20th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2004

1. D.Gusevs, I.Gvardina, A.Kristiņš, S.Zelenkovs, *The using of „Rabbit" microcontroller for remote objects control purposes* Abstracts, p.105.
2. P.Annus, A.Kristiņš, *Remote and secure updating of the firmware in microcontrollers.* Abstracts, p.108.
3. D.Gusevs, V.Narnicka, E.Petersons, *Web point optimization using amount of work evaluation.* Abstracts, p.109.

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

Staff
1. Dr. J.Kļaviņš
2. Dr.hab. J.Maniks
3. Dr. E.Pentjušs
4. J.Pinnis

Support Staff
1. Dr. V.Eglītis
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

Scientific publications

1. G.Vaivars, N.W.Maxakato, T.Mokrani, L.Petrik, J.Klavins, G.Gericke and V.Linkov, Zirconium Phosphate Based Inorganic Direct Methanol Fuel Cell, Materials Science (Kauņa, Lietuva), 2004, Vol. 10, No. 2, pp. 162 - 165.

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ORGANIZED CONFERENCES

20th Scientific Conference of the Institute of Solid State Physics, University of Latvia

Riga, February 16 – 18, 2004

The anual Scientific Conferences of the ISSP are held at the Institute of Solid State Physics in February the 16 – 18 and is a part of Scientific Conference of University of Latvia (UL).

The 20th Conference worked in 6 sections:
- non – linear optical properties and problems of optometry (15 reports),
- nuclear reactions and "EURATOM"projects (9 reports),
- structure and phase transitions (14 reports),
- nanomaterials and organic materials (14 reports).
- optical spectroscopy and luminescence (17 reports),
- materials and applications (17 reports),

Alltogether 95 reports of 15 – 30 minutes were presented. Apart from staff members of ISSP and the Department of Optometry, representatives 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

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The International Conference on Defects in Insulating Materials (ICDIM-2004)

Riga, July 11-16, 2004

The International Conference on Defects in Insulating Materials (ICDIM-2004) was held at the University of Latvia, Riga, Latvia from July 11-16, 2004. It was the 15th conference in a long series that began in 1956 in the Argonne National Laboratory, USA, as an International Conference on Color Centers in Alkali Halides. The following conferences with the expanding range of subjects and phenomena were held in Corvallis (1959), Stuttgart (1962), Urbana (1965), Rome (1968), Sendai (1971), Reading (1974), Gatlinburg (1977), Riga (1981), Salt Lake City (1984), Parma (1988). The title of the conference was finally changed to the present one in 1992, when it was held in Nordkirchen, Germany. ICDIM-2004 followed the most recent meetings held in Wake Forest University, USA (1996) and Johannesburg-Midrand, South Africa (2000).

The topics of ICDIM-2004 reflected the basic trends in the development of physics of condensed matter with the expanding involvement of various inorganic materials, from the systems with the widest gaps (metal fluorides, solid helium) to relatively narrow-gap materials, which are widely discussed at the conferences on semiconductors. Particularly large number of contributions were devoted to metal oxides (ABO3 perovskites, silica etc.) which are complex with respect to crystal structure and electronic structure. Following a common practice for ICDIM conferences, highly sensitive and informative optical methods for a wide spectral region (incl. VUV and XUV regions) were of special popularity. The use of novel nanoscopic instruments allowed to obtain structural data of thin films, real surfaces or interfaces and their defects at atomic level. Similar to previous conferences, theoretical studies were widely favoured. Many contributions were devoted to promising materials as fast and efficient scintillation detectors, highly sensitive detectors of various kinds of radiation, spectral transformers, elements for nanoelectronics, storage and memory devices, radiation-resistant dielectric materials for nuclear energetics.

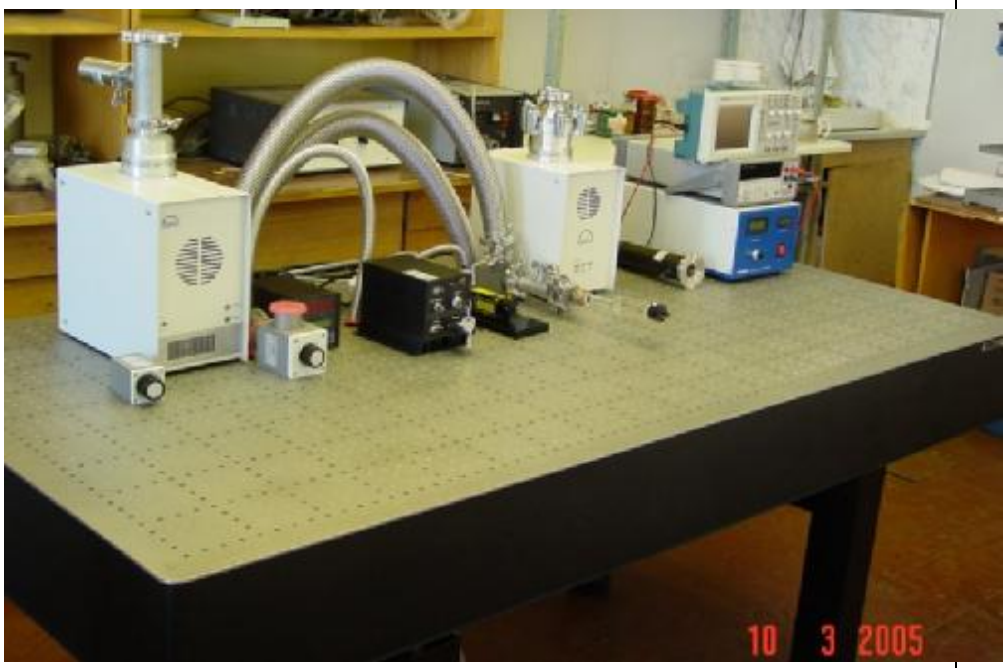
The ICDIM-2004 was jointly organized by the Institute of Solid State Physics, University of Latvia, chair Prof I. Tale, and the Institute of Physics, University of Tartu, Estonia, chair Prof. A. Lushchik. It was attended by 246 delegates of 30 countries. A large number of participants came from Germany, Italy, Russia, Ukraine, Latvia and Estonia, followed by a rather large number of delegates from USA, Japan, United Kingdom, Czech and France. The scientific programme included 7 plenary talks, 22 keynote talks, 62 oral and about 210 poster presentations, with 177 papers published in the refereed proceedings in journal "Physica Status Solidi (a) 177-260, (c) 15-724 (2005) Compared to the preceding conference, more young scientists participated, 33 of them were supported by the European Community under the Marie Curie Action Large Conferences Project. For the first time in the ICDIM series the scientific programme was preceded by a tutorial day for the young scientists.

Conference chairman
Prof. I.Tale

Appendix 1

New scientific equipment, purchased by EU Structural funds

Instrument title:	**Optical microscope ECLIPSE L150** **equipped with Color Matrix CCD and PC**
Photo:	
Technical details:	§ **Magnification up to 1000x** Reflected light objectives 10x, 20x, 50x, 100x § **Nikon Digital Camera DS-L1 for obtaining the photomicrographic images** 5 megapixels, Image size 2560x1920 pixels § **External PC, networking** § **Software for image processing, length measurements and indentation hardness tests** § **Simplified polarization microscopy**
Application example:	§ **Digital photo-images for structural studies;** § **Processing and analysis of images** § **High accuracy measurements of the linear dimensions, area, angle, circle radii, surface profile**
Responsible: (name, second name, e-mail, phone, room number)	**Dr. Ilze Manika** E-mail:**manik@latnet.lv** Phone +371 7261132 Room number **319**

Instrument title:	**Facility for Vacuum Ultraviolet Region and Laser Spectroscopy**
Photo:	
Technical details:	§ **VUV monochromator, model 234/302 (McPherson)** 1200 g/mm aberration corrected concave grating for 30 -500 nm range; Focal lengh 200mm; Resolution 0.1 nm; Accuracy 0.1 nm; reproducibility 0.05 nm. § **Light source: MgF_2 windowed deuterium lamp** Spectral range 120 – 400 nm § **Diode pumped solid state laser FQSS 266 Q (CryLas)** Pulse with 2 ns; Wavelength 266 nm, 532nm, switchable. § **Time-correlated photon counting (Multiscaler P7888 from Fast ComTec, Photon counting head H8259 from Hamamatsu)** Time resolution 2 ns; Spectral region 190-680 nm, max. counting rate (at 10% deviation from linear output) $2X10^6$ s^{-1}**.**
Application example:	§ **Optical properties of wide band gap materials. Optical absorption, reflection and luminescence excitation spectra in vacuum ultraviolet (VUV) spectral range.** § **Luminescence decay kinetics (excitation by laser pulses).**
Responsible: **(name, second name, e-mail, phone, room number)**	**1.Dr. Linards Skuja, (VUV spectroscopy)** E-mail: skuja@latnet.lv; Phone +371 7260756; Room number 327. **2. Dr.Larisa Grigorjeva, (time-resolved spectroscopy)** E-mail: lgrig@latnet.lv; Phone +371 7261880; Room number 432.

Instrument title:	**The Pulse Laser System for Spectroscopy of Material Ablation**
Photo:	
Technical details:	**NL300** series electro-optically **Q-switched nanosecond Nd:YAG** lasers provide up to **800 mJ** per pulse with excellent stability. These nanosecond lasers can be operated from a standard outlet and with **water-air** heat exchanger eliminating the need for external cooling water. The **NL300** series Q-switched nanosecond lasers are an excellent choice for many applications, including laser **ablation** and **OPO pumping.** The optional second (SH) (for **532 nm**), third (TH) (for **355 nm**) and fourth (FH) (for **266 nm**) harmonic generator modules are designed for easy attachment and removal. For customer convenience the q-switched laser is controlled through its RS232 type **PC interface** with **LabView** drivers (included) or a user-friendly **remote control** pad. Both options enable easy control of laser settings. Pulse duration (FWHM) 0.15 - 5ns. Pulse energy, mJ:

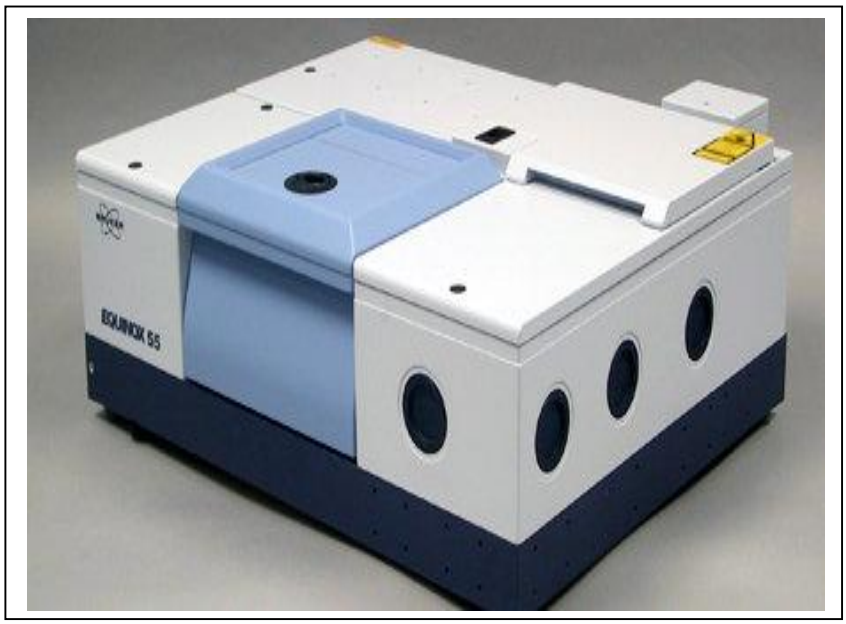
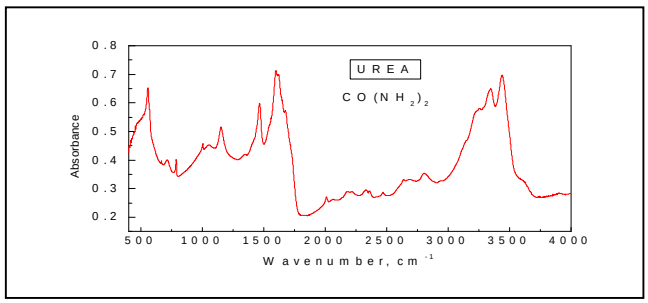
Model	NL303HT 10/20 Hz versions.
at 1064 nm	800/700
at 532 nm	360/310
at 355 nm	240/210
at 266 nm	80/60

OPO characteristics

OPO for tunable excitation	
Pump beam wavelength, nm	355
Tuning range VIS, nm	420 - 709
Tuning range IR, nm	710 - 2300
Tuning range UV, nm	210 - 355
Max. efficiency, %	20- 30 % depending tuning range
Spectral bandwidth, cm^{-1}	<5
Tuning control	external keypad/ internal PC

Details look at : www.ekspla.com

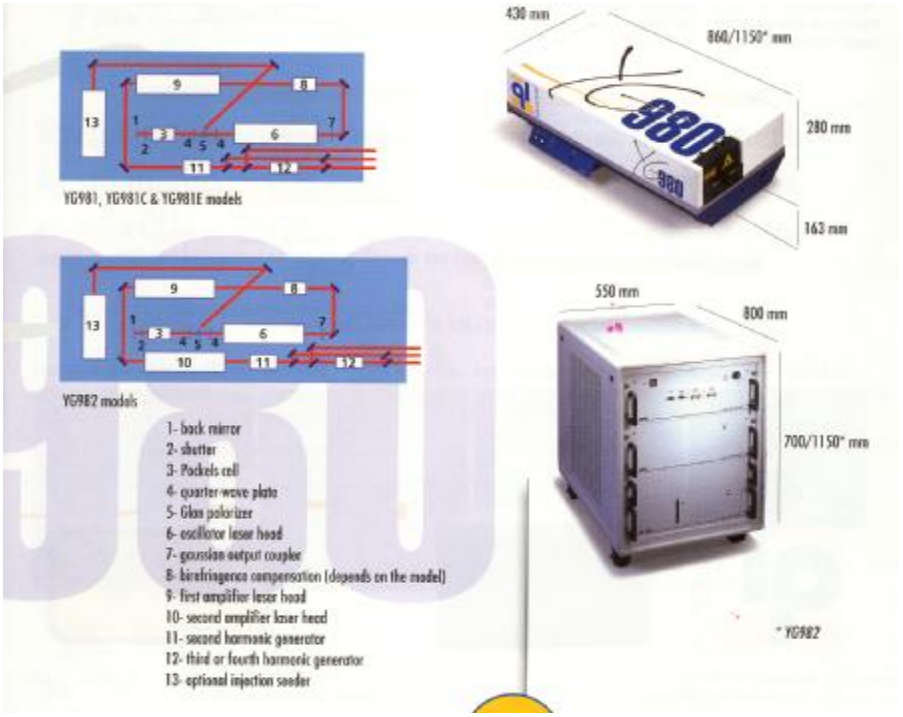
Application example:	The **NL300** series lasers are excellent for laser ablation and OPO pumping. OPO for tunable excitation of photoluminescence and time resolved spectroscopy.
Responsible: **(name, second name, e-mail, phone, room number)**	**Prof. Ivars Tale**, E-mail: iatale@latnet.lv, phone +371 7260639, Room number 331

Instrument title:	**FT - IR spectrometer Bruker Equinox 55**
Photo:	
Technical details:	**Frequency range: 370-25000 cm^{-1}** **Resolution : better than 0.5 cm^{-1}** **Variable temperature cell: 80K – 400K** **Samples: solid, liquids, powders, gas phase** **OPUS/IR software**
Application example:	**§** 
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr. Larisa Grigorjeva** E-mail:**lgrig@latnet.lv** Phone: +371 7260880 Room number **432**

Instrument title:	**Compact diode pumped solid state YAG:Nd laser EKSPLA NL640 / SH**
Photo:	
Technical details:	§ **Laser type** Electrooptically Q switched diode pumped all solid state (DPSS) laser with second harmonic (SH) option § **Wavelenth** fundamental - 1064 nm and second harmonic 532 nm § **Pulse parameters** pulse width 6 ns, repetition rate 0.2-40 kHz § **Average power** Max 6W @ 1064 nm, 40kHz rep. rate, (single beam) Max 3W @ 532 nm , (single beam) 1W @1064 nm & 0.5W @ 532 nm (dual beam) § **Control** manual keypad or remote PC via USB or RS232 § **Operating voltage and cooling** 220V AC, power <200W, air cooled
Application example:	§ **Nonlinear optics** optical second harmonic generation for material analysis § **Micromachining** scribing of thin films and ceramics
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr. Vismants Zauls** **E-mail: vism@latnet.lv** **Phone: 371-7260803** Room number **438**

Instrument title:	**HELIUM-CADMIUM LASER Model IK5751I-G**
Photo:	
Technical details:	§ **Wavelength (nm):** 325.0/441.6 § **Initial power (mW):** 30/110 § **Transverse mode:** TEM_{00} § **Polarization:** Linear § **Polarization ratio:** 500:1
Application example:	§ **Holography** § **Lithography**
Responsible: (name, second name, e-mail, phone, room number)	**Dr. Janis Teteris** E-mail:**teteris@latnet.lv** Phone +371 9414553 Room number **309**

Instrument title:	**Coherent Solid-State Green Laser Verdi-6**
Photo:	
Technical details:	§ **Wavelength (nm):** 532 § **Output power (W):** 6 § **Transverse mode:** TEM_{00} § **Polarization:** Linear § **Polarization ratio:** >100:1 § **Linewidth:** < 5 MHz
Application example:	§ **Holography** § **Lithography**
Responsible: (name, second name, e-mail, phone, room number)	**Dr. Janis Teteris** E-mail:**teteris@latnet.lv** Phone: +371 9414553 Room number **309**

Instrument title:	**Q-Switched Nd:YAG laser YG981E**
Photo:	
Technical details:	§ **Wavelength (nm):** 266; 355; 532; 1064 § **Pulse energy (mJ):** 150; 490; 820; 1600 § **Repetition rate (Hz):** 10 § **Pulse Duration (ns):** 8-11 § **Polarization ratio:** >90
Application example:	§ **Holography** § **Lithography**
Responsible: (name, second name, e-mail, phone, room number)	**Dr. Janis Teteris** E-mail:**teteris@latnet.lv** Phone: +371 9414553 Room number **309**

Instrument title:	**CCD Detector for Raman Measurements**
Photo:	
Technical details:	§ **CCD Format:** 1024x256 § **Pixel Size:** 26µmx26µm § **Image Area:** 26,6mmx6,7mm § **Readout Noise (20kHz):** 3,5e⁻rms § **Dark Signal (LNT):** 0,3e⁻rms/pixel/hr
Application example:	§ **Raman measurements** § **Luminiscence**
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr. Jevgenijs Gabrusenoks** E-mail:**gabrusen@latnet.lv** Phone: +317 6405993 Room number **220**

Instrument title:	**“HR4000 UV-NIR” High resolution Spectrometer with “DT-Mini-GS” light source**
Photo:	
Technical details:	Dimensions: 148.6 mm x 104.8 mm x 45.1 mm Weight: 570 grams Detector: 3648-element linear silicon CCD array Wavelength Range: 200-1100 nm Grating: HC-1, 300 lines per mm grating Entrance aperture: 5 µm wide slit Order sorting filters: Installed OFLV-200-1100 Focal length: f/4, 101 mm Dynamic range: 2×10^8 (system); 2000:1 for a single scan Optical resolution: 0.7 nm (FWHM) Stray light: <0.05% at 600 nm; <0.10% at 435 nm Light source type combined deuterium tungsten halogen Light source range 200 –1100 nm
Application example:	Absorbance, reflectance, fluorescence spectroscopy and thin film thickness measurements
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr. Mārtiņš Rutkis** E-mail: martinsr@edi.lv Phone: +371 7260787 Room number 225

Instrument title:	**“Metricon 2010” Prizm coupler for thin film optical wave guiding technique**
Photo:	
Technical details:	Thickness range 0,5 – 150,0 µm Thickness accuracy ±(0.5% + 50 Å) Thickness resolution ±0.3% Refractive index range 1,4 – 2,45 Index accuracy ±0.001 Index resolution ±0.0005 Operating wavelength He-Ne laser (632.8 nm) Optional operating wavelength He-Ne laser (1523 nm) Operational modes TE and TM
Application example:	Thin film thickness, refractive index and birefringence measurement system
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr. Mārtiņš Rutkis** E-mail: martinsr@edi.lv Phone: +371 7260787 Room number 225

Instrument title: **Ierīces nosaukums:**	**"Scanning Electron Microscope (SEM) with energy dispersive detector for X-rays (EDX) and with an option of Electron Beam Lithography (EBL).**
Photo: **Foto:** **SEM**	
Technical details: **Tehniskā specifikācija:**	The **Scanning Electron Microscope** is of **Carl Zeiss** brand, model **EVO 50 XVP** with LaB6 filament. Main characteristics: • Possibility to inspect samples in both: Low and High vacuum modes (possibility to inspect insulating and gassing samples), with easy vacuum mode changeover, LV mode pressure range 1-750 Pa and HV mode pressure better than 10^{-4} Pa; and with LaB6 better than 10^{-7} Pa • Resolution of 3 nm (in LV mode 4.5 nm) for W filament, and 2 nm for LaB6 filament, compatibility to both filament types • Magnification from 5x – 1.000.000x • Acceleration voltage range from 0.2 kV to 30 kV, easy adjustable, continues variable in 10V steps • Beam current in range from 0.5 pA to 5 μA, easy adjustable, and with good stability in time (give possibility for long EBL exposures without substantial change in beam current) • Image modes: secondary electron image (SE), backscattered electron image (4QBSE), topography (TOPO), composition (COMPO), shadowed • Additional detectors: infrared camera, probe current and specimen current detector (SCM) • Specimen stage: motorized in 5 axis (X – 100 mm, Y – 125 mm, Z – 61 mm (35 motorized), tilt 90^{o} rotation 360^{o} continuous compucentric), computer controlled, positioning precision of 1.5-2 micrometer and good stability (gives possibility for long EBL

	exposures without substantial change in the sample position) • Easy and fast sample load/unload system, (quick-fit holder) with sample size up to 250 mm in diameter at analytical working distance • Modular, upgradable The **EDX** is of **Oxford instruments** brand, model **INCA 350**. Main characteristics: • 10mm2 area, INCA SATW Window (for detection of elements from Be upwards.). • Detector resolution **guaranteed** at 2,500cps provides reliable and accurate results over entire spectral range at typical microscope operating conditions: At C: 66eV or better At F: 70eV or better At Mn: 133eV or better • **Guaranteed** peak resolution change by <1eV at Mn Kα between 1,000 and 10,000cps ensures accuracy of results and speed of analysis whilst delivering greater user productivity and quality of information. • The only EDX detector that conforms to ISO 15632:2002 **guaranteeing** performance at a productive count rate. • Sensitivity of 1 Wt% for light elements and 0.1% for heavier elements. • A micrometer resolution. The **EBL** is of **Raith** brand, model **ELPHY Quantum**. Main characteristics: • Good quality pattern generator: 2.5 MHz writing speed with < 2 ns dwelltime • 2 high speed 16-bit DACs for X and Y main beam deflection • 6 multiplying 16-bit DACs for overlay alignment and write field calibration with sub-nm step size control • high speed image acquisition & mark registration (400 ns Video ADC) • Beamblanker control circuit TTL 5V • Convinient software • Should give possibility to obtain structures below 50 nm.
Application example: Lietošanas piemers:	Simultaneous / Multifunctional Analysis and nanostructures formation: • SEM imaging (different modes) • Local composition Measurements with EDX • Creation of nano-structures using EBL The system is proving indispensable to researchers in material analysis (semiconductors, insulators, metals), life sciences, healthcare, nanoscience.
Responsible	**Dr.Ivans Shorubalko**, E-mail: ish@lu.lv, Phone: +371 7260803 Room number 409

Instrument title: **Ierīces nosaukums:**	**"Nanofinder S" 3D Scanning Confocal Microscope with Spectrometer**
Photo: **Foto:**	
Technical details: **Tehniskā specifikācija:**	The "Nanofinder S" is a versatile system to carry out multifunctional analysis of micro-structures in 3 dimensions. It combines excellently the advanced features of conventional high-resolution optical microscopy and laser scanning confocal spectroscopy. The heart of the system is a confocal microscope coupled to a spectroscopy system enabling 3D-imaging with a spatial resolution of 200 nm. • High spatial resolution: 200 nm (X-Y axes); 500 nm (Z-axis) • Quick analysis in imaging mode: 4 µs per point • Raman shift measurements from low wavelengths: 80 cm^{-1} (633 nm); 90 cm^{-1} (488 nm) • Modular, upgradable • High thermal and mechanical stability • Polarization measurements • Fully automated • High spectral resolution: 0.008 nm (Echelle grating, 500 nm wavelength); 0.025 nm (1200 l/mm grating) • High-efficiency imaging spectrograph • Multiple laser input • Excitation laser wavelengths: 350 nm to 850 nm (up to five different lasers can be used with automatic switchover) • Low power excitation (µW to mW): non-destructive analysis • Optimized optics for your applications in VIS: 450 - 900 nm.
Application example: **Lietošanas piemers:**	Simultaneous / Multifunctional Analysis: • Raman Measurements • Luminescence Measurements • Laser Reflection & Transmission Measurements The "Nanofinder S" is proving indispensable to researchers in nanoscience, semiconductors, carbon nanotubes, liquid crystals, polymers, optical wave guides.
Responsible: **(name, second name, e-mail)** **Atbildīgais:** **(vārds, uzvārds, e-pasts)**	**Dr. Aleksejs Kuzmins**, E-mail: a.kuzmin@cfi.lu.lv, Phone: +371 7251691 Room number 240

<table>
<tr><td>Instrument title:
Ierīces nosaukums:</td><td>NT-MDT Stand Alone "SMENA" Scanning Probe Microscope</td></tr>
<tr><td>Photo:
Foto:</td><td>  </td></tr>
<tr><td>Technical details:
Tehniskā specifikācija:</td><td>
Measuring modes:
In air:
Contact AFM/ LFM/ ResonantMode AFM (semicontact + noncontact)/ Phase Imaging/ Force Modulation (viscoelastisity)/ Adhesion Force Imaging/ Spreading Resistance Imaging/ SCM/ SKM/ MFM/ EFM/ AFM, Voltage, RM Lithographies

Technical specification
<table>
<tr><td>Sample Size</td><td>Unlimited
Note: Small samples (up to 100x100x20mm) can be placed between the SMENA head legs.</td></tr>
<tr><td>Scanner</td><td>50x50x2.5µm</td></tr>
<tr><td>Min. Scanning Step</td><td>0.006nm; 0.012nm</td></tr>
<tr><td>Scan Type</td><td>By Probe</td></tr>
<tr><td>Sample positioning range</td><td>5x5mm</td></tr>
<tr><td>Positioning resolution</td><td>5µm</td></tr>
<tr><td>Optical viewing system</td><td>Numerical aperture 0.1
Magnification 58x to 578x
Horizontal field of view 2 to 0,51mm</td></tr>
<tr><td>Control System</td><td>SPM Controller</td></tr>
<tr><td></td><td></td></tr>
</table>
</td></tr>
<tr><td>Application example:
Lietošanas piemers:</td><td>Optical and Magnetic Storage, Coating and Polishing Quality Control, Large Optics, Polymers, Biology and Medicine, Semiconductors, Materials Science and many others.</td></tr>
<tr><td>Responsible:
(name, second name, e-mail)
Atbildīgais:
(vārds, uzvārds, e-pasts)</td><td>Dr. Aleksejs Kuzmins, E-mail: a.kuzmin@cfi.lu.lv,
Phone: +371 725169, Room number 240</td></tr>
</table>

Instrument title: **Ierīces nosaukums:**	**Closed-cycle cryostat** **Noslēgta cikla kriostats**
Photo: **Foto:**	
Technical details: **Tehniskā specifikācija:**	Closed cycle cryogenic system for investigation of electrical and photoelectrical properties in thin solid films. • Temperature range 10-350K • Temperature sensors 2 Si diode sensors • Sample holder 50x50mm • A port with 1 electrometric feedthrough for Keithley M617 electrometer for current measurement in range10^{-15} A - 1mA • A 12 instrumentation feedthrough port • Refrigeration capacity 2.5W at 20K
Application example: **Lietošanas piemers:**	Investigation of electrical and photoelectrical properties in thin organic solid films with high resistivity by space charge limited current method and thermally modulated space charge limited current method. The closed-cycle cryostat is available for researchers in nanoscience, semiconductors, organic materials and polymers dealing with electrical and photoelectrical properties.
Responsible: **(name, second name, e-mail)** **Atbildīgais:** **(vārds, uzvārds, e-pasts)**	**Dr. Inta Muzikante** E-mail: intam@edi.lv, Phone: +371 7260787 Room number 224

Instrument title:	Magneto-optical cryostat of Oxford Instruments
Photo:	 
Technical details:	SM4000-8 horizontal field split pair magnet system for optical studies, comprising: • Horizontal field split pair magnet • Central field 7 T at 2.2 K, 6 T at 4.2 K • Homogeneity 0.6% over a 10 mm diameter sphere • 0.23 l/hr helium consumption (with zero flow through insert and zero current in leads) • 1.0 l/hr helium consumption (with zero flow through insert and full current in leads) • 20 l usable helium volume providing > 100 hr hold time • OVC with 4 off horizontal optical access, two parallel to field, two perpendicular to field, fitted with Spec. B quartz windows • Overall system height 1.4 m approx. • Minimum height required to remove sample rod, 2.3 m • System weight ~135 kg (without cryogens) Integral Variable temperature insert with: • 25 mm diameter sample space • Temperature range (measured at heat exchanger) 4.2 – 300 K (with GF4 pump) 1.5 – 300 K (with EPS40 pump) • Temperature stability ± 0.1 K (measured over a 10 minute period) • Capillary fed heat exchanger fitted with heater and Cernox sensor • Automatic needle valve operated via ITC controller • 4 off horizontal optical access, two parallel to field, two perpendicular to field, fitted with Spec. B quartz windows IPS120-10 superconducting magnet power supply: • ± 120 A output current: ± 10 V output voltage • RS232 and IEEE interfaces TC 503 digital Temperature Controller
Application example:	For measurements at low temperatures down to 1.5K: - Magnetic circular dichroism: - Optically detected EPR Optically detected EPR technique allows find out a direct correlation between the data of the structure-sensitive EPR method and optical properties of luminescence and colour centres in solids.
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr.Uldis Rogulis**, E-mail: rogulis@latnet.lv, Phone: +371-7260553, Room number 518

Instrument title:	**Electrochemical System "VoltaLab 40"** **with software for different classical electrochemical methods** **"VoltaMaster 4"**
Photo:	
Technical details:	§ maximum output current ± 1 A § maximum output voltage ± 30 V § potential range ± 15 V § applied potential resolution 60 µV § current ranges 100 nA to 1 A in 7 ranges § measured current resolution 0.003%, 30 pA § potentiostat bandwidth >100 kHz § potentiostat rise-time/fall-time (1 V step, 10-90%) 12 µs § potentiostat modes Slow/medium/fast § input impedance of electrometer 1 GW § interfacing RS 232 (COM) § power requirements 115/230 V; 47-63 Hz § frequency range (Impedance Mod) 1 mHz – 100 kHz
Application example:	§ Potentiostatic, § Galvanostatic, § Culonometric, amperometric, § Impedance, § Battery testing, § pH measurements § etc
Responsibl	**Dr. Janis Kleperis**

e:	e-mail: **kleperis@latnet.lv** Phone: +371 7262145 Room number **212**

Instrument title:	***Model 6514 System Electrometer***
Photo:	
Technical details:	

Mode of action	*fA scale current mode measurements*
Resolution	*<1fA*
Lowest range in current mode	*20 10^-12 A*
Current range	*±100 aA to ±21 mA*
Speed	*Readings/ second=>1200*

Application example:

Standard application	*Measurements of dielectric polarization in nanometric scale samples*
Nonstandard	*Voltage and charge measurements*
Stage of implementation	*IEEE-488 interface connections & physical run-up*

Responsible: **(name, second name, e-mail, phone, room number)**	***Dr.Eriks Klotins*** *E-mail:klotins@cfi.lu.lv* *Phone: +371 7187866 Room number 434*

Appendix 2

Systems and equipment, developed at Institute of Solid State Physics