Institute of Solid State Physics
University of Latvia

ANNUAL REPORT 2005

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Riga 2006

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

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INTRODUCTION

The research in solid state physics at the University of Latvia restarted after World War II. The **Institute of Solid State Physics** (ISSP) of the University of Latvia was established on the basis of Laboratory of *Semiconductor Research* and Laboratory of *Ferro- and Piezoelectric Research* in 1978. Since 1986 the ISSP has the status of an independent organization of the University and now is the 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 2004 scientists from Latvian Institute of Physical Energetics joined ISSP and established Laboratory of Organic Materials (Table 1).

In mid 90-ties the ISSP has intensified its **teaching activities**. Three research staff members of the Institute have been elected as professors of the University of Latvia. Post graduate and graduate curricula are offered in solid state physics, material 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.

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

The research of the ISSP includes:

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

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

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

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

The interdisciplinary nature of research at the ISSP is reflected by its **highly qualified staff.** At present there are 180 employees working at the Institute, 28 of 87 members of the research staff hold Dr.habil.degrees, 45 hold Dr. or PhD. At the end of 2005 there were 10 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 2005.

Table 1

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2005

International Supervisory board

Council of Institute
Dr.phys. L.Trinklere

Director
*Dr.habil.phys. S*ternberg

Deputy director
Dr.habil.phys. A.Krumins

RESEARCH DIVISIONS AND LABORATORIES

Crystal Physics Division
Dr.phys P.Kulis

Disordered Material Physics Division
Dr.habil. phys .D.Millers

Ferroelectric Physics Division
Dr.habil.phys A.Sternberg

Semiconductor Materials Division
Dr.phys A.Lusis

Lab. of Nonlinear Processes Theory
Dr.habil.phys. J.Kotomin

Lab. of Optical Recording
Dr.chem J.Teteris

Lab. of Wide Band Gap Materials
Dr.habil.phys. B.Berzina

Lab. of Surface Physics
Dr.habil.phys. J.Maniks

Lab. of Optical Materials
Dr.habil.phys. I.Lacis

Lab. of Radiation Physics
Dr.habil.phys. J.Berzins

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

Table 2

The Council of the Institute

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

Table 3

International Advisory Board of the Institute

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

In 2004 the Institute finished its activities as a Centre of Excellence of the European Commission (Centre of Excellence for Advanced Material Research and Technologies). The ISSP was awarded this title by EC in December 2000. This honorary recognition with the accompanying financial support of 0,7 million EUR has increased our research activities, particularly extending the list of our research partners and scientists who come to work to our Institute from the leading European research centres.

In 2004 Institute succeeded in receiving a notable grant of 1 142,5 thous Ls (Lats) (exchange rate: 1 Ls =1,42 EUR) from EU Structural funds for update of scientific infrastructure (Fig.1). Now the modern technological and research equipment, listed in our 2004 year report, is installed including Electron Scanning Microscopy with EDX and EBL options and MOCVD thin film technology.

Extra expenditures from state budget 2005 were used for:

- reconstruction of conference hall and water installation system (120 thous. Ls);
- purchasing of modern research equipment (200 thous. Ls) ; see Appendix 1.

The annual report summarizes research activities of the ISSP in 2005. The staff of the Institute has succeed in 31 **national science grants** and in the **two national cooperation projects** (Functional Materials and Technologies for Microelectronics and Photonics and Nanomaterials and Nanotechnologies), with the total financing 245.5 thous. Ls.

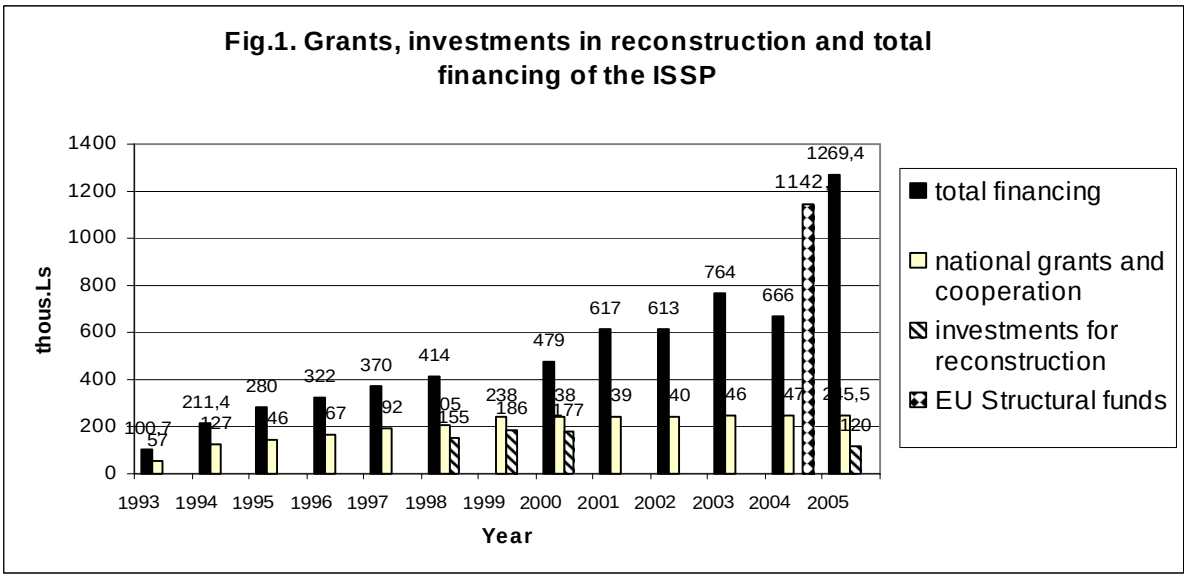
In 2005 the new Law of Science was passed by Parliament of Latvia. According to this law the state budgetary financing in Latvia for science have to increase yearly per 0.15% from GDP up to reaching a 1% value in the future. The budgetary increase was focused on scientific infrastructure financing and launching of National research programmes. One of the scientific priorities in Latvia is materialscience. During the last two months of 2005 the National research programme in materialscience was started with the total funding of 145 thous. Ls for that period. ISSP became coordinating institution for the Programme attracting 56 thous. Ls budget in 2005. The infrastructure financing for ISSP for three last months of 2005 was 69 thous. Ls. and it was partly used also for the salaries of the scientific and maintenance staff of the institute.

Table 4

INCOME OF ISSP, THOUSAND Ls, FROM 1993 - 2005

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Rent of space	Structural funds (ERAF) 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**
2005	**1 269,4**	**245,5**	**358,8 + 120)***	**172,8**	**387,6**	**4,7**	

*) – investment for building reconstruction



2005 was successful for **national contracts**. The market oriented contracts reached 95.8 thous. Ls, but contracts with Latvian companies including SMEs – 77.0 thous. Ls. The descriptions of some materials and devices developed at the ISSP as a result of contracts are enclosed in the Appendix 2.

The main source for international funding were the EC 6th Framework Programme contracts:

- for the Centre of Excellence CAMART – 105 thous. EUR;

- X-TIP project – 75 thous. EUR;
- for Green Rose project – 17 thous. EUR;
- for MIND projects – 43 thous. EUR.;
- for four EURATOM projects – 280 thous. EUR;
- for NERP project – 12 thous. EUR

The Institute obtained 4.7 thous. Ls from **leasing part of its space**.
The ISSP income dynamics for 1993 – 2005 is given in Table 4 and Figure 1.

Main achievements in 2005

1. Purchasing and installation of modern technological and research equipment (Mr.J.Pinnis);
2. Starting of National materialscience programme (Dr.habil.phys. A.Sternberg);
3. Reconstruction of some laboratories and Conference hall of the Institute (Dr.phys.J.Klavins);
4. Starting of infrastructure financing for Institute from state budget;
5. Dr.habil.phys. A.Sternberg was elected a member of the Latvian Academy of Science;
6. Dr.phys. A.Kuzmin was elected a correspondent member of Latvian Academy of Science;
7. Dr.habil.phys. D.Millers received 2005 years award from Ministry of Education and Science;
8. Dr.habil.phys. J.Berzins received the "Grindex" award for 2005;
9. Eight scientists from Institute got "scientist emeritus" grant with additional financing (D.Millers, J.Maniks, S.Chernov, V.Bondarenko, K.Bormanis, O.Veveris, O.Vilitis, E.Pentjuss);
10. M.Kundzins and E.Tamanis were acquired degree of doctor of physics University of Latvia;
11. 6 master students started PhD studies in physics at Institute;
12. Under the supervision of our scientists 12 M.Sc thesis and 7 B.Sc thesis in physics were defended.
13. About 40 young researchers, mainly students form 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: Science Department of the Latvian Ministry of Education and Science, Latvian Council of Science, University of Latvia, EC 6th Framework Programme, Programme of EU Structural funds, COST Programme, and to many foreign Universities and institutions for cooperation.

Prof. Dr. A.Krumins

Master of Science (M.Sc) and Bacalaur of Science (B.Sc)
Thesis prepared at the institute in 2005.

M.Sc. thesis:

No	Author	Title	Supervisor
1.	A.Auzina	Spectral characterization of AlN	Dr.habil.phys. B.Berzina
2.	T.Dudareva	Time – resolved spectral investigations on neodymium centers in complex lanthanum and yttrium oxides	Dr.habil.phys. L.Grigorjeva
3.	I.Gromuls	Thermoactivation of fluoride crystals LiF, BaF_2 and $LiBaF_3$	Prof., Dr.habil.phys. I.Tale
4.	A.Gulans	*Ab inito* calculation of defects in h - GaN	Prof.,Dr.habil.phys. I.Tale Dr.habil.phys. R.Evarestov
5.	J.Hodakovska	Research on gas sensors'sensivity, selectivity and working resources	Dr. phys. J.Kleperis
6.	O.Jancenko	Investigations of high – energy – ion – induced defects in LiF crystals	Dr. phys. I.Manika
7.	R.Krutohvostovs	Ultraviolet radiation induced processes in BN	Dr.phys. L.Trinklere
8.	J.Proskurins	The studies of quantum chaos in the framework interacting boson model	Dr.habil.phys. J.Tambergs
9.	A.Sharakovsky	Photo- and thermostimulated processes in $CsCdF_3$ crystals doped with Mn	Dr.habil.phys. M.Springis
10.	M.Shorohovs	Electronic excitation and its correlation with ionizing radiation detectors parameters in TlBr crystals	Dr.habil.phys. L.Grigorjeva
11.	K.Smits	Luminiscence of zirconia oxide nanocrystals	Dr.habil.phys. D.Millers
12.	V.Vorohobovs	Physical and chemical processes in ozone generators: ozone sensors and possible applications in Latvia	Dr.phys. J.Kleperis

B.Sc. thesis:

No	Author	Title	Supervisor
1.	R.Dobulans	Electric properties of ozone and ammonia gas sensing thin films of phtalocianine derivates	Dr.habil.phys. I.Muzikante
2.	D.Haberkorne	Computer-generated Fresnel and Fourier holograms	Dr.phys. J.Harja
3.	V.Korsaks	Spectral characterization of BN nanomaterials	Dr.habil.phys. B.Berzina
4.	N.Laskovs	X-ray absorption spectroscopy study of local atomic structure in oxide materials	Dr.phys. A.Kuzmins
5.	A.Mikulis	Electrocaloric effect in ferroelectric (1-x)$PbMg_{1/3}Nb_{2/3}O_3$ – $xPbTiO_3$ solid solutions	Dr.phys. E.Birks
6.	L.Pekse	Ozone and methods of it's determination	Dr.phys. J.Kleperis
7.	A.Voitkans	Time-resolved spectroscopy of spectroscopy of BN thin film carhode luminiscence	Dr.habil.phys. I.Tale

DISSERATATIONS PREPARED AT THE INSTITUTE

1. M.Kundzins *„Optical and electrophysical properties of heterostructure ferroleletric materials"* (PhD., solid state physics)

Supervisors: Prof.G.Liberts (Univ. of Daugavpils), Prof. A.Krumins (ISSP)
Referees: Dr.habil.phys. J.Banys (University of Vilnius), Prof., Dr.habil.phys. M.Knite (Riga Technical University), Prof., Dr.habil.phys. U.Rogulis (ISSP)

2. E.Tamanis *"Nanostructure layers deposition in Penning discharge source, their modifications and physical properties investigation''* (PhD., solid state physics)

Supervisors: Dr.phys. L.V. Kozlovskis (Daugavpils Univ.), Prof., Dr.habil.phys. G.Liberts (Daugavpils Univ.), Dr.phys. J.Maniks (ISSP)
Referees: Prof., Dr.phys. Priit Kulu (Tallin Technical University), Prof., Dr.habil.phys. I.Tale (ISSP), Dr.habil.ing. J.Grabis (Riga Technical University).

CRYSTALS PHYSICS

Head of Division Dr. P. Kulis

Research Area and Main Problems

1. Recombination mechanisms of the electronic excitations in new optical binary and ternary compounds – the project is aimed to investigate the exact mechanisms of annihilation, localization and recombination of the electronic excitations and their relationships in new binary and ternary inorganic compounds (nominally pure and doped with some active impurities).
2. Magnetic resonance (EPR, optically detected EPR) investigations of the structure of the intrinsic and radiation defects, and their recombination process in some actual wide gap scintillator, x-ray storage phosphor and dosimeter materials. The scientific cooperation with other magnetic resonance groups, especially with the University of Paderborn, Germany. A contribution to the better understanding of the defects and processes in luminescent detector materials is expected.
3. Investigations on a new class of materials- oxifluoride composites. One of the goals is to obtain fluoride micro- and nanocrystals with controlled size and properties in the oxide glass matrix. First samples of oxifluorides on the basis of lithium borate glasses with lantanum fluoride component have been obtained; investigations of their properties are in progress.
4. Technology of Al-Ga nitride semiconductor heterostructures for light-emitting and laser diodes for violet and ultraviolet spectral regions - the goal of the project is the development of light-emitting diodes and laser diodes for violet and ultraviolet spectral region. The project involves installation of new MOCVD equipment AIXTRON AIX200 RF, synthesis and design of corresponding new materials on the basis of the third group nitrides, elaboration of the thin film heterostructures and further development of production of multifunctional fotonic devices in joint stock company ”Alfa”.
5. The main goals of EURATOM project are investigation and characterization of the impurity content in fusion plasmas and reactor hot wall. The objectives of this project require study of the influence of the liquid metal limiter on the main plasma parameters, including concentration of evaporated metal atoms in plasma. Laser spectroscopy techniques are proposed for development of procedures for research of impurities in plasma and plasma facing materials. According to the objectives emission of Ga metal vapours in plasmas during the evaporation of the metal gush has been considered. Density of metal vapours in plasma can be obtained using two spectroscopic methods: the steady state emission of the multiple ionised metal ions and the charge exchange emission during ionization of evaporated metal ions.

Scientific Staff

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

Technical Staff

1. E. Tale
2. M. Veispale

PhD Students

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

Students

1. Dz. Berzins
2. G. Marcinshs
3. A. Voitkans
4. P. Zarans

Scientific visits abroad

1. Dr. hab. phys. U. Rogulis, University of Paderborn, Germany (4 months);
2. Dr. hab. phys. I. Tale, Aixtron, Achen, Germany (2 weeks);
3. Dr. hab. phys. I. Tale, University of Rostock, Germany (1,5 week);
4. Dr. hab. phys. I. Tale, Alushta, Ukraine (1 week);
5. Dr. phys. P. Kulis, Alushta, Ukraine (1 week);
6. A. Sharakovsky, Alushta, Ukraine (1 week);
7. A. Fedotovs, Alushta, Ukraine (1 week);
8. L. Dmitrichenko, Alushta, Ukraine (1 week);
9. J. Butikova, Culham, UK (2 weeks);
10. J. Butikova, Garching bei Munich, Germany (10 weeks);
11. A. Sharakovsky, Instituto Superior Tecnico (IST), Lisbon Portugal (8 weeks);
12. A. Sharakovsky, Primorsko, Bulgaria (1 week);
13. A. Gulans, Helsinki, Finland (1 week);
14. G. Marcinshs, Aixtron, Achen, Germany (0,5 week)

Cooperation

Latvia

Joint stock company “Alfa”

Czech Republic

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

Germany

1. University of Paderborn, Germany (Prof. Dr. R. Wehrspohn, Prof. Emeritus, J.-M. Spaeth, Dr. hab. S. Schweizer, Dr. hab. S. Greulich-Weber).
2. University of Rostock, Germany (Prof. H.-J. Fitting).

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

EPR OF F TYPE CENTRES IN $LiBaF_3$

A.Fedotovs, E.Elsts, U.Rogulis, I.Tale, M.Nikl[1], N.Ichinose[2], K.Shimamura[2]
[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[2]*Laboratory of Material Sciences and Technology, Waseda University, Tokyo, Japan*

In this research we studied EPR spectra of pure $LiBaF_3$ sample of high quality. For EPR measurements $LiBaF_3$ sample was X-irradiated at room temperature, but spectra could be observed at low temperatures - at 77K. We could well resolve all hyperfine structure lines of F-type centre. Qualitative analysis with *g*-tensor parameters derived from magneto-optical measurements show that the F-type centre observed earlier by MCD-EPR techniques is the same F-type centre we observe in the EPR.

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

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

Perovskite type fluoride crystals doped with rare-earth ions and other activators are promising materials for laser hosts and detectors of ionising radiation. The radiation-induced effects have been studied in a number of fluorides and the main defects (F- and V_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.

LUMINESCENT OXYGEN-VACANCY COMPLEX IN Mn-DOPED $LiBaF_3$ INVESTIGATED BY OPTICALLY DETECTED MAGNETIC RESONANCE

U. Rogulis, B. Henke[1], S. Schweizer[1]
[1]*Department of Physics, University of Paderborn, Germany*

Upon ultraviolet photoexcitation, Mn-doped $LiBaF_3$ shows different luminescence bands in the visible range. The luminescence, which can be attributed to Mn^{2+}, is at 712 nm, whereas two additional bands appear at 423 and 480 nm. The peaks at 423 and 480 nm have completely different excitation spectra than the one for the 712 nm emission, which shows the typical Mn^{2+} excitation bands. Photoluminescence detected electron paramagnetic resonance measurements yielded that the bands at 423 and 480 nm can be attributed to an oxygen-vacancy complex. Its principal axis, *z*, of the fine structure tensor is aligned along a <110> direction. The Mn^{2+}-dopant can be found in the vicinity of this complex. We assume that Mn^{2+} substitutes for a Ba^{2+} ion.

EPR OF RADIATION DEFECTS IN $LiYF_4$ CRYSTALS

A. Fedotovs, L. Dimitrocenko, U. Rogulis

The EPR studies of pure $LiYF_4$ crystal have been done after x-ray irradiation at room temperature. Obtained results showed presence of radiation-induced defect which is stable at room temperature. The broad EPR band in the X-microwave range is structureless at RT. A structure could be resolved by measurements at 77 K, it is angular dependent on two perpendicular planes and could be explained mainly by g-anisotropy. We discuss the possibility that the observed spectrum could be the F centre.

RECOMBINATION PROCESSES IN $LiBaF_3$ CRYSTALS

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

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.

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

E.Elsts, U.Rogulis

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.

CARRIER LOCALIZATION EFFECT IN POLARIZED INGAN/GAN MULTIPLE QUANTUM WELLS

M. Springis, I. Tale, C. C. Yang[1], S. Jursenas[2]
[1]Graduate Institute of Electro-Optical Engineering, Department of Electrical Engineering, National Taiwan University
[2]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

A. Gulans, I. Tale, R. Evarestov[1], C.C Yang[2]

[1] Chemistry Department, St.-Petersburg State University, St.-Petersburg, Russian Federation

[2] 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.

INVESTIGATION OF METAL IONS IN FUSION PLASMAS USING EMISSION SPECTROSCOPY

I. Tale, A. Sharakovsky, M.Springis

The Latvian and Portugal Associations are performing development of advanced plasma – facing system using the liquid metal limiter. The objectives of this project require study of the influence of the liquid metal limiter on the main plasma parameters, including concentration of evaporated metal atoms in plasma.

The fusion plasmas are related to the dense hot plasmas. The required average ion temperature according to the ITER project (International Thermonuclear Experimental Reactor) is 8.0 keV (9.3 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.

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

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

Particle fluxes from the plasma (ions, electrons, atoms) results in complex processes of the plasma-wall interaction. They are crucial for possibility of application of the material in the fusion devices. Understanding these processes is necessary for improving of the wall materials as well as leads to optimize plasma discharge operation conditions. Investigation of the material modification under plasma exposure, development of new plasma facing materials and development of methods of their characterization are actual tasks into the development of plasma facing components. It is stated that plasma – wall material interaction results in several processes such as: erosion of material, migration of materials in fusion devices involving tungsten migration, deposition of carbon layers, tritium co-deposition, and diffusion of hydrogen isotopes in plasma facing materials.
Several methods for investigation of the surface and impurity content in near-surface layers are applied. They involves X-ray photoelectron spectroscopy, the deuterium depth profiling by analysis of energy spectrum of alpha particles resulting the nuclear reaction $D(^3He,p)^4He$ in the near-surface layers of solids. Using different ^3H energy depth

profiles from 1 μm up to >10 μm can be obtained. For obtaining of composition of hydrocarbon layers and their optical properties ion beam techniques is applied

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

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

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

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

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

Scientific publication

Published in 2005

1. M. Springis, A. Sharakovsky, I. Tale, and U. Rogulis, X-irradiation induced photo- and thermostimulated luminescence of CsCdF3:Mn crystals, - phys. stat. sol. (c) 2, No. 1, 511–514 (2005).
2. A. Žukauskas, K. Kazlauskas, G. Tamulaitis, J. Mickevièius, S. Juršenas, G. Kurilèik, S. Miasojedovas, M. Springis, I. Tale, Yung-Chen Cheng, Hsiang-Chen Wang, Chi-Feng Huang, and C. C. Yang, Carrier localization effect in polarized InGaN multiple quantum wells, - phys. stat. sol. (c), 2 No.7, 2753-2756, (2005).
3. K. Kazlauskas, G. Tamulatis, S. Juršenas, A. Žukauskas, M. Springis,Yung-Chen Cheng, Hsiang-Chen Wang, Chi-Feng Huang, and C. C. Yang, Monte Carlo simulation approach for a quantitative characterization of the band edge in InGaN quantum wells, - phys. stat. sol. (c) 2, No. 3, 1023– 1026 (2005).
4. K. Kazlauskas, G. Tamulaitis, P. Pobedinskas, and A. Žukauskas M. Springis, Chi-Feng Huang, Yung-Chen Cheng, and C. C. Yang, Exciton hopping in In*x*Ga1-*x*N multiple quantum wells, - Phys. Rev. B71, 5306-5310 (2005).
5. A. Trukhin, P. Kulis, J. Jansons, T. Dyuzheva, L. Lityagina, and N. Bendeliani, Host-defect luminescence of stishovite, - phys. stat. sol. (c) 2, No. 1, 584–587 (2005).
6. I. Manika, J. Maniks, P. Kulis, and L. Gailite, Hardening in LiF induced by fast Ni ions and recovery of properties under annealing, - phys. stat. sol. (c) 2, No. 1, 430–433 (2005).
7. B. Henke, M. Secu, U. Rogulis, S. Schweizer, and J.-M. Spaeth, Optical and magneto-optical studies of Mn-activated LiBaF3 phys. stat. sol. (c) 2, No. 1, 380–383 (2005).
8. A. Gulans, R. A. Evarestov, I. Tale, and C. C. Yang, Ab initio calculations of charged point defects in GaN, - phys. stat. sol. (c) 2, No. 1, 507–510 (2005).
9. E. Elsts. and U. Rogulis, EPR hyperfine structure of the Mo-related defect in CdWO4, - phys. stat. sol. (c) 2, No. 1, 69–72 (2005).
10. A. Fedotovs, U. Rogulis, Perturbed Cd centre in BaF_2 crystal, Latvian Journal of Physics and Technical Sciences, 2005, vol. 3, pp. 62-67.

11. A. Sharakovsky, M. Springis, U. Rogulis, I. Tale, Photostimulated recombination processes in X-ray irradiated $CsCdF_3$:Mn crystals, Proceedings of SPIE: 4th International Conference on Advanced optical Materials (AOMD-4), 2005, vol. 5946, pp. 112-118.
12. I. Manika, J. Maniks, P. Kulis, L. Gailite, Hardening in LiF induced by fast Kr and Ni ions, and recovery of the structure and properties under annealing, - Proceedings of SPIE: 4th International Conference on Advanced optical Materials (AOMD-4), 2005, vol. 5946, pp.81-86.

Lectures on Conferences

21th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 7–9, 2005.

1. A. Gulans, *Modeling of Impurities in GaN*, - Abstracts of the 21th Scientific Conference dedicated to the International Year of PHYSICS, Riga, 2005, p.6, (oral presentation).
2. A. Trukhin, J. Jansons, *SiO_2 Rutile-like Crystals UV Luminescence: Comparison with Luminescence of a-Quartz,* - Ibid. p. 7, (oral presentation).
3. E.Elsts, U. Rogulis, A. Fedotovs, *EPR Spectra of SrF_2:Ce Crystals,* - Ibid. p.8, (oral presentation).
4. A. Fedotovs, U. Rogulis,
5. A. Sharakovsky, M. Springis, *Photo- and Thermostimulated Processes in CsCdF3:Mn Crystals,* - Ibid. p. 10, (oral presentation).
6. A. Voitkans, I. Tale, J. Jansons, *Catodoluminescence of BN films,* - Ibid. p. 11, (oral presentation).
7. I. Gromuls, P. Kulis, I. Tale, *Thermostimulated Recombination Processes in Fluoride Crystals,* - Ibid. p. 12, (oral presentation).
8. I. Tale, J.Butikova, *Investigation of Metal Ions in Fusion Plasmas Using Emission Spectroscopy,* - Ibid. p. 75, (oral presentation).
9. Dz. Berzins, U. Rogulis, *EPR measurements at Low Temperatures,* - Ibid. p. 95, (oral presentation).
10. U. Rogulis, *Magnetooptical Setup,* - Ibid. p. 96, (oral presentation).

The 42nd Plasma Physics Summer School, Culham, UK, ,2005

1. J. Butikova, I. Tale, *Laser ablationspectroscopy for impurity depth profiling in plazma,* - (poster presentation).

Seminar of Max-Planck-Institut für Plasmaphysik (IPP), Material science department, Garching bei Munich, Germany, November, 2005.

1. J. Butikova, *Laser ablation spectroscopy for impurity depth profiling and concentration imaging in plasma facing components,* - (oral presentation).

InternationalConference on Inorganic Scintillators and their Industrial Application SCINT2005, Alushta, Ukraine, September 19-23, 2005.

1. P. Kulis M. Springis, I. Tale, A. Sharakovsky, L. Dimitrichenko, Recombination Processes in $LiBaF_3$ Crystals, - Book of Abstracts, SCINT2005 International Conference on Inorganic Scintillators and their Industrial Application, Alushta, Ukraine, September 19-23, 2005, p 59 (poster presentation).
2. A. Fedotovs, E. Elsts, U. Rogulis, I, Tale, M. Nikl, N. Incinose, K. Shimamura, *EPR of F-Type Centres in $LiBaF_3$,* - Ibid. p. 60, (poster presentation).
3. A. Fedotovs, L. Dimitrocenko, U. Rogulis, *EPR of Radiation Defects in $LiYF_4$ Crystals,* - Ibid. p.62 (poster presentation).

4. A. Sharakovsky, M. Springis, I. Tale, *Luminescence of $CsCdF_3$:Mn Crystals*, - Ibid. p.65 (poster presentation).

International Student Conference on Development in Optics and Photonics DOP-2005, Latvian University, Riga , Latvia, April 30 – May 1, 2005.

1. A. Sharakovsky, M. Springis, U. Rogulis, Photo- and thermostimulated Processes in $CsCdF_3$:Mn Crystals, - (oral presentation).

Popular scientific articles

1. J. Jansons, *Latvijas Universitātes sagatavoto fiziķu Pētera Auziņa un Friča Dravnieka dzīves krustceļi sakarā ar Otrā Pasaules kara izraisīto Latvijas valsts okupāciju,*. –Zvaigžņotā Debess, 2005. gada vasara, 58. - 64. lpp.
2. J. Jansons, *LU docents Jānis Fridrichson, – 100,* – Zvaigžņotā Debess, 2005./2006. gada ziema, 44. - 58. lpp.

DISORDERED MATERIAL PHYSICS

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

Solid state radiation physics laboratory

Head of Laboratory, Dr.hab.phys.L.Grigorjeva

Defect studies group

Head of Group, Dr.hab.phys. L.Skuja

Solid state optics laboratory

Head of Laboratory, Dr. hab. phys. A. Trukhin

Research area and the main problems

Medium- and wide-band gap materials, mainly oxides, in the form of crystals, ceramics and fibers are investigated by various spectroscopic methods. The main materials studied are: $KTaO_3$, $LiNbO_3$, YVO_4, TlBr, YAP, $CaWO_4$, $LaGaO_3$, ZnO, ZrO_2, glassy SiO_2, Ge-doped silica.

The main experimental methods employed are:

- Time-resolved optical absorption and luminescence spectroscopy to study fast relaxation processes responsible for excited states formation, excited states radiative and nonradiative decay, charge and energy transfer.
- The Fourier-transform infrared (FTIR) spectroscopy was used for detection of molecular species and dopants.
- Electron paramagnetic resonance (EPR) spectroscopy to study the structure of paramagnetic species.
- Vacuum-ultraviolet absorption spectroscopy to investigate optical properties of wide-band gap compounds (e.g., SiO_2).
- X-ray induced luminescence spectroscopy to study emission centers, recombination processes, and migration of electronic excitations.

Solid state radiation physics laboratory

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

Defect studies group

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

Laboratory of solid state optics

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

Technical Staff

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

Students

1. A.Kalinko
2. T. Dudareva
3. M.Shorohov
4. K.Smits

Scientific Visits Abroad

1. Dr.hab.phys. L.Grigorjeva, Poland, (7 days).
2. Dr.hab.phys.D.Millers, Poland, (7 days).
3. Dr.phys.V.Pankratov, USA. (6 month).
4. Dr.V.Pankratov, France, (5days)
5. K.Smits, Bulgaria, (7days)
6. Dr.hab.phys. S.Chernov, Alushta, Ukraine, (7 days)
7. Dr.hab.phys. L.Grigorjeva, Alushta, Ukraine, (6 days).
8. Dr.hab.phys.D.Millers, Alushta, Ukraine, (6 days).
9. Dr. hab. Phys. A. Trukhin, Russia (3 weeks)
10. Dr.hab.phys. L.Skuja Germany (3 days)
11. Dr.hab.phys. L.Skuja USA (5 days)
12. Dr.hab.phys. L.Skuja Japan (4 months).

Visits from Abroad

Dr.L.Maksimov, GOI, St.Peterburg, (3 days).

Cooperation

Latvia

University of Latvia, Institute of Biology (Dr. O.Mutere).
SIA "Baltic Scientific Instruments" (Dr.V.Gostillo).
Riga Technical University, Institute of Inorganic Chemistry (Dr.habil.sc.ing. J.Grabis).
SIA "OPTICS", (V.Jakovlev).
Institute of Chemical Physics, University of Latvia (Dr. D.Erts)

USA

Wake Forest University (Prof. R.T. Williams).
Department of Physics and Engineering, Sweet Briar College (Prof. Hank Yochum).
Montana State University (Prof. G.Malovichko).
Solid State Division, Oak Ridge National Laboratory. Oak-Ridge, TN. 37831 (Dr. Lynn A. Boatner)
University of Central Florida, CREOL (Professor, Dr.L.B.Glebov)

Czech Republic

Academy of Sciences, Institute of Physics (Dr. M.Nikl, Dr.V.Trepakov)
Charles University (Dr.M. Zvara, Dr .P.Hlidek, Dr. J.Bok)

Estonia

Institute of Physics, Tartu (Dr.V.Nagirnyj, M.Kirm, Prof.C. Luschchik, Dr. R.Kink, Dr. Yu. Maksimov)

France

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

Germany

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

Hungary

Hungarian Academy of Sciences, Research Inst. for Solid State Physics & Optics, Crystal Physics Laboratory (Dr.G.Corradi, Dr.K.Polgar, Dr.A.Watterich).

Italy

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

Japan

Tokyo Institute of Technology (Prof. H.Hosono)

Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), (Dr. K.Kajihara, Dr. M. Hirano)

Poland

Polish Academy of Science, UNIPRESS (Prof.W.Łojkowski)

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

Institute of Low Temperatures and Structure Researches, PAS, Wroclaw (Prof.W.Strek)

Romania

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

Russia

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

Ioffe Phys.Techn.Inst. RAS, (Dr.V.Trepakov, Dr. A.Badaljan).

Burjatija State University (A.V.Nomoev)

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

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

Ukraine

Lviv Polytechnic National University (Prof. S.Ubizskii)

The main results

TIME-RESOLVED LUMINESCENCE STUDIES FOR THE SOL-GEL PREPARED $CaWO_4$

L.Grigorjeva, D.Millers, V.Pankratov
Linas Vilciauskas [1], Aivaras Kareiva[1] , Arturas Katelnikovas[1]
[1]University of Vilnius, Lithuania

In tungstate crystals the intrinsic luminescence arises due to self-trapped exciton (STE) annihilation in WO_4^{2-} or WO_6^{6-} complex in sheelite or wolframite structure. The luminescence properties and details of STE creation were widely studied.

The fabrication of scintillating nanocrystals opens new opportunities – the scintillating ceramics as well as composites for different application might be manufactured. On the other hand sol-gel technologies for nanocrystal production is not expensive and complicate. The powders with sub-micrometer grain sizes (300 nm – 1 μm) were produced by two different chemical reactions via sol-gel process. For the powders

testing the SEM images and FTIR absorption was used. The luminescence properties (spectra and decay kinetics) were studied under pulse electron beam excitation (250 keV, 8 ns). The results were compared with those obtained and known for single $CaWO_4$ crystal.
In FTIR absorption spectra two bands (440 cm-1 and 800 cm-1) were analyzed. It is shown that for the powders with grain sizes ~350 nm and ~800 nm the structure of WO_4^{2-} complex is strongly distorted and this distortion depends on grain size. The STE luminescence decay consists of two components: 7.3 μs and 0.55 μs in $CaWO_4$ single crystal.

TLBR DETECTOR CRYSTALS: OPTICAL PROPERTIES AND SPECTROMETRIC PERFORMANCE

M.Shorohov[1], L.Grigorjeva, D.Millers
[1]Baltic Scientific Instruments, (BSI), Riga

The following optical methods of crystals investigation were used: 1) absorption at the edge of fundamental absorption; 2) luminescence excited either by X-rays or by electronic beam. Some crystals were studied for the efficiency of colloid formation under UV excitation. After the optical examination the crystals were used for production of ionizing radiation detectors, whose characteristics were investigated by conventional spectrometric methods.
The best spectrometric characteristics (the energy resolution 6.592 keV for Am-24 radionuclide 59.5 keV line) were obtained. It is shown that best detector was made from the specimen with the best optical parameters (the position of the maxima and halfwidth of the ALE luminescence band, Urbach's tail position and the efficiency of colloid formation was controlled).

LUMINESCENCE AND FTIR SPECTROSCOPY OF ZNO NANOCRYSTALS

L.Grigorjeva, D.Millers, W.Łojkowski[1], A.Tomaszewska-Grzeda[1], T. T.Strachowski
[1]Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland

ZnO has been attractive material for potential applications, for example, lasers and optoelectronic devices. The excitonic luminescence with decay times in ps range will be observed up to room temperature. It is expected high quantum yield for fast luminescence due to exciton quantum size effects on nanostructured ZnO. The ZnO nanocrystals (NC) and thin films were synthesized and characterized by FTIR, x-ray diffraction and SEM methods. The luminescence spectra and decay kinetics were studied under pulsed laser (266 nm, 2 ns) and pulse electron beam (10 ns 250 keV) excitation. NC powders with controlled grain size 10-40 nm was prepared by microwave driven hydrothermal process using different chemical reactions.
The FTIR spectroscopy results and luminescence spectra shows that fractions of chemicals used in synthesis process could be found as impurities in nanopowders. The bounding of fragments from organic compounds used in synthesis reaction could be used for the NC surface engineering as well as for luminescence spectral distribution control.

LUMINESCENCE OF ZrO_2 AND YTTTRIA STABILIZED ZrO_2 NANOCRYSTALS

D.Millers, L.Grigorjeva, K.Smits W.Lojkowski[1], A.Opalinska[1], J.Fidelius[1]
[1]Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland

The study of luminescence from nanostructured ZrO_2 was carried out. The luminescence spectra and decay kinetics were measured for free standing ZrO_2 nanopowders with different grain size, crystal and defect structure. Time-resolved measurements were conducted using YAG-Nd laser beam (266 nm, 2 ns) and high density (up to 20 MW/cm2) pulsed electron beam excitation.

It is shown the luminescence spectra are similar for all nanocrystal sizes, whereas the intensity of luminescence is nanocrystal size dependent. The decay of luminescence did not obey a simple exponential or hyperbolic rule, indicating more complicated recombination process. The luminescence intensity and decay time dependence on temperature gives an evidence that two processes – the luminescence center destruction and non-radiative electron transitions – were responsible for luminescence quenching observed. The relative contribution of these processes in luminescence quenching depends on nanocrystal size.

It is shown that the luminescence intensity strongly depends on oxygen deficiency: most sensitive to the deficiency of oxygen was cubic phase ZrO_2 nanocrystals. The oxygen exchange between environment and ZrO_2 was nanocrystal is size dependent: for smallest nanocrystals exchange starts at lower temperature**.**

INTRINSIC LUMINESCENCE OF PURE AND DOPED YAG NANOPOWDERS

V.Pankratov, D. Millers, L.Grigorjeva, W.Lojkowski[1],
R. Fedyk[1], T.Chudoba[1], W.Strek[2], D.Hreniak[2], P.Mazur[2]
[1]Institute of High Pressure Physics, Warsaw, Poland
[2]Institute of Low Temperature and Structure Research, Wroclaw, Poland

The nominally pure and doped by Nd^{3+} or Eu^{3+} nanocrystalline YAG powders were studied. Luminescence spectrum of undoped YAG powders under pulsed electron beam excitation at room temperature reveals broad band peaking near 3.9 eV and having two shoulders at ~3.3 and ~4.7 eV. The time evolution of the spectra leads to the considerable shift of its maximum to low energy side already in 100 ns and tend to the position of steady-state (X-ray) luminescence at 3.45 eV. Intrinsic defect luminescence intensity and relaxation kinetics is strongly depended on Nd^{3+} and Eu^{3+} concentration. Luminescence intensity decreases but luminescence decay becomes faster if the concentration of impurity increases. The origin of luminescence was comparing result for nanocrystals and well-studied YAG single crystals.

TIME-RESOLVED TRANSIENT ABSORPTION SPECTROSCOPY OF UNDOPED YVO_4 WITH VARIED AS-GROWN DISCOLORATION

H.M. Yochum[1], L.Grigorjeva, D. Millers, V. Pankratov, K.T. Stevens[2]
[1]Department of Physics and Engineering, Sweet Briar College, Sweet Briar, VA, USA
[2]Northrop Grumman - Synoptics, Charlotte, NC, USA

Induced transient absorption spectra and relaxation kinetics in undoped Czochralski grown YVO_4 single crystals for probe energies from 1.1 eV to 3.5 eV were measured under electron beam excitation (8 ns, 270 keV). These experiments were completed at room temperature on four YVO_4 samples with different levels of as-grown absorption in the 380 nm – 430 nm region. It was found that the broad induced absorption can be fit to three overlapping transient absorption bands at approximately 1.3 eV, 2.0 eV, and 3.0 eV. The peak value of each of these transient absorption bands varies with as-grown

sample discoloration. Using recent electron paramagnetic resonance (EPR) based models for electron-hole traps in YVO_4, we offer a preliminary defect assignment to each induced absorption band in YVO_4. The anti-Stokes luminescence in undoped YVO_4 was studied also. It is found that anti-Stokes luminescence lifetime depends on as-grown sample absorption.

VACUUM-ULTRAVIOLET ABSORPTION OF HYDROGENATED AND DEUTERATED SILANOL GROUPS AND INTERSTITIAL WATER MOLECULES IN AMORPHOUS SiO_2

K.Kajihara,[1] M.Hirano[1], L.Skuja, H. Hosono[2]

[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;

[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.

Vacuum-ultraviolet (VUV) absorption cross sections of hydrogenated and deuterated silanol groups (SiOX, where X=H or D) as well as interstitial water molecules (X_2O) in amorphous SiO_2 (a-SiO_2) were determined between photon energies of 7 and 8.2 eV. The absorption bands for the deuterated species are blue-shifted compared to those for the hydrogenated ones by ≈0.1-0.2 eV as a result of a decrease in the zero-point energy associated with the OX groups. The VUV absorption of interstitial X_2O below 8 eV is ≈1-2 orders of magnitude stronger than that of SiOX groups, and is blue-shifted with respect to that of X_2O trapped in rare-gas solids because of the formation of hydrogen bonding, most likely between X_2O and oxygen atoms in a-SiO_2 network.

REACTIONS OF SiCl GROUPS IN AMORPHOUS SiO_2 WITH MOBILE INTERSTITIAL CHEMICAL SPECIES: FORMATION OF INTERSTITIAL Cl_2 AND HCl MOLECULES, AND ROLE OF INTERSTITIAL H_2O MOLECULES.

K.Kajihara,[1] M.Hirano[1], L.Skuja, H. Hosono[2]

[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;

[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.

Reactions of the network-bound chloride SiCl groups in amorphous SiO_2 with mobile interstitial oxygen O_2, water H_2O, and hydrogen H_2 molecules thermally loaded from ambient atmosphere and with mobile radicals created by exposure to F_2 laser light (157 nm, 7.9 eV) were investigated. Reactions of the SiCl groups with O_2 and H_2O produce interstitial chlorine Cl_2 and hydrogen chloride HCl molecules, respectively. An infrared-absorption band appearing at 2815 cm^{-1} is assigned to the interstitial HCl. The SiCl groups do not react with H_2 below 400° C. However, sequential gas loading first with O_2 , then with H_2 leads to the production of interstitial H_2O, which decomposes the SiCl groups into HCl. Furthermore, the formation of the interstitial HCl with exposure to F_2 laser light, most likely due to the cracking of the Si–Cl bonds with photogenerated hydrogen atoms H^0, was demonstrated. These findings yield a general picture of the reactions of the chlorine-related species in a-SiO_2 and demonstrate the significant influence of even minor amounts (10^{18} cm^{-3}) of interstitial H_2O on defect formation and annihilation processes.

DEFECTS IN OXIDE GLASSES

L.Skuja, M.Hirano[1], H. Hosono[2] K.Kajihara,[1]

[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;

[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.

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 re-duce 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.

DECOMPOSITION OF PEROXY RADICALS IN SiO_2 GLASS WITH X-RAYS OR KrF LASER LIGHT

K.Kajihara,[1] M.Hirano[1], L.Skuja, H. Hosono[2]

[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;

[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.

Reactions of the network-bound chloride SiCl groups in amorphous SiO_2 with mobile interstitial oxygen O_2, water H_2O, and hydrogen H_2 molecules thermally loaded from ambient atmosphere and with mobile radicals created by exposure to F_2 laser light (157 nm, 7.9 eV) were investigated. Reactions of the SiCl groups with O_2 and H_2O produce interstitial chlorine Cl_2 and hydrogen chloride HCl molecules, respectively. An infrared-absorption band appearing at 2815 cm^{-1} is assigned to the interstitial HCl. The SiCl groups do not react with H_2 below 400° C. However, sequential gas loading first with O_2 , then with H_2 leads to the production of interstitial H_2O, which decomposes the SiCl groups into HCl. Furthermore, the formation of the interstitial HCl with exposure to F_2 laser light, most likely due to the cracking of the Si–Cl bonds with photogenerated hydrogen atoms H^0, was demonstrated. These findings yield a general picture of the reactions of the chlorine-related species in a-SiO_2 and demonstrate the significant influence of even minor amounts (10^{18} cm^{-3}) of interstitial H_2O on defect formation and annihilation processes.

INTERSTITIAL OXYGEN MOLECULES IN AMORPHOUS SiO_2. I. QUANTITATIVE CONCENTRATION ANALYSIS BY THERMAL DESORPTION, INFRARED PHOTOLUMINESCENCE, AND VACUUM-ULTRAVIOLET OPTICAL ABSORPTION

K.Kajihara,[1] M.Hirano[1], M. Uramoto[3], Y. Morimoto[3], L.Skuja, H. Hosono[2]
[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;
[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.
[3]Research and Development Center, Ushio Inc. Bessho-cho, Himeji, Japan

The amount of interstitial oxygen molecules O_2 in amorphous SiO_2 was quantitatively measured by combining thermal-desorption spectroscopy (TDS) with infrared photoluminescence (PL) measurements of interstitial O_2 at 1272 nm while exciting with 1064-nm Nd: yttrium aluminum garnet laser light. It was found that the amount of O_2 released by the TDS measurement is proportional to the intensity decrease of the PL band, demonstrating that a-SiO_2 easily emits interstitial O_2 during thermal annealing in vacuum. This correlation yielded the proportionality coefficient between the absolute concentration of interstitial O_2 and its PL intensity normalized against the intensity of the fundamental Raman bands of a-SiO_2 . This relationship was further used to determine the optical-absorption cross section of the Schumann–Runge band of the interstitial O_2 located at photon energies 6.5 eV. This band is significantly redshifted and has a larger cross section compared to that of O_2 in the gas phase

INTERSTITIAL OXYGEN MOLECULES IN AMORPHOUS SiO_2. II. THE INFLUENCE OF COMMON DOPANTS SiOH, SiF, AND SiCl GROUPS AND FICTIVE TEMPERATURE ON THE DECAY OF SINGLET PHOTOLUMINESCENCE

K.Kajihara,[1] H. Kamioka[1], M.Hirano[1], T. Miura[3], L.Skuja, H. Hosono[2]
[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;
[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.
[3]Extreme Ultraviolet Lithography System Development Association,Hiratsuka, Japan

Time decay of photoluminescence due to interstitial oxygen molecules O_2 in synthetic amorphous SiO_2 (a-SiO_2) was studied by varying the fictive temperature and the concentrations of common dopants, SiOH, SiCl, and SiF groups. The decay constant is insensitive to the fictive temperature, but strongly depends on the type of dopants: it is reduced by the nonradiative decay via an energy transfer from O_2 to the vibrational modes of the dopants. The increases in the non-radiative decay rate due to SiOH, SiF, and SiCl groups are strong, slight, and negligible, respectively, which correlate with their vibrational energies. The quantum yield decreases by 20% as the SiOH content increases from 10^{17} to 10^{20} cm^{-3} . The deviation from the single exponential decay is due to the shape variation in the a-SiO_2 network cages that surround O_2, and to the distance distribution between O_2 and SiOH groups.

INTERSTITIAL OXYGEN MOLECULES IN AMORPHOUS SiO_2. III. . MEASUREMENTS OF DISSOLUTION KINETICS, DIFFUSION COEFFICIENT, AND SOLUBILITY BY INFRARED PHOTOLUMINESCENCE

K.Kajihara,[1] H. Kamioka[1], M.Hirano[1], T. Miura[3], L.Skuja, H. Hosono[2]
[1]Transparent Electro-Active Materials Project, Japan Science and Technology Agency (ERATO-SORST), Nagatsuta, Midori-ku, Yokohama, Japan;
[2]Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama, Japan.
[3]Extreme Ultraviolet Lithography System Development Association,Hiratsuka, Japan

Concentration changes of interstitial oxygen molecules O_2 in amorphous SiO_2 (a-SiO_2) thermally annealed in oxygen atmosphere were examined by the O_2 photoluminescence at 1272 nm excited with 765-nm light of titanium sapphire laser. This highly sensitive technique allows the time- and temperature-dependent concentration changes of interstitial O_2 due to their incorporation from an oxygen atmosphere to be directly measured. The data provide the dissolution rate, the diffusion coefficient, and the solubility of interstitial O_2 in a-SiO_2 and are able to exclude interferences from other forms of mobile oxygen species in a-SiO_2. These observations confirm that O_2 molecules are incorporated into a-SiO_2 without separating into monoatomic species, diffuse in a-SiO_2 without extensive interaction with the a-SiO_2 network, and play a primary role in the thermal oxidation of silicon.

E-BEAM INDUCED DAMAGE IN SiO_2 - GE CRYSTALLINE a-QUARTZ, COMPARISON WITH SILICA GLASS

A.Trukhin, C. Haut[*], A.-S. Jacqueline [*], B. Poumellec[*]
**Physico-Chimie de l'Etat Solide, Bat. 414, Université Paris Sud, Orsay 91405 France*

Electron beam induced transformation in crystalline α-quartz doped with germanium was studied by mean of cathodoluminescence and of phase shift interferometric microscope. E-beams with low current (below 50 nA), defocused (diameter of spot about 40 μm) and with acceleration energy of 15 kV produce swelling of the irradiated volume about 100 nm above the non-irradiated surface. The luminescence of the self-trapped near germanium exciton (GeSTE) is observed mainly. No luminescence of the germanium related oxygen deficient center) with bands at 290 and at 395 nm, usual for Ge-doped silica glass (GeODC), was observed. defocused e-beam with higher current (about 200 nA), the same energy and similar dose, produces depression about 100 nm deep. In this case, we observed the band at 280 nm typical for SiODC in pure silica glass in the same time than the GeSTE already appearing for low current. However, we could not detect the band at 460 nm also typical for SiODC. It was, probably, obscured by the intensive band of GeSTE. We deduced that high density e-beam produces glass-like phase in the irradiated volume of α-quartz exhibiting the luminescence characteristic of pure silica glass. We explain, the absence of both bands related to GeODC in glass-like phase by a disappearance of germanium from this phase under irradiation. 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.

THE USE OF X-RAY INDUCED AND THERMOSTIMULATED LUMINESCENCE FOR OPTIMIZING THERMAL POLING OF PRE-X-RAY IRRADIATED SILICA GLASSES

Raphael Blum[1], Anatolijs Truhins, Bertrand Poumellec[1], Suling Zhao[1]
[1]Physico-Chimie de l'Etat Solide, Bat. 414, Université Paris Sud, Orsay 91405 France

The increase of the worldwide needs for communication and fiber optics have created a need for silica glass optical components such as modulators and switches. But the modulation and switching of light proved to be a difficult task to perform in silica glass systems due to their low optical nonlinearity. However, poled silica glass exhibits a linear electro-optic effect that can be used for the modulation and switching of light.
The nonlinearity of silica glasses is produced with poling techniques such as thermal poling, corona poling, electron beam (EB) poling, and UV-excited poling. For this paper, we used a new method to pole silica glasses by mean of the conjugate action of x-ray irradiation and high external electric field which results in the charge migration in materials. In order to understand the charge trapping mechanism in x-ray poling and hence of the building of internal electric field, we studied the x-ray induced luminescence (XRL, during x-ray irradiation), afterglow (after x-ray was shut off) and thermostimulated luminescence (TSL). TSL experiments were carried out on a 1mm thick suprasil sample in a vacuum chamber specially designed to allow X-ray irradiation or poling, and simultaneous temperature and luminescence measurement. An external electric field of 1.5 kV was applied for poling. The typical TSL curve for an x-ray irradiated sample presents two peaks centered at 90 and 280 ^{o}C respectively. The relative intensity of these two peaks is x-ray dose dependant differently, therefore corresponding traps are independent. The external electric field enhances the XRL, but no effect on the afterglow. The TSL and afterglow spectrum are similar with XRL spectrum and contains the bands at 3.25 eV and 4.25eV. That shows on existence of only one type of recombination center with spectral content witnessing GeODC or the twofold-coordinated germanium center in silica incorporated into different types of clusters. The UV band at high temperature is thermally quenched already in intracenter photoluminescence, therefore it could be observed only in low temperature TSL peak. The XRL intensity exhibits dose dependence depending on thermal treatment prehistory supporting assumption of different clusters existence. Both charge carriers are trapping within clusters and therefore no electric field influence on afterglow.

RAMAN AND OPTICAL REFLECTION SPECTRA OF GERMANATE AND SILICATE GLASSES

A.Trukhin, B. Capoen[1]
[1]Laboratoire de Physique des Lasers, Université des Sciences et Technologies de Lille, France

Pure, made in oxygen surplus conditions germanate and phosphosilicate glasses were studied by Raman and optical reflection methods. We found that the optical reflection spectra of germanate glasses are quite similar to the one of a GeO_2 crystal with the α-quartz structure. The reflection of phosphosilicate glasses is very close to the silica glass-related spectra. Hence, the determining influence of the tetrahedral structure on reflection spectra is revealed. The Raman spectra of germanate samples are rather similar to the one known in the literature. Octahedral entities, namely bands similar to stishovite vibration modes, were difficult to detect in phosphosilicate glasses through Raman spectroscopy.

HOST-DEFECT LUMINESCENCE OF STISHOVITE

A. Trukhin, P. Kulis, J. Jansons, T. Dyuzheva[1], L. Lityagina[1], N. Bendeliani[1]
[1]F.Verechshagin Institute of High pressure Physics of RAS, Troitsk, Russia

A detailed study of the 4.75 eV luminescence band of stishovite single crystal (SiO_2 with rutile structure) is reported. Kinetics of luminescence intensity is studied at durable (tens of minutes) X-ray excitation. The observed behaviour of the band intensity is explained by creation and destruction of luminescence centres depending on temperature both being determined by radiation stimulated diffusion of atomic particles. The luminescence decay is observed to last for minutes after X-ray irradiation while only for ns and hundreds of μs under pulsed e-beam irradiation suggesting a complicated recombination of the created defects. The UV band of stishovite is compared with the 4.9 eV luminescence band in α-quartz, which could not be created by x-ray. The latter being associated with transient centres created by destructive electron-beam irradiation or with permanent centres at neutron or γ-irradiation, and with oxygen-deficient luminescence of silica glass.

LUMINESCENCE OF GeO_2 GLASS, RUTILE-LIKE AND a-QUARTZ-LIKE CRYSTALS

A. Trukhin, M. Kink[1], Y. Maksimov[1], J.Jansons, R. Kink[1]
[1]Institute of Physics, University of Tartu, Estonia

The luminescence of GeO_2 rutile-like crystals was studied. Crystals were grown from melt of germanium dioxide and sodium bicarbonate mixture. Luminescence of the crystal was compared with that of sodium germanate glasses produced in reduced and oxidised conditions. A luminescence band at 2.3 eV was observed under N_2 laser (337 nm). At higher excitation photon energies and x-ray excitation an additional band at 3 eV appears in luminescence. The band at 2.3 eV possesses intra-center decay time constant about 100 μs at 290 K and about 200 μs at low temperature. Analogous luminescence was obtained in reduced sodium germanate glasses. No luminescence was observed in oxidised glasses under nitrogen laser, therefore the luminescence of rutile-like crystal and reduced sodium germanate glass was ascribed to oxygen deficient luminescence center modified by sodium. The band at 2.3 eV could be ascribed to triplet-singlet transition of this center, whereas the band at 3 eV, possessing decay about 0.2 μs, could be ascribed to singlet-singlet transitions. Both bands could be excited in recombination process with decay kinetics determined by traps, when excitation realised by ArF laser or ionising irradiation with x-ray or electron beam. Another luminescence band at 3.9 eV in GeO_2 rutile-like crystal was obtained under ArF laser in the range 100 – 15 K. Damaging e-beam irradiation of GeO_2 crystal with α-quartz structure induces similar luminescence band.

ENERGY TRANSPORT IN a-QUARTZ CRYSTAL AT 10 K

A.N. Trukhin, V.Kisand[1], R. Kink[1], I. Kink[1]
[1] Institute of Physics, University of Tartu, Estonia

Optical reflectivity, photoluminescence as well as excitation spectra of crystalline α-quartz were studied with the use of synchrotron radiation at 10 K for the first time. The samples were synthetic crystal nominally pure, germanium doped and natural crystal - morion. It was found, as previously, that the first excitonic absorption band at 10.5 eV is sensitive to temperature and it becomes sharper and shifts towards higher energy when cooling from 293 K to 10 K. However, relative changes are very small relatively to bands' width being very wide (~1 eV). Energy transport efficiency was studied using its sensitivity to the absorption rate. Different luminescence centers were used as detectors

of electronic excitations. The luminescence of the self-trapped exciton, germanium and aluminum related centers in crystal were studied. The main feature, witnessing that energy absorbed by the host material is transported to the luminescence center, is observation of a quantum yield decrease in the range of intensive absorption bands, showing competition between migration of the electronic excitation to detector and their radiation-less annihilation on the surface. The result of this work shows that the transport of electronic excitation is not frozen when the samples are cooled to 10 K. It is in good agreement with previous study of energy transport in α-quartz in shorter spectral range at higher temperatures. The energy transport spectrum was simulated from absorption spectrum and compared with experimentally measured one. The comparison reveals that strong increases of energy transport efficiency above 22 eV could not be explained by excitation light penetration depth only. It is proposed that this increase in efficiency could be explained by several factors. One is multiplication of the electronic excitations when photon energy exceeds the double energy gap. The E_g is estimated about 11 eV, being much higher than it is accepted in literature. Another factor of strong efficiency increase could be manifestation of a gap between upper valence band created by so called "non-bonding" p orbital of oxygen and valence band corresponding to "bonding orbital" of silicon dioxide.

Scientific Publications

Published in 2005

1. D.Millers, L.Grigorjerva, W.Lojkowski and A.Opalinska· Luminescence of ZrO_2 nanocrystals. Solid State Phenomena. From Nanopowders to Functional Materials. Trans Tech Publications,vol.106, 2005, p.103-107.
2. S.Chernov, D.Millers, L.Grigorjeva. Formation of luminescence centers under excitation with electron beams in $PbWO_4$ and $ZnWO_4$ crystals. Phys.Stat. Sol. (c), vol.2, No.1, p.85-88, 2005.
3. P.Potera, A.Matkovskii, L.Grigorjeva, D.Millers, T.Lukasiewicz, Z.Galazka. Transient color centers in complex oxide crystals. Ibid, p.163-166.
4. D.Millers, L.Grigorjeva, V.Trepakov, S.E.Kapphan, L.A.Boatner. X-ray and pulsed electron beam excited luminescence and optical absorption in $KTaO_3$ crystals. Ibid.p.200-203.
5. T.Dudareva, L.Grigorjeva, D.Millers. Radiation defects in undoped and Nd-doped $LaGaO_3$ crystals. Ibid, p.264-267.
6. V.Pankratov, MT.Kirm, H.von Seggern. Exciton emission and defect formation in yttrium trifluoride. Ibid, p.371-374.
7. V.Pankratov, M.Kirm, H.von Seggern. Intrinsic luminescence in yttrium trifluoride. J.Lumin., vol.113, p. 143-150, 2005.
8. L.Grigorjeva, D.Millers, V.Pankratov. Polaron state characterization in $LiNbO_3$ crystals by means of time-resolved absorption spectroscopy. In Technical digest "Lithium niobate from materials to device, from device to system", p. 95-96, Metz, 2005.
9. L.Skuja, M.Hirano, H.Hosono, K.Kajihara, Defects in Oxide Glasses. phys. stat. sol. (c) vol. 2, No. 1, p. 15 –24 (2005)
10. 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).
11. K. Kajihara, M.Hirano, M. Uramoto, Y. Morimoto, L. Skuja, H. Hosono, Interstitial oxygen molecules in amorphous SiO_2. I. Quantitative concentration analysis by thermal desorption, infrared photoluminescence, and vacuum-ultraviolet optical absorption. J.Appl.Phys. v.98, p.013527(1-6) (2005).

12. K. Kajihara, H. Kamioka, M. Hirano, T. Miura, L. Skuja, H. Hosono, Interstitial oxygen molecules in amorphous SiO_2 . II. The influence of common dopants (SiOH, SiF, and SiCl groups) and fictive temperature on the decay of singlet photoluminescence. J. Appl.Phys. v.98, p.013528(1-5) (2005).
13. K. Kajihara, H. Kamioka, M. Hirano, T. Miura, L. Skuja, H. Hosono, Interstitial oxygen molecules in amorphous SiO_2 . III. Measurements of dissolution kinetics, diffusion coefficient, and solubility by infrared photoluminescence. J. Appl.Phys. v.98, p.013529(1-7) (2005).
14. K.Kajihara, M.Hirano, L.Skuja, H. Hosono, Reactions of SiCl groups in amorphous SiO_2 with mobile interstitial chemical species: Formation of interstitial Cl_2 and HCl molecules, and role of interstitial H_2O molecules. J. Appl. Physics v.98, p.043515-(1-9) (2005).
15. K.Kajihara, M.Hirano, L.Skuja, H. Hosono, Vacuum-ultraviolet absorption of hydrogenated and deuterated silanol groups and interstitial water molecules in amorphous SiO_2. Phys. Rev. v. B72, p.214112 (1-4) (2005).
16. A.Trukhin, P. Kulis, J. Jansons, T. Dyuzheva, L. Lityagina and N. Bendeliani, Host-defect luminescence of stishovite, phys. stat. sol. (c) 2, No. 1, 584 –587 (2005)
17. A.Trukhin, C. Haut, A.-S. Jacqueline, B. Poumellec, E-beam induced damage in SiO_2 - Ge crystalline α-quartz, comparison with silica glass, Journal of Non-Crystalline Solids, 351/30-32(2005) pp. 2481-2484.
18. A.Trukhin, and B. Capoen Raman and optical reflection spectra of germanate and silicate glasses, Journal of Non-Crystalline Solids 351, (2005) 3640-3643.

Lectures in Conferences

21th Scientific Conference dedicated to the International Year of Physics, Institute of Solid State Physics, University of Latvia, February 7-9, 2005, Riga, Latvia.

1. V.Pankratov. Phosphors for dielectric barrier discharge excimer lamps. Abstracts, p.16.
2. S.Chernov, D.Millers, L.Grigorjeva. Influence of Iron Impurities on $ZnWO_4$ scintillation pulse parameters. Ibid, p.17 (oral).
3. T.Dudareva. Spectral and kinetic properties of YVO_4 and YVO_4;Nd crystals. Ibid, p.18 (oral).
4. B.Polyakov, B.Daly, J.Prikulis, L.Grigorjeva, D.Millers, J.Holmes, D.Erts. Conductive and photoconductive properties of Ge nanowires in anodic aluminium oxide membranes. Ibid, p.35 (oral).
5. K.Smits, D.Milers, L.Grigorjeva. Time-resolved luminescence of ZrO2 nanocrystals (the structure and dopand effects). Ibid, p.40 (oral)
6. Anatoly Trukhin, Janis Jansons, SiO_2-rutile-like crystals UV luminescence: comparison with luminescence of α-quartz, Ibid. p.7 (oral).

The 15 international conference on vacuum ultraviolet spectroscopy and radiation interaction with condensed matter (VUVS 2005, Irkutsk, Russia, July 2005)

A.N. Trukhin, V.Kisand, R. Kink, I. Kink Energy transport in α-quartz crystal at 10 K, Book of Abstract International Conference on Vacuum Ultraviolet and radiation interaction with condensed matter, p.58. (oral).

International student conference on Development in Optics and Photonics, DOP-2005, 30 April - 1 May, 2005, Riga.

1. T.Dudareva. Optical absorption and luminescence in Nd doped oxides.
2. K.Smits. Luminescence of pure and doped ZrO_2 nanocrystals.

3. M.Shorohov. Application of luminescence and absorption methods for TlBr detectors material testing.
4. A.Kalinko. Software for data processing of the time–resolved solid state optical properties.

XII Portuguese Material Society Meeting, III International Materials Symposium (MATERIALS 2005), 20-23 March, 2005, Aveiro, Porugal.

1. D.Millers, L.Grigorjeva, V.Pankratov. Transient absorption and luminescence of polaron states in complex oxide crystals. Book of abstracts, p. 111.
2. L.Grigorjeva, D.Millers. Luminescence and FTIR spectroscopy of ZnO nanocrystals. Ibid, p.260.

First Latvian Conference "Nanomaterials and nanotehnologies", 30-31 March, 2005, Riga, Latvia.

1. D.Millers, L.Grigorjeva, K.Smits. ZrO_2 nanocrystals for oxygen sensors. Proceedings, p.117(oral).

International workshop "Lithium niobate from materials to device, from device to system", 23-25 May, 2005, Metz, France.

1. L.Grigorjeva, D.Millers, V.Pankratov. Polaron state characterization in $LiNbO_3$ crystals by means of time-resolved absorption spectroscopy.

International conference on luminescence ICL'05 Beijing, China, July 2005

R. Blum, A. Truhins, B. Poumellec, Suling Zhao, The Use of X-ray Induced and Thermostimulated Luminescence for Optimizing Thermal Poling of Pre-x-ray Irradiated Silica Glasses, book of abstract, p. 69. (oral).

European Material Reserch Society Fall Meeting (E-MRS 2005), 5-7 September, 2005, Warsaw, Poland.

1. D.Millers, L.Grigorjeva, K.Smits, W.Lojkowski, A.Opalinska. Yttria stabilized zirconia nanocrystals luminescence. Book of abstracts, p.229 (oral).
2. L.Grigorjeva, D.Millers, A.Kuzmin, R.Kalendarev, W.Lojkowski, A.Tomaszewska-Grzeda. Time-resolved luminescence of nanostructured ZnO. Ibid, p.229 (oral).

International Conference on Inorganic Scintillators and their Industrial Application (SCINT2005), 19-23 September, 2005, Alushta, Ukraine.

1. S.Chernov, L.Grigorjeva, D.Millers, V.Pankratov. Luminescence center formation under pulse electron beam excitation in $CaWO_4$ crystal. Book of abstracts, p.50.
2. L.Grigorjeva, D.Millers, V.Pankratov, L.Vilciauskas, A.Kareiva, A.Katelnikovas. Time-resolved luminescence studies for the sol-gel prepared $CaWO_4$. Ibid, p.51.
3. V.Pankratov, D.Millers, L.Grigorjeva, W.Lojkowski, R.Fedjuk, T.Chudoba, W.Strek, D.Hreniak, P.Mazur. Intrinsic Luminescence of pure and doped YAG nanopowders. Ibid, p.117 (oral).

First Conference on Advances in Optical Materials AIOM-2005, Tucson, Arizona, U.S.A., Oct.12-15, 2005

1. L.Skuja, K. Kajihara, M.Hirano, A.Saitoh, H.Hosono, An increased F_2 laser damage in "wet" silica glass due to atomic hydrogen: a new hydrogen-related E'-center. Abstract O1 (oral).
2. K. Kajihara, M.Hirano, L.Skuja, H.Hosono, Vacuum-ultraviolet optical absorption of interstitial O_2 and H_2O molecules in SiO_2 glass. Abstract O2 (oral).

3. K. Kajihara, M.Hirano, L.Skuja, H.Hosono, Temperature dependence of infrared and vacuum-ultraviolet optical absorptions of SiOH groups in SiO_2 glass. Abstract O3 (oral).

Popular scientific articles

A. Siliņš "Gaismas akumulatori", Enerģija un pasaule, 2005, Nr.1,
64-67.lpp. (A.Silin, "Accumulators of light", in Latvian popular science journal).

PHYSICS OF FERROELECTRICS

Head of Division Dr. hab. phys. Andris Sternberg

Research Area

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

Main research topics in 2005

Toward Critical Dynamics of Ferroelectrics: Diffusion Approach

Synthesis of Ferroelectric Ceramics and Investigation of Microstructure

- New Ceramic Compositions Based on $PbSc_{1/2}Nb_{1/2}O_3 - PbLu_{1/2}Nb_{1/2}O_3$ System;
- Investigation of Lead Contaning Rare-Earth Niobates;
- 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 and Roughness Effects on Optical Properties of PST and PMNT Thin Films;
- Optical Constants of PST and PMNT Thin Films in 200-1200 nm Range

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

- Passive and Active Light Scattering Obstacles Used for Simulation of Vision Pathologies;
- Dynamics Of Eye Aberration Detected By High-Speed Hartmann-Shack Aberrometer;
- Application of PLZT and PDLC Passive and Active Optical Elements in Infrared Laser Systems for Bio-Optical Experiments and Medicine.

Scientific staff

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

Technical staff

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

Doctorants

1. Mg. phys. Ilze Aulika
2. Mg. phys. Romans Krutohvostovs

Students

1. Reinis Arajs
2. Marija Dunce
3. Martins Granats
4. Eriks Klotins (junior)
4. Ainars Kuznecovs
5. Peteris Spels

Visitors from Abroad

1. Linas Vilčiauskas, University of Vilnius (3 months).

Scientific Visits Abroad

Mg. sc. **Maija Antonova**

1. International Conference “Modern Aspects of Solid State Physics”, Minsk, Belorussia, October (1 week).

Mg. sc. **Ilze Aulika**

1. Experimental Physics, University of Vienna, Vienna, Austria, February–March (1 month).
2. Institute of Physics, Academy of Sciences of the Czech Republic, Prague, May–June (1 month).
3. University of Oulu, Finland, September–December (4 months).
4. “Winter-School on Piezoelectric”, Chateau-d’Oex, Switzerland, February (1 week).

Dr. phys. **Karlis Bormanis**

1. XVII Всероссийская конференция по физике сегнетоэлектриков (ВКС-XVII-2005), Пенза: Пенз. Гос. Ун-т, Россия, июнь-июль (1 week).
2. International Conference “Modern Aspects of Solid State Physics”, Minsk, Belorussia, October (1 week).

Mg.phys. **Laila Chakare** - Samardžija

1. Jozef Stefan Institute, Univ. of Ljubljana (11 months)

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

1. International Conference "Modern Aspects of Solid State Physics", Minsk, Belorussia, October (1 week).

Mg. chem. **Anna Kalvane**

1. International Conference "Modern Aspects of Solid State Physics", Minsk, Belorussia, October (1 week).

Dr. phys**. Eriks Klotins**

1. III International Material Symposium, Aveiro, Portugal, March (1 week).
2. Colloquium 468, APM – 2005 / EUROMEH, St. Petersburg, Russia, June-July (10 days).
3. 3rd NEXT Sigma Phy International Conference, Greece, August (1 week).
4. 11-th International Meeting on Ferroelectricity, Iguassu Falls, Argentine/Brazil, September (1 week).
5. 94th Statistic Mechanics Conference, Piscataway, New Jersey, USA (1 week).

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

1. Institute of Physics, University of Tartu, Tartu, Estonia (1 week).
2. International Exhibition "Hanover Messe", Hanover, Germany (1 week).

Mg. sc. **Karlis Kundzins**

1. ESRF Grenoble, France, November (3days).
2. Centre de Recherche de la Matiere Condensee et des Nanosciences (CRMC-N) Luminy, Marseilles, France, December (10 days).

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

1. Conference on Education and Training in Optics and Photonics, ETOP-2005, Marseille (1 week).
2. The 18th Symposium of the International Colour Vision Society, Lyon, France (1 week).
3. European Conference on Visual Perception, A Coruña, Spain (1 week).
4. Conference on Optical Complex Sytems, OCS-2005, Marseille (1 week).

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

1. 11-th International Meeting on Ferroelectricity, Iguassu Falls, Argentine/Brazil, September (1 week).
2. 7-th International Summer School-Conference "Advanced Materials and Technologies", Palanga, Lithuania, August (1 week).
3. International Symposium Micro- and Nano-Scale Domain Structuring in Ferroelectrics, Ural State University, Ekaterinburg, Russia, November (1 week).
4. WTZ-Meeting Praha-Ljubljana-Wien-Budapest "Dynamics of Complex Systems", Vienna, October (1 week).
5. Institute of Physics, University of Tartu, Tartu, Estonia (1 week).
6. IX Conference &Exhibition of the European Ceramic Society, Portorož, Slovenia, June (1 week).

Dr.phys. **Marina Tjunina**

1. University of Oulu, Finland (11 months)

Dr. phys. **Vismants Zauls**

3. "Winter-School on Piezoelectric", Chateau-d'Oex, Switzerland, February (1 week).
4. Experimental Physics, University of Vienna, Vienna, Austria, February (1 week).
5. Institute of Physics, Academy of Sciences of the Czech Republic, Prague, February (2 days).
6. ESRF Grenoble, France, November (3days).
7. Centre de Recherche de la Matiere Condensee et des Nanosciences (CRMC-N) Luminy, Marseilles, France, December (10 days).

Cooperation

Latvia

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

Austria

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

Belorussia

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

Czech Republic

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

Denmark

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

Estonia

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

Finland

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

Italy

1. Department of Material Engineering & Industrial Technology, University of Trento (Prof. Paolo Skardi, Dr. Matteo Leoni).

Japan

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

Lithuania

1. Vilnius University, Vilnius (Prof. J.Grigas, Prof. J. Banys, Prof. A. Kareiva).

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).
4. X-ray group of Institute of Organic Chemistry, Polish Academy of Sciences (Dr Z. Lipkowska).

Portugal

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

Russia

1. Ural State University, Ekaterinburg (Prof. V. Shur).
2. Volgograd State Architectural and Engineering Academy, Volgograd (Dr. phys. A. Burkhanov).
3. Joint Institute for Nuclear Research, Dubna (Dr. S. Tiutiunnikov, Dr. V.V. Jefimov).
4. Institute of Chemistry and Technology of Rare Elements and Minerals, Apatity (Prof. N.V. Sidorov).

Slovenia

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

Spain

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

Ukraina

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

Expert referees

Anatolijs Mishnovs – expert referee of Journal “Acta Crystallographica, Sec. D” (editor Z.Dauter).

Andris Sternberg - expert referee of Journal “Ferroelectrics”;
- expert referee of Journal “Materials Letters”.

Main Results

ANTIFERROELECTRICS OF LEAD CONTAINING RARE-EARTH NIOBATES AND SOLID SOLUTIONS ON THEIR BASES

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

The physical characteristics of compounds with chemical formula $Pb(B'_{1/2}B''_{1/2})O_3$ ($B'= Fe^{3+}$, In^{3+}, Sc^{3+}, Lu^{3+}, Yb^{3+}, Tm^{3+} etc., $B''= Nb^{5+}$, Ta^{5+}) have been of interest due to different types of phase transition. With the degree of order between

the B-site cations in the perovskites, diffuse phase transitions or sharp ones are frequently observed in these compounds.

The purpose of the present study is as follows: 1) producing and investigating properties of little studied antiferroelectrics of $PbB'_{1/2}Nb_{1/2}O_3$, where B' – rare earth ions (Lu^{3+}, Yb^{3+}, Tm^{3+}, Er^{3+}, Ho^{3+}, etc.); 2) investigation of possibility of producing binary solid solutions of antiferroelectrics with $PbSc_{1/2}Nb_{1/2}O_3$ (PSN); 3) producing ceramic samples of high density and single phase perovskite structure, studying the microstructure of ceramics and measuring dielectric and ferroelectric properties.

The data of X-ray diffraction and differential thermal analysis (DTA) were used to select conditions for solid phase synthesis of the pure compounds and solid solutions. The effect of technological factors on the synthesis of $PbB'B''O_3$ compounds and solid solutions were studied: 1) by varying the temperature, soaking time and over-stoichiometric amount of PbO and B'_2O_3 of traditional solid phase reaction; 2) by using two-stage wolframite ($B'NbO_4$) route, the so called Swartz – Shrout method, and 3) by applying carbonates and carbonates hydroxides as B'_2O_3 source. The calcination temperature was about 900 ^{0}C for 2 – 4 h. Ceramic samples were hot pressed under the pressure of 20 MPa during 1 – 4 h, the temperature being adjusted within the 1050 – 1200^{0}C, depending on the composition.

The antiferroelectrics belong to a subgroup of complex perovskites with a highly ordered arrangement of B-site cations. They undergo a ferroelectric - antiferroelectric phase transition within 250 - 300 ^{0}C intervals. Solid solutions $xPbB'_{1/2}Nb_{1/2}O_3$ – $(1-x)PbSc_{1/2}Nb_{1/2}O_3$ have morphotropic phase region extending over the x = 0.5 – 0.6 interval. The value of dielectric permittivity of solid solutions decrease rapidly with the concentration of antiferroelectrics. The investigation of $PbB'_{1/2}Nb_{1/2}O_3$, (where B'- Ho^{3+}, Tb^{3+}, Gd^{3+}, Eu^{3+}, Sm^{3+}) showed a failure of the synthesis. The nearly dense packing of the crystallographic structure in $PbB_{1/2}Nb_{1/2}O_3$ accounts the geometric peculiarities in the composition range B = Lu, Er, Ho, Tb, Gd, Eu, Sm causing a gradual "hardening" of parameters of synthesis in the compositions. The gradually decreasing low values of tolerance factors (t=0.83; 0.82; 0.81 etc.) became critical for the perovskite structure revealing a remarkable B-O bonds strain in BO_6 octahedra and perovskite structure become thermodynamically unstable. The metastable perovskite phases of compounds $PbB_{1/2}Nb_{1/2}O_3$ (B = Tb, Gd, Eu, Sm) were firstly obtained under high pressures at high temperatures, and their stability at atmospheric pressure were limited [1].

References

[1] A.N.Salak, A.D.Shilin, M.V.Bushinski, N.M.Olekhnovich, N.P.Yyshatko. Structural regularities and dielectric phenomena in the compound series $PbB^{3+}{}_{1/2}Nb_{1/2}O_3$. Materials Research Bulletin, 2000, 35, pp.1429 – 1438.

INFLUENCE OF AXIAL PRESSURE ON ELECTRIC PROPERTIES OF PluN AND 0.6PLuN-0.4PSN CERAMICS

J. Suchanicz[1], M. Dambekalne, A. Sternberg, B. Garbarz-Glos[1], W. Smiga[1], K. Konieczny[1], and Cz. Kus[1]

[1] *Institute of Physics, Pedagogical Academy, Krakow, Poland*

Lead-based ferroelectric materials have been intensively studied due to their great technical importance. In this group of materials, $PbLu_{0.5}Nb_{0.5}O_3$ (PLuN) and PLuN-based solid solutions are promising compounds for active elements in different devices. As the hysteresis in field-polarization and field-strain limits the application of ferroelectric ceramics, it is important to know how combined electric and stress fields can effect the properties of the material. The present paper, being the continuation of investigations started in [1], reports the studies in which the axial pressure influence on

electric properties of PLuN and 0.6PLuN-0.4PSN compounds have been checked.

PLuN and PSN have antiferroelectric and ferroelectric order, respectively. Powder of pure PLuN was synthesized by two-stage calcination via wolframite $LuNbO_4$ at 1250 ^{0}C for 1h, the second stage-reaction between PbO and $LuNbO_4$ at 800 ^{0}C for 2h. Ceramic samples were sintered by hot pressing. Details connected with samples preparation are in reference [1]. Ceramic samples have a high density (96-98% of the theoretical value), a low total porosity (less than 1.0%), and negligible water absorption (about 0.02%).

The Hitachi S-4700 scanning electron microscope (SEM) suitable for X-ray energy dispersion spectroscopy (EDS) with Si(Li) X-ray detector was used for the investigation of the microstructure of ceramics. The microanalysis was performed with the Noran-Vantage system. X-ray diffraction measurements were performed by DRON-UM1 diffractometer with Co K_α - radiation and Feβ filter. The powdered ceramics were investigated.

The weak field (3V/cm) dielectric measurements were made using HP 4284A LCR meter for the frequency range 20Hz to 1MHz and for the temperature range from 30 ^{0}C to 350 ^{0}C. Axial pressure was applied parallel to measuring electric field with the use of lever and a weight within the range 0-1.5 kbar. The remanent and spontaneous polarizations were obtained from pyroelectric and from current loops measurements, respectively. Pyroelectric measurements were performed in quasistatic method on heating.

Microstructure investigations show that PLuN and 0.6PLuN-0.4PSN ceramics have average grain sizes 1μm and 1.5μm, respectively. The example of EDS analysis, obtained for one of the grain indicated a homogeneous distribution of all the native elements of the ceramics within the grains.

The X-ray diffraction study shows that the obtained samples have single phase of perovskite-type structure with rhombohedral and pseudomonoclinic symmetry for 0.6PLuN-0.4PSN and for PLuN, respectively. The unit cell parameters are: a= 4.1223Å, α=89.98° and a=c=4.1450Å, b=4.1120Å, β=90.52° for 0.6PLuN-0.4PSN and for PLuN, respectively.

Figure1. shows the temperature/pressure variation of the dielectric permittivity ε for PLuN and 0.6PLuN-0.4PSN, respectively. As it can be seen from Fig.1, after rapid increase of ε, broad maximum at about 275°C can be observed. Axial pressure shifts these both anomalies to higher temperature (~19 ^{0}C/kbar). Another effect of pressure application is a reduction of thermal hysteresis of dielectric permittivity (insert in Fig.1). This means that character of the transition seems to change to that of the second order.

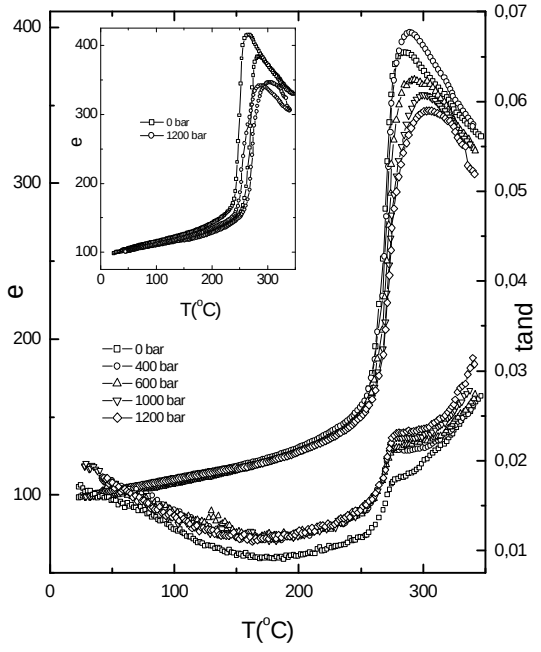


Figure 1. Tempereture dependence of ε and tanδ of PLuN ceramic (on heating, f=10kHz) at various axial pressure.

Dense ceramic samples of PLuN and 0.6PLuN-0.4PSN with very good mechanical properties have been prepared. The dielectric (for both materials), pyroelectric and hysteresis loops (for 0.6PLuN-0.4PSN) measure-ments in the stress-free state or under stress have been performed. It was found, that 0.6PLuN-0.4PSN ceramic has ferroelectric-ferroelectric phase transition at about 100°C and polar regions can exist at temperatures above

T_m. The main effect of axial pressure is the shifts of the T_m, the decrease of the polarization and the reduction of thermal hysteresis of electric permittivity. This influence can be mainly connected with domain walls moving and with switching of the polarization under action of axial pressure. The possibility of alteration of properties of the investigated materials by axial pressure can be utilized for device application.

References

[1] J.Suchanich, M.Dambekalne, L.Shebanovs, A.Sternberg, B.Garbarz-Glos, W.Smiga, Cz.Kus. Effect of Compressive Stress on Dielectric and Ferroelectric Properties of 0.25 PSN – 0.75 PLuN Ceramics. Ferroelectrics, 2003, Vol. 289, pp. 53-60.

TOWARD CRITICAL DYNAMICS OF FERROELECTRICS: DIFFUSION APPROACH

E. Klotins

Developments in microscopic size structures crucially depend on solution of conceptual and technical problems which encounter if going from the conventional thermodynamic description of homogeneous, infinite systems to the time evolution of microscopic scale objects. Reconciling the macroscopic and microscopic scale description has become a central issue in physics during the last decades.

Application of some of its essential results to ferroelectric based systems yields the diffusion (Fokker-Planck) approach for the model Hamiltonian constituted of microscopically large/ macroscopically small blocks each of which exhibiting metastability and ergodicity breaking. This basic research is focused on critical kinetics of ferroelectrics as initiated by attractive interaction between adjacent blocks and the impact of thermal bath. The mathematical technique is definitely nonstandard and is supported by original codes based on symplectic integration technique.

In spite of its simplicity and the Boltzmann-Gibbs axiomatic level, the diffusion approach displays fine details of polarization/electroelastic response at arbitrary driving and boundary conditions. Its extension toward quantum-statistical description of a block is a highly motivated and challenging future problem.

STUDY OF RELAXOR FERROELECTRIC THIN FILMS BY MICRO-RAMAN AND FAR INFRARED SPECTROSCOPY

I. Aulika

Relaxor ferroelectric thin films of $PbSc_{1/2}Ta_{1/2}O_3$ (PST) of various order (Disordered, annealed at 700 ^{0}C for 1 min, slightly ordered, annealed at 850 ^{0}C for 1 min, 50% ordered, annealed at 850 ^{0}C for 1 hour) at the perovskite B-sites prepared at EPFL Lausanne by chemical solution deposition on Al_20_3 (0001) substrates and $PbMg_{1/3}Ta_{2/3}O_3$ (PMT) and solid solution of $PbMg_{1/3}Nb_{2/3}O_3$ with $PbTiO_3$ (PMNT) prepared by pulse laser deposition on Mg0 (001) single crystal substrates at the University Oulu were investigated. The following measurements were performed in the Department of Dielectrics: 1) Temperature dependence of micro-Raman spectroscopy using RENISHAW spectrometer (10-800 K); 2) Transmission far infrared spectroscopy using BRUKER IFS 113v Fourier transform spectrometer (10-800 K). These measurements gave a possibility to study the ferroelectric soft mode behavior, which is known to be very sensitive to the film strains, granularity and other defects. Relation with the dielectric constant and with the behavior in bulk samples was discussed. Complementary spectral ellipsometric measurements using the spectral ellipsometer J.A. WOOLLAM (wide spectral range 193 nm to 2200 nm) in the Department of Multilayer

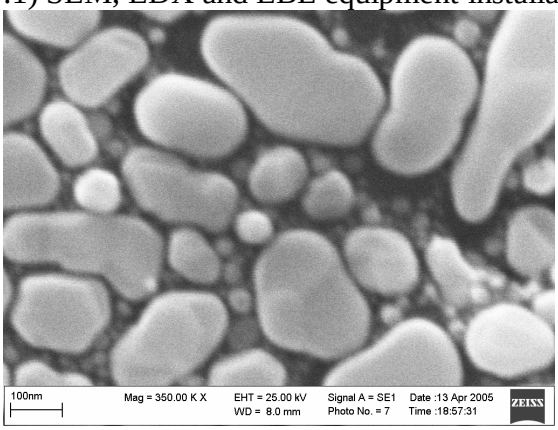
Structures was performed to determine the film thickness and homogeneity. The difference in Raman spectrum has been obtained for the ordered and disordered PST films. The in intensities of the peeks and the frequency of Raman shift increases with increasing of B-site ordering. The new mode has been detected for PMT film which can be related to second phase attendance in the film. These measurements gave possibility to study the ferroelectric soft mode behaviour, which is known to be very sensitive to the film strains, granularity and other defects. Relation with the dielectric constant and with the behaviour in bulk samples will be discussed. With spectral ellipsometry measurements the film thickness, optical properties at the spectrum range from 500 nm till 800 nm, and surface roughness have been determined.

SCANNING ELECTRON BEAM MICROSCOPY

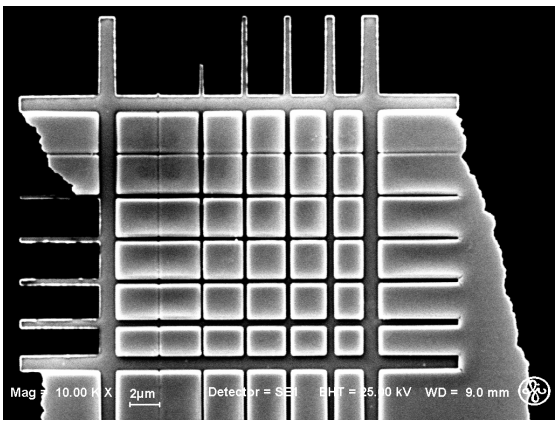
R. Krutohvostovs, K. Kundzins, I.Shorubalko, and M.Dunce

The Scanning Electron beam Microscope (SEM) has been installed in our laboratory serving as a reseach technique for imaging of surfaces and material characterization. The main characteristics of Carl Zeiss model EVO 50 XVP microscope include possibility to inspect samples in both: low and high vacuum modes with magnification from 5x to 1.000.000x; acceleration voltage range from 0.2 kV to 30 kV and adjustable beam current in range from 0.5 pA to 5 mA. The instrument is equiped with energy dispersive X-ray (EDX) detector (Oxford Instruments INCA 350) and Electron Beam Lithography EBL option (Raith ELPHY Quantum). Some example applications are illustrated in figures below indicating collaborations with other research teams.

.1) SEM, EDX and EBL equipment installation and calibration

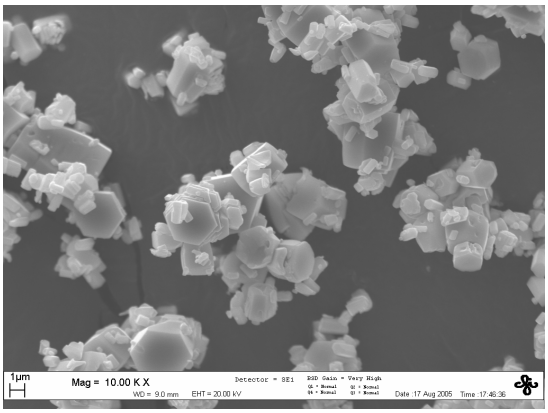


Gold particles on carbon substrate

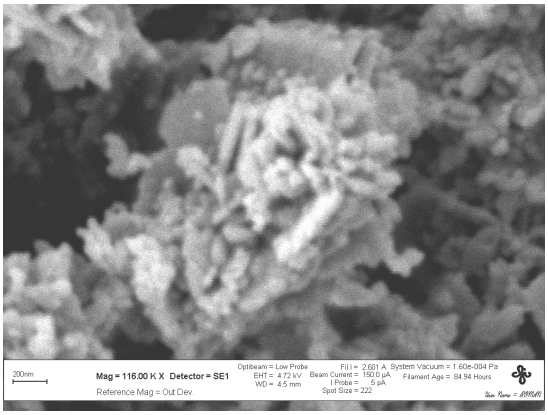


Example of e-beam lithography resolution test – patterned resist on silicon substrate metallized with gold/palladium sputter coating

2) Comparison of Zinc oxide (ZnO) macro- and nanopowder particles - size measurements (in collaboration with Solid State Radiation Physics laboratory)

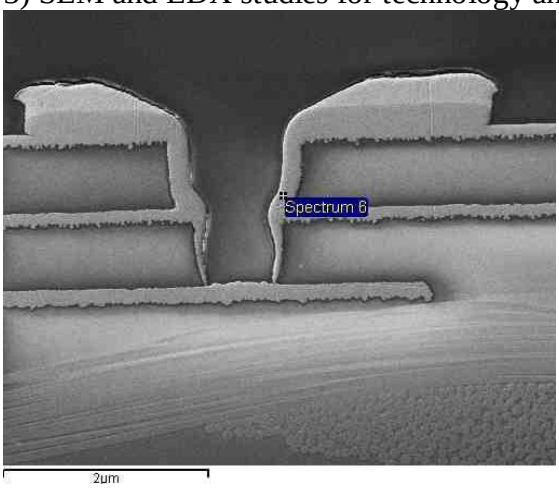


Zinc oxide macropowder

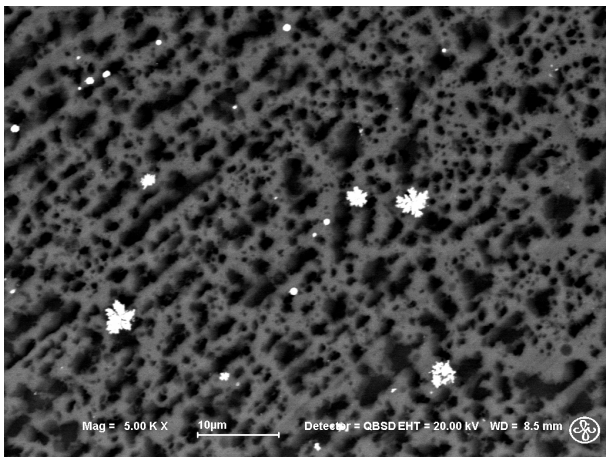


Zinc oxide nanopowder

3) SEM and EDX studies for technology and nanoscience



EDX investigations of tin-copper (Cu-Sn) lead-free contact lead-free brazing technique (**Jointly with Semiconductor Materials and Solid State Ionics Division**)

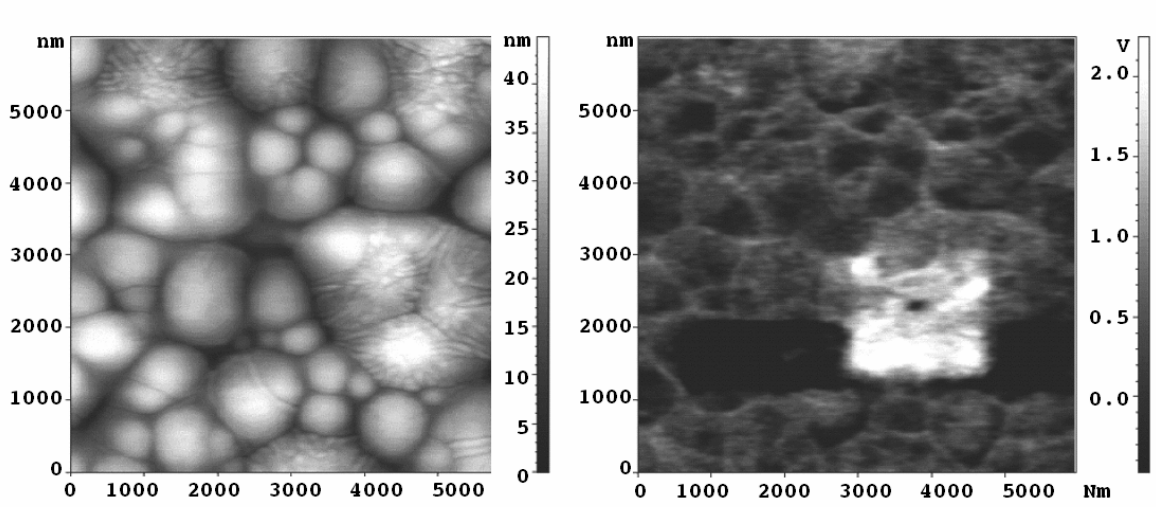


Studies of growth of Au nanowire fillers in nanoporous Al_2O_3 matrix (jointly with **Institute of Chemical Physics)**

SCANNING PROBE MICROSCOPY INVESTIGATIONS OF FUNCTIONAL MATERIALS

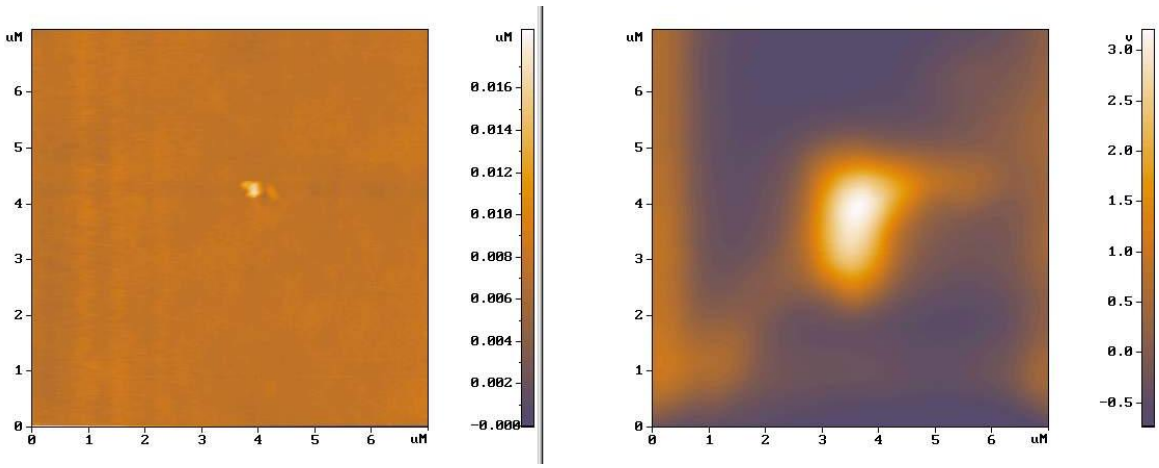
K. Kundzins, V. Zauls, and M.Granats

Wide range of functional materials including ferroelectric thin films, electrodes, ion bombarded interfaces of ionic crystals, photoresists for optical holography and poled polymer layers, has been investigated by adapting specific modifications of Scanning Probe Microscopy (SPM) technique, combining topographic imaging with multipass scanning modes such as local contact mechanic or piezoelectric response, electrostatic force measurements and voltage lithography. Collaborations within ISSP include Ferroelectric Physics division, Surface Physics group, Optical Recording laboratory, Surface Physics group and Laboratory of Organic Materials.



Example1. Direct electric poling by scanning probe *writing* of PZT 50/50 + 2% Fe sol-gel thin film surface microregions. Left – surface topography. Right – piezoresponse imaging of regions poled by calibrated +8V voltage pulses applied to AFM tip in electrolithographic mode (dark region). Part of the poled scan area has been later erased and poling reversed by –8V voltage (light region).

Another part of work is devoted towards development of SPM setup suitable for measurements in demanding environment to achieve chemical element specific contrast via detection of electrostatic force variation induced by direct X-ray or syncrotron irradiation of local area under SPM tip (jointly with X-TIP project in collaboration with *Centre de Recherche de la Matiere Condensee et des Nanosciences* (CRMC-N) Luminy,



Example 2. Imaging of the host-guest polymer (1wt.% DMABI - PMMA) surface potential in Kelvin probe scanning mode. Left – topographic image shows small particle just a few nm high used as target spot on the flat surface of polymer for electrical poling.

Marseilles, France).

HIGH FREQUENCY DIELECTRIC AND OPTICAL PROPERTIES OF THIN-FILM FERROELECTRICS

I. Aulika

A method of analyzing variable-angle null-ellipsometry and spectrophotometry measurement data were proposed for pure perovskite relaxor ferroelectric lead magnesium niobate $Pb(Mn_{1/3}Nb_{2/3})O_3$ (PMN 33/67) thin films grown on MgO/ $La_{0.5}Sr_{0.5}CoO_3$ substrate by pulsed laser ablation (PLD) technique varying the temperature of deposition. The refractive and extinction coefficients of the samples were determined in the photon energy range of 0.45 – 4.45 eV. Spectrophotometry and ellipsometry techniques were combined to detect optical properties of $La_{0.5}Sr_{0.5}CoO_3$ (LSCO) bottom electrode. Variation of optical properties and surface roughness in order of deposition temperature for PMN films were observed. Lower surface roughness was established for the films, which were deposited at higher temperature. Higher optical band gap energy, oscillator energy, and average oscillator strength were determinate for films with lower strain.

PASSIVE AND ACTIVE LIGHT SCATTERING OBSTACLES

M. Ozolinsh, J. M. Bueno[1], V. Karitans[2], and G. Ikaunieks[2]
[1]Laboratorio de Óptica (Dpto. Física), Universidad de Murcia, Spain
[2]Department of Optometry and Vision Science, University of Latvia

Simulation of vision pathologies and adverse viewing conditions in laboratory conditions requires optical phantoms with different level of light scattering. Such obstacles are designed as passive or active elements applying several technologies. We used for studies two kinds of solid state smart materials with electrically controllable light scattering – electrooptic PLZT ceramics, polymer dispersed liquid crystals PDLC and obstacles with fixed light scattering – composite of polymer methylmethaacrilat PMM together with grinded glass microparticles. Report analyzes optical characteristics of such obstacles – attenuation, scattering, depolarization of different wavelength light at various scattering levels and changes of visual performance applying obstacles in vision science studies.

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

M. Ozolinsh and G. Ikaunieks[1]
[1] Department of Optometry and Vision Science, University of Latvia

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

Published in 2005

1. J. Banys, J. Macutkevic, A. Brilingas, J. Grigas, K. Bormanis, and A. Stenberg. Radio and Microwave Spectroscopy of 0.2PMN-0.4PSN-0.4PZN Relaxor Ceramics. Ferroelectrics, 2005, Vol. 318, pp.141–146.
2. J. Banys, J. Macutkevic, A. Brilingas, J. Grigas, K. Bormanis, and A. Sternberg. Broadband Dielectric Spectroscopy of 0,2PMN-0,4PSN-0,4PZN Relaxors Ceramics. Materials Science (Medžiagotyra), 2005, Vol. 11, No. 1, pp. 3-8.
3. R. Bittner, K. Humer, H.W. Weber, K. Kundzins, A. Sternberg, D.A. Lesnyh, D.V. Kulikov, and Y.V. Trushin. Neutron Irradiation Effects in PZ and PZT Thin Films. Integrated Ferroelectrics, 2005, Vol. 72, pp. 47-51.
4. K. Bormanis, A. Kalvane, A. Burkhanov, A. Alpatov, M. Dambekalne, and A. Shil'nikov. Dielectric polarization in xPbZn$_{1/3}$Nb$_{2/3}$O$_3$–(1–x)PbSc$_{1/2}$Nb$_{1/2}$O$_3$ ferroelectric solid solutions. Proceedings of SPIE, Optical materials and applications, 2005, Vol. 5946, edited by Arnold Rosental, pp. 594604-1 – 594604-6.
5. 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, 2005, Vol.318, pp. 209–214.
6. M. Dambekalne, M. Antonova, M. Livinsh, B. Garbarz-Glos, W. Smiga, and A. Sternberg. Production and Properties of PLZT Ceramics. Proceedings of International Conference "Modern Aspects of Solid State Physics", Minsk, Belorussia, 2005. Vol. 1, c. 261-264.
7. M.Dambekalne, M.Kalnberga, M.Livinsh, L.Shebanovs, K.Bormanis, and A.Sternberg. Studies of PbSc$_{1/2}$Nb$_{1/2}$O$_3$ – PbYb$_{1/2}$Nb$_{1/2}$O$_3$ Solid Solutions. Proceedings of International Conference "Modern Aspects of Solid State Physics", Minsk, Belorussia, 2005. Vol. 1, pp. 257-260.
8. V.V. Efimov, E.A. Efimova, S.S. Khasanov, Y.S. Kovalev, B.N. Mavrin, A.O. Pogosov, A. Sternberg, and S.I. Tiutiunikov. Mechanism of Pulsed Electron Irradiation of the PLZT X/65/35 Ceramics. Phys. Stat. Sol. (C), 2005, Vol. 2, No. 1, pp. 449-452.
9. E. Klotins. Symplectic Integration Approach to Nonadiabatic Polarization Response in Ferroelectrics: Scalar Theory. PHYSICA E, 2005, Vol. 29, pp. 237.-242.
10. E. Klotins, and J. Kaupuzs. Theory and Modeling of Polarization Switching in Ferroelectrics. Journ. of the European Ceramic Society (ELECTROCERAMICS), 2005, Vol. 25, pp. 2553.-2557.
11. A. Krumins. International Year of Physics in the World and Latvia. Proceedings of First Latvian Conference Nanomaterials and Nanotechnologies, Riga, 2005, pp. 3-6.
12. G. Krumina, M. Ozolinsh, I. Lacis, and V. Lyakhovetskii. Estimation of Stereovision in Conditions of Blurring Simulation. Proceedings of SPIE, Optical materials and applications, 2005, Vol. 5946, edited by Arnold Rosental, pp. 59461N-1 – 59461N-10.
13. K. Kundzins, V. Zauls, and M. Granats. Nanoscale Piezoelectric and Electrostatic Force Imaging of Dielectric Surfaces. Proceedings of First Latvian Conference Nanomaterials and Nanotechnologies, Riga, 2005, pp. 161-166.
14. J. Levoska, M. Tyunina, and I. Jaakola. Compositional Evolution of Structure and Dielectric Properties in Ba1−Xsrxtio3 Epitaxial Thin-Film Heterostructures. Ferroelectrics, 2005, Vol. 318, pp. 49–53.
15. G. Liberts, G. Ivanovs, V. Dimza, and E. Tamanis. Thermo-Optical Investigation of Sodium-Bismuth Titanate Single Crystal and PLZT Ceramics. Ferroelectrics, 2005, Vol. 319, pp. 87–93.

16. J. Macutkevic, S. Lapinskas, J. Grigas, A. Brilingas, J. Banys, R. Grigalaitis, K. Meskonis, K. Bormanis, A. Sternberg, and V. Zauls. Distribution of the Relaxation Times of the New Relaxor 0.4PSN-0.3PMN-0.3PZN Ceramics. Journal of the European Ceramic Society, 2005, Vol. 25, pp. 2515-2519.
17. M. Ozolinsh, K. Anisko, G. Ikaunieks, and G. Krumina. Assessment of Ocular Stereovision Prevalence and Eye Dominance Stability. Proceedings of SPIE, Optical materials and applications, 2005, Vol. 5946, edited by Arnold Rosental, pp. 59461Q-1 – 59461Q-6 (pp. 510-515).
18. M. Ozolinsh, G. Ikaunieks, and S. Fomins. Colour Vision Experimental Studies in Teaching of Optometry. Proc. „Education and Training in Optics and Photonics." Pôle Optique et Photonique, Marseille, 2005, pp. 295-297.
19. M. Ozolinsh, G. Ikaunieks, and D. Fridrihsone. Dynamics of eye aberration detected by high-speed Hartmann-Shack aberrometer. Proc. „Optical Complex Systems." Pôle Optique et Photonique, Marseille, 2005, pp. 51-54.
20. 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), 2005, Vol. 2, 1, pp. 212-215.
21. M. Rutkis, I. Muzikante, B. Stiller, A. Vembris, and V. Zauls. Indandione Derivatives as a Cromophores for the Non-Linear Optical Applications and Photonics. Proceedings of First Latvian Conference Nanomaterials and Nanotechnologies, Riga, 2005, pp. 125-129.
22. V.Y. 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, 2005, Vol. 314, pp. 245-253.
23. V.Y. Shur, E.L.Rumyantsev, G.G. Lomakin, O.V. Yakutova, D.V. Pelegov, A. Sternberg, and M. Kosec. Field Induced Evolution of Nanoscale Structures in Relaxor PLZT Ceramics. Ferroelectrics, 2005, Vol. 316, pp. 23-29.
24. V.Ya. Shur, G.G. Lomakin, E.L. Rumyantsev, O.V. Yakutova, D.V. Pelegov, A. Sternberg, and M. Kosec. Polarization Reversal in Heterophase Nanostructures: Relaxor PLZT Ceramics**.** Physics of Solid State, 2005, Vol. **47**(7), pp. 1340-1345.
25. V.V. Shvartsman, A.L. Kholkin, A. Orlova, D. Kiselev, A.A. Bogomolov, and A. Sternberg. Polar Nanodomains and Local Ferroelectric Phenomena in Relaxor Lead Lanthanum Zirconate Titanate Ceramics. Applied Physics Letters, 2005, Vol. 86, 1, p. 202907 (1-4).
26. N.V. Sidorov, M.N. Palatnikov, V.T. Kalinnikov, I.V. Biryukova, and K. Bormanis. Effects of Ionising Radiation on Optical Properties of Lithium Niobate Single Crystals. Ferroelectrics, 2005, Vol.318, pp.113–118.
27. N. V. Sidorov, M. N. Palatnikov, and K. Bormanis. Ferroelectric-Antiferroelectric Phase Transition in $Li_{0.12}Na_{0.88}Ta_{0.4}Nb_{0.6}O_3$ Ceramics. Ferroelectrics, 2005, Vol. 319, pp. 27–34.
28. N.V. Sidorov, P.G. Chufyrev, M.N. Palatnikov, V.M. Voskresensky, and K. Bormanis. Photorefractive Effect in Lithium Niobate Crystals of Variable Composition and Its Manifestation in Raman Spectra. Proceedings of International Conference "Modern Aspects of Solid State Physics", Minsk, Belorussia, 2005. Vol. 2, c. 146-148.
29. J.Suchanich, M.Dambekalne, L.Shebanovs, A.Sternberg, B.Garbarz-Glos, W.Smiga, and Cz.Kus. Influence of axial pressure on electric properties of PLuN and 0.6PSN-0.4PSN ceramics. Ferroelectrics, 2005, Vol.322, pp. 3-10.
30. M. Tyunina, and J. Levoska. Epitaxial Films of Relaxor Ferroelectric $PbMg_{1/3}Nb_{2/3}O_3$ in Strong Electric Fields. Ferroelectrics, 2005, Vol.318, pp.29–34.

31. M. Tyunina, and J. Levoska. Compositional Evolution of Properties in Epitaxial Films of Relaxor $PbMg_{1/3}$ $Nb_{2/3}$ O_3 -$PbTiO_3$. Ferroelectrics, 2005, Vol.318, pp.63–66.
32. C. Ziebert, H. Schmitt, J.K. Kruger, A. Sternberg, and K.-H. Ehses. Grain-Size-Induced Relaxor Properties in Nanocrystalline Perovskite Films. Phys. Rev., 2004, Vol. B69, pp. 214106(1-10).
33. К. Борманис, А.И. Бурханов , А. Калване, М. Дамбекалне, А.В. Алпатов, А.В. Шильников, А. Штернберг. Нелинейность диэлектрического отклика в сегнетокерамике скандониобата свинца. Сборник докладов Международной научной конференции «Актуальные проблемы физики твердого тела» ФТТ-2005, Минск, Том 1, с. 275-277.
34. А.И. Бурханов, П.В.Бондаренко, К. Борманис, А. Калване, А. Штернберг. Низко- и инфранизкочастотные диэлектрические свойства керамики PLZTS. Материалы IV Международной научно-технической конференции «INTERMATIC – 2005», МИРЭА, 4 стр.
35. А.И. Бурханов, А.В. Алпатов, К. Борманис, А. Калване, А. Штернберг. Диэлектрическая нелинейность в сегнетоэлектрическом твердом растворе (1-x)Pb(Ti,Zr)O_3-xBi(Sr,Ti)O_3. Материалы IV Международной научно-технической конференции «INTERMATIC – 2005», МИРЭА, 4 стр.
36. М.Н. Палатников, Н.В. Сидоров, И.В. Бирюкова, К.Я. Борманис, В.Т. Калинников. Оптические характеристики легированных монокристаллов ниобата лития. Сборник докладов Международной научной конференции «Актуальные проблемы физики твердого тела» ФТТ-2005, 2005, Минск, Том 2, с. 217 – 219.

Lectures on Conferences

21. Zinātniskā konference, veltīta Starptautiskajam Fizikas gadam. LU Cietvielu fizikas institūts, Rīga, 2005.gada 7.-9. februāris.

21th Scientific Conference Dedicated to the International Year of Physics. Institute of Solid State Physics, University of Latvia, Riga, February 7-9, 2005.

1. A. Krūmiņš. Starptautiskais fizikas gads pasaulē un Latvijā. International Year of Physics in World and Latvia. Referātu tēzes, 4. lpp.
2. A. Mišņovs. Kristalītu izmēru noteikšana ar rentgendifrakcijas metodi. Crystallite Size Determination by X-Ray Diffraction. Referātu tēzes, 22. lpp.
3. Ē. Klotiņš. Simplektiskās integrēšanas pielietojumi polarizācijas kinētikas modelēšanā segnetoelektriķos. Symplectic Integration Approach to Nonadiabatic Polarization Response in Ferroelectrics. Referātu tēzes, 24. lpp.
4. I. Aulika, V. Zauls, K. Kundziņš, M. Granāts. Lāzeruzputinātu $BaTiO_3$, $Ba_{0.8}Sr_{0.2}TiO_3$ un $SrBi_2Ta_2O_9$ plāno kārtiņu optisko īpašību un virsmas morfoloģijas pētījumi. Studies of Optical Properties and Surface Morphology of Laser Deposited $BaTiO_3$, $Ba_{0.8}Sr_{0.2}TiO_3$ and $SrBi_2Ta_2O_9$ Thin Films. Referātu tēzes, 25. lpp.
5. V. Zauls, A. Krotkus, J. Banys, K. Bormanis. Relaksoru materiālu dielektrisko īpašību pētījumi terahercu frekvenču diapazonā. Dielectric Characterization of Relaxor Materials in the Terahertz Frequency Domain. Referātu tēzes, 26. lpp.
6. M. Dambekalne, M. Kalnberga, M. Līviņš, A. Mišņovs, A. Spūle. Jauns segnetoelektriskais materiāls uz $PbSc_{1/2}Nb_{1/2}O_3$ – $PbTm_{1/2}Nb_{1/2}O_3$ bāzes. New Ferroelectric Materials on the Basis of $PbSc_{1/2}Nb_{1/2}O_3$ – $PbTm_{1/2}Nb_{1/2}O_3$. Referātu tēzes, 27. lpp.
7. A. Šternbergs. Sadarbības projekts "Nanomateriāli un nanotehnoloģijas": mērķi, uzdevumi, izpildītāji. Cooperation Project: "Nanomaterials and Nanotechnologies": Objectives, Challenges, Contractors. Referātu tēzes, 33. lpp.

8. A. Šternbergs. Nanotehnoloģijas: vides un sociālie atbildības aspekti pētniecībā. Responsible Research in Nanotechnologies: Environmental and Social Aspects. Referātu tēzes, 34. lpp.
9. M. Ozoliņš, H.M. Bueno, G. Ikaunieks, V. Karitāns. Izkliedes elipsometrija elektriski vadāmai izkliedei PDLC-polimēros disperģētos šķidros kristālos. Elipsometry of Electricaly Controled Scattering in PDLC-polymer Dispersed Liquid Crystals. Referātu tēzes, 54. lpp.
10. M. Rutkis, V. Zauls. Nelineāro optisko koeficientu D_{ij} noteikšana – metodika, problēmas un to risinājumi CFI. Determination of the Nonlinear Optical Coefficients D_{ij} – methodology, problems and Solutions at the ISSP. Referātu tēzes, 55. lpp.
11. I. Gvardina, A. Kristiņš, J. Melderis, G. Pikurs, J. Tībergs, J. Zvirgzds. Elektrodzinēju mīkstā starta ierīces. Soft Start Devices for Electric Motors. Referātu tēzes, 87. lpp.
12. M. Kundziņš. Telekonferences iespējas EURATOM projekta dalībniekiem. Teleconferencing Facilities for EFDA Members. Referātu tēzes, 91. lpp.
13. I. Šorubalko. Skanējošais elektronu mikroskops LU CFI: tehniskie parametri un izmantošanas iespējas. Referātu tēzes, 92-93. lpp.

Pirmā Latvijas konference Nanomateriāli un nanotehnoloģijas, Rīga, 30.-31. marts 2005.
First Latvian Conference Nanomaterials and Nanotechnologies, Riga, March 30-31, 2005.

1. A. Krumins. International Year of Physics in the World and Latvia. Proceedings, pp. 3-6.
2. A. Sternberg. Responsible Research in Nanotechnologies: Environmental and Social Aspects. Proceedings, p. 116.
3. M. Rutkis, I. Muzikante, B. Stiller, A. Vembris, and V. Zauls. Indandione Derivatives as a Cromophores for the Non-Linear Optical Applications and Photonics. Proceedings, pp. 125-129.
4. K. Kundzins, V. Zauls, and M. Granats. Nanoscale Piezoelectric and Electrostatic Force Imaging of Dielectric Surfaces. Proceedings, pp. 161-166.

International student conference on "Developments in optics and photonics" Riga, April 30– May 1, 2005.

1. I. Aulika, V. Zauls, K. Kundzins, M. 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 the International student conference on "Developments in optics and photonics", Riga, p. 50.

IX Conference &Exhibition of the European Ceramic Society, Portorož, Slovenia, June 19-23, 2005.

1. M. Dambekalne, M. Antonova, M. Livinsh, B. Garbarz-Glos, W. Smiga, and A. Sternberg. PLZT – Synthesis, Sintering and Ceramics Microstructure. Abstract book, Abstract COST-M-12, pp. 270-271.

XVII Всероссийская конференция по физике сегнетоэлектриков (ВКС-XVII-2005), Пенза: Пенз. Гос. Ун-т, Россия, 27 июня-1 июля 2005 года.

1. Бурханов А.И., Алпатов А.В., Шильников А.В., Борманис К., Калване А., Дамбекалне М., Штернберг А. Реверсивные зависимости диэлектрической проницаемости в сегнетокерамике xPZN-(1-x)PSN. Тезисы докладов, с.153.
2. К.Борманис, М.Дамбекалне, А.Калване, А.И.Бурханов. Получение и свойства слоистых соединений типа перовскита. Тезисы докладов, с.217.

3. В.Я. Шур, Д.В. Пелегов, Е.Л. Румянцев, Г.Г. Ломакин, О.В. Якутова, Е.И. Шишкин, В.А. Шихова, А. Штернберг, М. Косец. Индуцированная полем эволюция наноразмерных структур в релаксорной PLZT керамике. Тезисы докладов, с.163-164.
4. В.В. Ефимов, Е.А. Ефимова, Д.И. Кочубей, В.В. Кривенцов, Б.Н. Маврин, Н.Н. Новикова, С.И. Тютюнников, С.С. Хасанов, А. Штернберг. Структура и динамика решетки сегнетокерамики ЦТСЛ 4 и 9,75/65/35, облученной сильноточным импульсным электронным пучком. Тезисы докладов, с. 97.
5. Е.В. Николаева, В.Я. Шур, Г.Г. Ломакин, Д.В. Пелегов, О.В. Якутова, Е.А. Родина, А. Штернберг. Нанодоменная структура в релаксорных сегнетоэлектриках: керамика PLZT (6-9)/65/35. Тезисы докладов, с.175.
6. А.В. Сопит, А.И. Бурханов, А. Штернберг. Влияние радиационных дефектов на характер диэлектрического отклика сегнетокерамики PSN. Тезисы докладов, с. 238.
7. Д.К. Кузнецов, В.Я. Шур, И.С. Батурин, А.А. Адыгамов, N. Menou, C. Muller, A. Sternberg. Кинетика переключения поляризации в облученных тонких пленках PZT. Тезисы докладов, с. 260.

3rd NEXT SigmaPhy International Conference, Greece, August 13-18, 2005.

1. E. Klotins. Nonlinear Fokker-Planck Equation for Nonlocal and Nonconservative Model Hamiltonians: Symplectic Integration and Applications to Metastable Systems. Abstracts of 3rd NEXT SigmaPhy International Conference, Greece, p. 25 (oral).

7-th International Summer School-Conference "Advanced Materials and Technologies", Lithuania, Palanga, August 27-31, 2005.

1. A. Sternberg, and V. Zauls. Functional Dielectric Thin Films and Coatings: Nanoscale Approach. Book of Abstracts, p. 33.

11-th International Meeting on Ferroelectricity, Iguassu Falls, Argentine/Brazil, September 5-9, 2005.

1. V. Zauls, A. Sternbergs, K. Kundzins, and L. Cakare-Samardzija. Studies of Local Induced Polarization in Modified Ferroelectric Thin Films. Abstract IMF-06-059.
2. J. Petzelt, and S. Kamba. Complete Dielectric Spectra of PMN-PSN-PZN Relaxor Ceramics. Abstract IMF-18-005.
3. M. Tyunina, and J. Levoska. New Mechanism of Dielectric Nonlinearity in Thin-Film Perovskite Relaxors and Ferroelectrics. Abstract IMF-17-036.
4. K. Bormanis, A. Sternberg, A.I. Burkhanov, M.Dambekalne, and A. Kalvane. Production and Properties of Layered Aurivillius Perovskite Compounds. Abstract IMF-05-020.
5. I. Jaakola, J. Levoska, and M. Tyunina. Multilayers and Superlattices of Perovskite Ferroelectric Barium Strontium Titanate. Abstract IMF-06-039.
6. E. Klotins. Nonadiabatic Polarization Response in Finite Bodies: Symplectic Integration and Application to Domain Switching. Abstract IMF01-010.
7. K. Bormanis, A. Burkhanov, A. Sternberg, A. Shilnikov, A. Kalvane, A. Alpatov, and M. Dambekalne. Reversive Dielectric Response in xPZN – (1-x)PSN Ceramics. Abstract IMF-17-034.
8. V. Shur, E. Nikolaeva, E. Shishkin, E. Rumyantsev, D. Pelegov, G. Lomakin, and A. Sternberg. Nanoscale Domain Structure in Relaxors: Statics and Field-Induced Kinetics of Nanodomains in PLZT Ceramics. Abstract IMF-17-037.

III Международная научно-техническая школа-конференция "Молодые ученые - науке, технологиям и профессиональному образованию", МИРЭА, Москва, Россия, 26-30 сентября 2005. г.

1. Алпатов А.В., Бурханов А.И., Шильников А.В., Борманис К., Штернберг А., Дамбекалне М., Калване А. Влияние смещающих электрических полей на диэлектрический отклик в сегнетопьезокерамике xPZN-(1-x)PSN. Материалы школы-конференции "Молодые ученые - науке, технологиям и профессиональному образованию", Москва, 2005, 4 стр.

IV Международная научно-техническая конференция «INTERMATIC – 2005», МИРЭА, Москва, Россия, 25-28 октября 2005. г.

1. А.И. Бурханов, А.В. Алпатов, К. Борманис, А. Калване, А. Штернберг. Диэлектрическая нелинейность в сегнетоэлектрическом твердом растворе $(1-x)Pb(Ti,Zr)O_3$-$xBi(Sr,Ti)O_3$. Материалы конференции «INTERMATIC – 2005», МИРЭА, 4 стр.
2. А.И. Бурханов, П.В.Бондаренко, К. Борманис, А. Калване, А. Штернберг. Низко- и инфранизкочастотные диэлектрические свойства керамики PLZTS. Материалы конференции «INTERMATIC – 2005», МИРЭА, 4 стр.

International Conference “Modern Aspects of Solid State Physics”, Minsk, Belorussia, October 26-28, 2005.

1. M. Dambekalne, M. Antonova, M. Livinsh, B. Garbarz-Glos, W. Smiga, and A. Sternberg. Production and Properties of PLZT Ceramics. Materials of Conference, Vol. 1, pp. 261–264.
2. M. Dambekalne, M. Kalnberga, M. Livinsh, L. Shebanovs, K. Bormanis, and A. Sternberg. Studies of $PbSc_{1/2}Nb_{1/2}O_3$ – $PbYb_{1/2}Nb_{1/2}O_3$ Solid Solutions. Materials of Conference, Vol. 1, pp. 257–260.
3. К. Борманис, А.И. Бурханов, А. Калване, М. Дамбекалне, А.В. Алпатов, А.В. Шильников, А. Штернберг. Нелинейность диэлектрического отклика в сегнетокерамике скандониобата свинца. Сборник докладов, том 1, с. 275-277.
4. N.V. Sidorov, P.G. Chufyrev, M.N. Palatnikov, V.M. Voskresensky, and K. Bormanis. Photorefractive Effect in Lithium Niobate Crystals of Variable Compositions and its Manifestation in Raman Spectra. Materials of Conference, Vol. 2, pp. 146-148.
5. М.Н. Палатников, Н.В. Сидоров, И.В. Бирюкова, К.Я. Борманис, В.Т. Калинников. Оптические характеристики легированных монокристаллов ниобата лития. Сборник докладов, том 2, с. 217-219.

International Symposium Micro- and Nano-Scale Domain Structuring in Ferroelectrics, Ural State University, Ekaterinburg, Russia, November 15-19, 2005.

1. V. Zauls, A. Sternberg, K. Kundzins, and L.C. Samardzija. Local Induced Polarization in Modified Ferroelectric Thin Films. Abstract and Program Book, p. 62-63.
2. V.Ya. Shur, D.V. Pelegov, G.G. Lomakin, E.L. Rumyantsev, O.V. Yakutova, E.V. Nikolaeva, V.A. Shikhova, and A. Sternberg. Polarization Reversal in Relaxor PLZT Ceramics: Role of Nano-Scale Nonpolar Inclusions. Abstract and Program Book, p. 72-73.
3. E. Nikolaeva, V. Shur, E. Shishkin, and A. Sternberg. Nanoscale Domain Structure in Relaxor PLZT x/65/35 Ceramics. Abstract and Program Book, p. 102-103.
4. D.K. Kuznetsov, V.Ya. Shur, I.S. Baturin, N. Menou, Ch. Muller, and A. Sternberg. Effect of Penetrating Irradiation on Polarization Reversal in PZT Thin Films. Abstract and Program Book, p. 110-111.

Workshop on the Coupling of Syncrotron Irradiation and X-Rays with Tip based Scanning Probe Microscopies, Grenoble, France, November 16-18, 2005.

1. A. Kuzmin, J. Purans, R. Kalendarev, L. Grigorjeva, K. Kundzins, V. Zauls, F. Jandard, and D. Pailharey. X-Tip:Development of Laboratory Setup for X-Ray AFM Experiments. Abstracts, p.18.

Lectures on conferences without theses

Conference on Education and Training in Optics and Photonics, ETOP-2005, Marseille, 2005.

1. M. Ozolinsh, J. M. Bueno, V. Karitans, and G. Ikaunieks. Passive and Active Light Scattering Obstacles.

The 18th Symposium of the International Colour Vision Society, Lyon, France, 2005.

1. M. Ozolinsh, M. Colomb, G. Ikaunieks, and V. Karitans. Colour Stimuli Perception in Presence of Light Scattering.

European Conference on Visual Perception, A Coruña, Spain, 2005.

1. M. Ozolinsh, M. Colomb, G. Ikaunieks, and V. Karitans. Different Colour Contrast Stimuli Perception in Fog.

Conference on Optical Complex Sytems, OCS-2005, Marseille.

1. M. Ozolinsh, G. Ikaunieks, and D. Fridrihsone. Dynamics of Eye Aberration Detected by High-Speed Hartmann-Shack Aberrometer.

Rīgas Tehniskās universitātes 46. Starptautiskā zinātniskā konference, Rīga, 13.-15. oktobris, 2005.

1. M. Dambekalne, M. Kalnberga, M. Līviņš, K. Bormanis. Jauni segnetoelektriskie materiāli uz $PbSc_{1/2}Nb_{1/2}O_3 – PbTu_{1/2}Nb_{1/2}O_3$ bāzes.
2. M. Dambekalne, M. Antonova, M. Līviņš, A. Šternbergs. PLZT caurspīdīgās keramikas iegūšana un mikrostruktūras pētījumi

SEMICONDUCTOR MATERIALS AND SOLID STATE IONICS

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

Research Area and Main Problems

Research areas:

- Resource science – resource physics and chemistry
- Electrophysics and electrochemistry of specific semiconductor materials, mixed conductors, ion conductors (transition metal oxides, bronzes, metal hydrates, solid electrolytes, etc.);
- Material preparation methods: thin and thick film technologies, sol-gel process;
- Material characterization by spectroscopic methods (Raman scattering, optical and X-ray absorption, electrical and electrochemical impedance, ESR, etc);
- Solid state ionics:
  - electro-, photo-, chemo- or gaso-chromic phenomena,
  - structural changes due to ion intercalation,
  - lattice dynamics and structural and electronic phase transitions,
  - solid state reactions at interfaces electrode – solid electrolyte,
  - gases and ions sensing phenomena and detection technologies;
- Functional coatings and multi layer electrochemical systems;
- Hydrogen absorption phenomena in metals, semiconductors and insulators;
- Development of new nano structured materials for hydrogen storage;
- New measurement technologies and instruments with artificial intelligence;
- Miniaturisation of solid state ionic devices;
- Application specific semiconductor materials and solid-state ionic devices in micro systems for electronic nose.

Research problems and tasks:

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

Postgraduate students:

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

Students:

1. J. Gaidelene

Laboratories of Semiconductor Material Department

Laboratory of Solid State Ionics – Head of Laboratory Dr. phys. E.Pentjuss

Laboratory of EXAFS Spectroscopy – Head of Laboratory Dr. hab. phys. J.Purans

Laboratory of Electrophysics – Head of Laboratory Dr.J.Klavins

Laboratory of Sensors – Head of Laboratory Dr.J.Klepers

Cooperation

Latvia

1. University of Latvia - Department of Chemistry (Prof. J.Tīliks, Dr. A.Vīksna)
2. University of Latvia - 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. Certification Centre of Latvian Academy of Science (Prof. J.Matīss)
9. Ulbroka Scientific Institute of Agricultural Machinery of the Latvia University of Agriculture, Ulbrok
10. Riga City Council - Environmental Department.

Brasil

National Laboratory of Synchrotron Radiation (LNLS) (Campinas, Brazil) – Dr. E. Avendaño.

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
2. Max-Planck-Institut für Festkörperforschung, Stuttgart (Germany) – Prof. J. Maier, Dr.R.Merkle, M. Vracar

Great Britain

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

Italy

1. University of Trento (Trento, Italy) - Prof. G.Mariotto, Prof. G.Dalba.
2. IFN-CNR CeFSA (Trento, Italy) - Dr. F. Rocca.
3. Universita della Calabria (Arcavacata di Rende, Italy) - Prof. E.Cazzanelli.
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. Joint Instute for Nuclear Research, Dubna (Dr. S.I. Tjutjunnikov)
2. Moscow State Engineering Physics Institute, Moscow (Prof. A.Menushenkov)

Sweden

Linkoping University – Laboratory of Applied Physics (Prof. I.Lundstrom)

Stockholm University, Arrhenius laboratory (Dr. J.Greens)

Uppsala University, Angstrom Laboratory, Uppsala, Prof. C.G. Granqvist, Dr. A. Azens.

South Africa

West Cape University, Institute of Advanced Material Chemistry, 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).

Main results

SOLID STATE IONICS – RESOURCE SCIENCE AND SUSTAINABLE DEVELOPMENT

G. Bajārs, A. Lūsis, Ē. Pentjušs

Participation of ISSP in two EC financed projects "GreenRoSE" and "EcoDesign" as well as in activities organized by Ministries of Economics and Environment (for example, investigation contract EM 2005/141: "Strategy for development of innovative friendly to environment technologies and implementation of RoHS directive in Latvian industry"), from one side, and from other side - EU concept of Sustainable Development and Lisbon strategy give us possibility to start ***new research area related to resources science.***

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

The first steps to build up some framework as driving force is EU directives and activities of implementation of them.

Ecodesign drivers and tools in electrical and electronics sector.

The basic idea of ecodesign is the reduction of environmental impacts throughout entire product life cycle by improved product design. The legal compliance is a major driver for ecodesign efforts. Discovering the benefits associated with a green product strategy as more and more important drivers became business and private customers, the market, and other stakeholders. In addition, ecodesign approach leads to innovative strategies. Ecodesign tools such as checklists, material declarations and environmental indicators could be used to improve the environmental performance of the product.

Implementation of RoHS directive in electrical and electroinics sector of Latvia.

Shortly considered RoHS Directive demands to electric and electronic goods and ways to achieve a compliance with them for small and medium enterprises. Presented results of inquiry among enterprises about getting ready to compliance with RoHS. Inquiry results showed that main part of enterprises are at the beginning of process

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

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

There are was developed concept based on amorphous thin films of tungsten oxide as a model for nanostructured mixed electron-ion conductors.

Transition metal oxides (TMO or $T_\alpha O_\beta$) as well as their thin films have applications in different solid-state electronic and ionic devices based on ion insertion/extraction and mixed (ion and electron) conduction phenomenon. The typical representative of such TMO is tungsten oxide, which belongs to group of materials with wide non-stoichiometry. Therefore for the tungsten oxide is used formula WO_{3-y}, where $3-y = 0 \div 2$.

One of the structural peculiarities of tungsten oxide, related to oxygen-based non-stoichiometry, is a variety of phases based on $[WO_6]$-octahedron sharing in structural units of pure tungsten oxide compounds with crystalline patterns. The sharing type of the $[WO_6]$-octahedron, and structure of different non-stoichiometric phases depend on oxygen deficiency. The ion insertion or extraction phenomenon (ion insertion based non-stoichiometry) is an other basic common peculiarity of tungsten oxide phases.

In general the basic mechanism of oxygen deficiency of transition metal oxides ($T_\alpha O_\beta$) is crystallographic shear (CS) [1]. Annihilation of oxygen vacancies is moving force of formation of a regular block structure of ideal stoichiometric $T_\alpha O_\beta$ crystals separated by CS planes. By that non-stoichiometry has influence on formation of particles of tungsten oxide compounds in the thin film during thermal evaporation of WO_3 and deposition on substrate.

The model for performance of thin film electrochemical cells have been generalized, 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 WO_3 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 symmetry of the vibrations of WO_3 crystal have been determined for different polimorphous phases. The infrared and Raman spectra have been applied to calculate the parameters of lattice dynamics for WO_3 and ReO_3 crystals. The calculated phonon spectra are used to determine the mean square displacement of tungsten and oxygen ions. The mean square relative displacements 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. The calculated phonon spectra are used to determine the mean square displacement of rhenium and oxygen ions. The mean square displacement of an oxygen ion shows the well-pronounced anisotropy. The mean square relative displacement are calculated for ion pairs Re-O and Re-Re.

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

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

EXAFS Spectroscopy Laboratory is involved in the research and development of new nano-sized materials, new experimental methods as well as new procedures for x-ray absorption spectra data analysis. We use complex approach based on a combination of modern experimental techniques with advanced data analysis methodologies, including the use of high performance cluster computing. Our experimental possibilities cover x-ray absorption spectroscopy (EXAFS/XANES) using synchrotron radiation, atomic force microscopy and 3D confocal spectromicroscopy (2D/3D high-speed imaging with Raman and luminescence spectroscopy) as well as conventional optical absorption/luminescence spectroscopies and electrochemical techniques. Main our results, obtained in 2005, are described below.

Element-Specific Contrast in Local Probe Microscopy via X-Ray Spectroscopy

The extremely high lateral resolution of the Local Probe Microscopies (LPM) makes them among the most largely used in all the domains of nanoscience. However, these tools suffer of a total lack in chemical sensitivity. On the other hand, XAS techniques probe the chemical and structural properties of materials. Therefore, a *combination* of X-rays and LPM techniques would be the ideal answer to many structural problems in nanosciences.

The different combination of XAS and LPM as a local detector was proposed by J.Purans. First STM and SNOM experiments under *focused* synchrotron-radiation (SR) were performed at ESRF on the microbeam line ID-22. Further progress we have achieved in the framework of the European X-TIP project (STRP FP6) by the focussing SR beam to increase the density of the incident photons. We have started with three types of experiments : (i) XAS-AFM x-ray excited secondary electrons detection by conductive tip in AFM mode ; (ii) XAS-SNOM x-ray excited optical luminescence (XEOL) detection by SNOM in AFM mode ; (iii) XAS-AFM x-ray excited photoconductivity of sample detection by conductive tip in AFM mode.

EXAFS study with femtometer accuracy: "negative" thermal expansion in ReO_3

Temperature dependent (from 30 to 603 K) EXAFS study of ReO_3 was performed at the Re L_3-edge in at the European Synchrotron Radiation Facility. The EXAFS signals were analyzed using two approaches: (i) the ab initio multiple-scattering formalism and (ii) the single-scattering cumulant approximation with the experimental amplitude and phase shift functions. High-quality experimental spectra and accurate EXAFS analysis procedure allowed us to obtain a precise information on the lattice thermal expansion and local dynamics. No distortion of the ReO_6 octahedra was observed at all temperatures that makes the rigid unit model (RUM) to be a good approximation for the ReO_3 lattice dynamics. The large amplitude of the oxygen vibrations in the direction perpendicular to the Re-O-Re bonds was determined. It is responsible for that the thermal expansion coefficient of ReO_3 in the probed range of temperatures is very small, being below 10^{-6} K^{-1}.

Our experience at the beam-line BM-29 on ReO_3 and Ge shows that also *10 femtometer (*10^{-4}Å) "barrier" is now attainable (see ESRF report HS-2270), even though such determination is far from trivial. Very recently, Pettifer et.al. (Nature 435 (2005) 78) have confirmed our idea that femto-meter scale XAFS experiment is now attainable!!!

Raman spectroscopy of rhenium trioxide ReO_3

The Raman scattering in single-crystal, polycrystalline powder and thin film ReO_3 samples was studied using micro-Raman setup. The origin of the Raman bands was interpreted on the basis of the rigid-ion vibrational model within the quasiharmonic approximation by comparison with calculated phonon density of states (PDOS). The importance of the rhenium ions effective charge on the shape of the calculated PDOS was investigated.

INTEGRATION OF ELECTROLYTIC HYDROGEN INTO THE HYDROGEN STORAGE DEVICES

L. Grinberga, Janis Kleperis, G. Vaivars, A. Nechaev[1], F. W. Poulsen[2], A. S. Pedersen[2]

1 - University of the Western Cape, Institute of Advanced Material Chemistry, Cape Town, South Africa

2 – RISÕ National Research Centre, Denmark

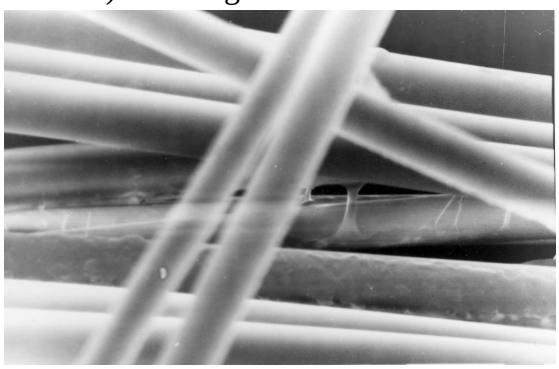
The metal hydride electrodes are of a particular interest due to their potential and practical application in batteries. A large number of the hydrogen storage materials have been characterized so far. Nevertheless only selected composite structures were synthesized. Our work deals with the effect of the hydrogen sorption capability and electrochemical characterisation of specific AB_5 alloy composites - AB_5 with SiO_2, B_2O_3, WO_3 and C. The hydrogen storage capacity and kinetics of hydrogen sorption-desorption in the solid phase/gas and solid phase/electrolyte solution systems are investigated and described.

The electrochemical properties of different nickel based materials (bulk, porous, foamed tapes) were examined to state the hydrogen adsorption/absorption phenomena and possibility to use them as negative electrode in hydrogen devices (electrolyser, rechargeable battery, fuel cell) . Voltamperometric and impedance measurements showed the important role of activated nickel (electroplated) and composite additives (Raney Ni, metal hydride alloy, carbon) in the surface activation of electrode materials and promotion of hydrogen absorption.

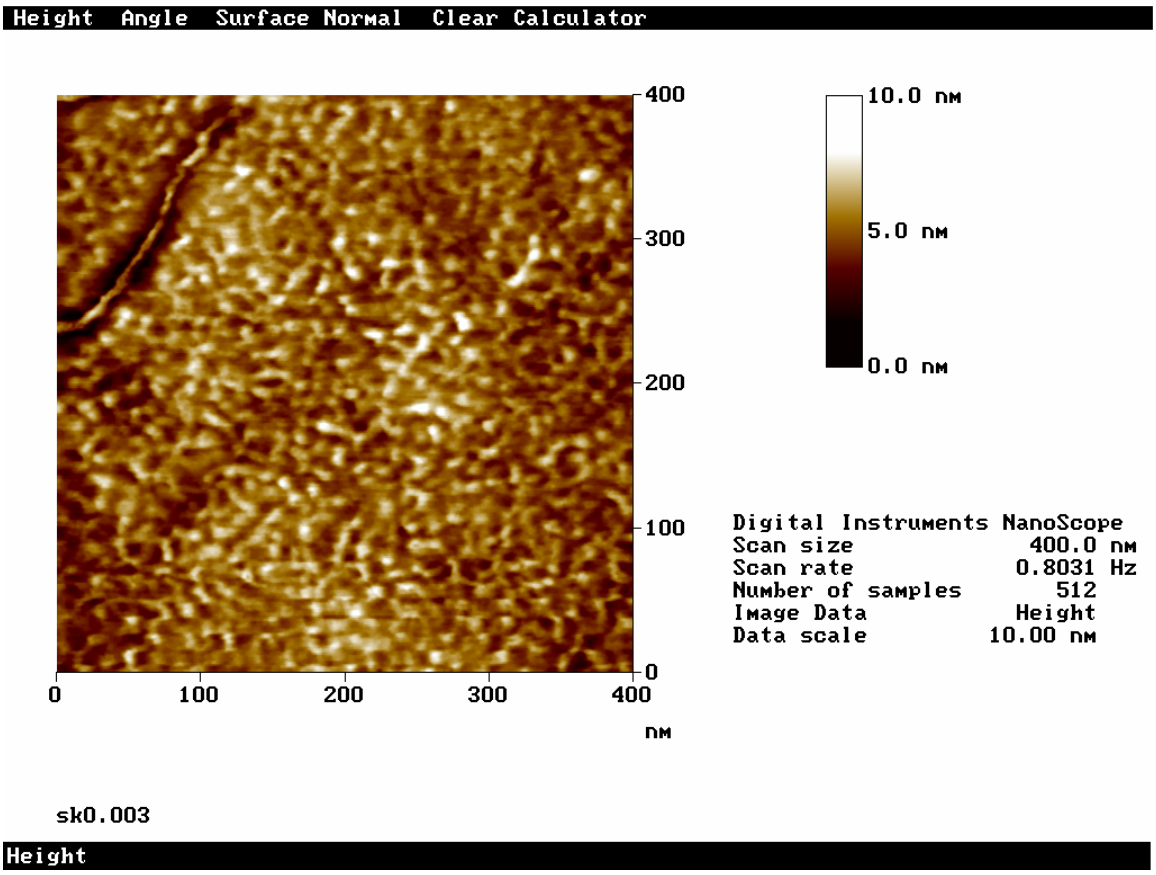
MODIFICATION OF SURFACE PROPERTIES OF GLASS FIBERS

V. Eglitis, A. Lusis, G. Veveris

The glass fibers (look below ESM graph of industrial glass fibers: diameter of fibers 6-8 microns) with high content of SiO2 before leaching process of the alkali metals was



treated and activated in “Amsonic” ultrasonic tank. After leaching 0,1 N HCl solution have been obtained nanostructured glass fibers: content of SiO2 - 94-96% and surface with porous structure. Substructure of microporous sodium alumosilicate glass fibers are investigate by AFM and by gas isothermal desorption using gas chromatography. From AFM graph of leached glass fibers surface have micropores ranging from 1-2 to 15 nm with depth at least 5 nm.



ODOUR NUISANCE PROBLEMS AND CHEMICAL GAS SENSORS: SELECTIVITY AND RESPONSE/RECOVERY TIMES

J. Kleperis, L. Grinberga, J. Hodakovska, A. Plate[1], A.Laurs[2]
1 - Latvian Ministry of Environment, Riga, Latvia
2 - Latvian University of Agriculture, Jelgava, Latvia

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).

HUMIDITY SENSORS AND OZONE GENERATORS, - APPLICATION TECHNOLOGIES IN AGRICULTURE

J. Kleperis, V. Vorohobovs, J. Hodakovska, S. Cesnieks[1], A. Vilde[1], A. Cesnieks[1]
1 - Ulbroka Scientific Institute of Agricultural Machinery of the Latvia University of Agriculture, Ulbroka, Latvia

The self-made ecological barn in an individual Agricultural Farm “Mazkalnini” from Tervete region (Latvia) with grain storage–drying facility was equip with computerized monitoring of moisture, temperature and ozone concentrations. Special constructions were made to prepare an air with desirable temperature and moisture by preheating with sun and/or oven heated with wood. Preliminary results were collected during 3 months in Autumn 2004 and summarised in this report. An influence of ozone is discussed theoretically because only generator with small power was test yet.

Our experimental work and practice shows that air – cooling for ozone generator is always simpler and cheaper than water – cooling. But it can be as much effective. On the other hand it demands good adhesion between dielectric enamel and aluminium radiator. Such adhesion was achieved in our laboratory. It appeared that the most reliable are ozone generators with two dielectric barrier coated both electrodes. In our report the reason of this experimental fact, geometry and character of discharge is analysed. Frequency can be risen till 30000 Hz without any disturbance for ozone generators work. Meanwhile necessary size of high voltage transformer diminishes and whole design simplifies. It makes a sense to increase speed of oxygen, but at the same time

partially recycle oxygen turning it from exit to entrance. Discharge from needle allows generate ozone from non prepared air, but its efficiency is small. Its efficiency can be sufficiently risen up by placing additional electrode in discharge zone. It is very reasonably to install little compressor in ozone sensor, which allows to inhale air probes from any narrow places. Pocket-size sensor of this type was created in our laboratory.

ACTIVITIES FOR IMPLEMENTATION OF THE EURATOM PROJECT ON THE MAGNETIC FIELD AND RADIATION EFFECTS ON THE TRITIUM RELEASE FROM IRRADIATED BE PEBBLES

A.Vītiņš

Participation in experiments on the tritium release from the beryllium pebbles irradiated in the BERYLLIUM experiment. Treatment of data of experiments of tritium release and pebble dissolution by means of the computer software "Microsoft Excel for Windows". The main results of the investigations are summarized the following abstract:

Beryllium pebbles irradiated in the BERYLLIUM experiment in 1994 (irradiation neutron fluence $1.24 \cdot 10^{25}$ m^{-2}, irradiation temperature 780 K, ^{3}H content 7 appm) were investigated in this study. The total amount of tritium in a separate pebble, the chemical forms of localised tritium (T^0, T_2, T^+) and the tritium distribution in the pebble volume were determined by a dissolution method. Annealing experiments were performed at a constant temperature 1123 K for 2 h under the following conditions: separately both in magnetic field of 1.7 T and in fast electron radiation of energy 5 MeV and the dose rate P=14 MGy/h as well as under the action of all the three factors. Tritium in the Be pebbles is localised for the most part as T_2 (85%-94%). The abundances of T^+ (4%-5%) and T^0 (5%-10%) are little. Tritium distribution in a pebble is not uniform, the most part of tritium is localised in an inner part of a pebble. Magnetic field of 1.7 T decreases slightly the fractional release of tritium under the given conditions of annealing (from 30% to 25%), the fast electron radiation increases it (from 30% to 40%), but the simultaneous action of the magnetic field and radiation increases it (from 30% to 54%). The effects observed are explained that magnetic field and radiation affect concentration of main diffusing particles T^0 in a beryllium matrix.

RAISING ECO-DESIGN AWARENESS FOR SMALL AND MEDIUM SIZED ENTERPRISES OF THE ELECTRICAL AND ELECTRONIC SECTOR

G.Bajars, A.Lusis

On behalf of the European Commission, DG Enterprise, Fraunhofer IZM, Plan Miljø and partners have carried out a project „Promoting Eco-Design Activities in the Small and Medium Sized Enterprises (SMEs) of the Electrical/Electronic Sector". The partners have been universities, chambers of commerce, industry associations, consultants, etc. Through 28 awareness raising workshops in 21 countries in Europe the project has informed electrical and electronics SMEs about Eco-Design.

One of the outcomes of the project is the teaching material, providing an introduction to all relevant aspects of Eco-Design: integration of Eco-Design in the design process, the economic aspects of Eco-Design, the legal framework, development of an Eco-Design strategy.

During the project a number of Eco-Design case studies has compiled with relevance for electrical and electronics SMEs. Presentations within the workshops and the case study promotion via the website (www.ecodesignarc.info) and the teaching

material will help SMEs to reach requirements of new EU legislation and to achieve success in their business.

The workshop "Business Benefits through Eco-Design" in Riga was organized at 3rd June, 2005 by ISSP in conjunction with Fraunhofer IZM. The workshop materials was presented in:

- The 9th International Exhibition and Conference on Information Technologies and Telecommunications in the Baltic Sea and CEE Region "Baltic IT&T 2005", Riga, April 6-9, 2005.
- The Ministry of the Environment of Republic of Latvia during the round table discussion on Environmental Technologies, Riga, December 14, 2005.

LEAD-FREE SOLDERING QUALITY AND RELIABILITY LABORATORY

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

According tasks of FP6 project "GreenRoSE" in ISSP have been set up soldering quality laboratory to help the local small and medium enterprises to change the technologies to lead-free and solve associated problems.

Available services for quality and reliability testing

Tests for lead-free materials applied in PCB assemblies

1. Chemical test methods
2. Mechanical test methods
3. Flammability
4. Miscellaneous for analysis of RoHS Directive restricted elements and materials:

Tests for PCB with lead-free finishes

1. Visual and dimensional examination
2. Surface conditions tests
3. Mechanical test methods*
4. Electrical tests
5. Environmental tests

Tests for lead free components for SMT and THT

1. Visual and dimensional examination
2. Surface conditions tests

Tests for PCB assemblies

1. Visual and dimensional examination
2. Miscellaneous test (Analysis of metallographic cross-section of solder joints; Pull test*)
3. Environmental tests

* Using Computer- controlled Test System Multitest1-I for force measurements.

ACTIVITIES FOR IMPLEMENTATION OF THE "GreenRoSE" PROJECT ON LEAD-FREE SOLDERING

A.Vītiņs

As ITR suggested, possibilities to test solder pastes according to the standard EN 61190-1-2 „Attachment materials for electronic assembly - Part 1-2: Requirements for solder pastes for high-quality interconnections in electronics assembly" in the Institute of Solid State Physics (ISSP) of the University of Latvia (UL) were evaluated. A report

has been written and sent. It is noteworthy that only the requirements for solder pastes are given in the standard EN 61190-1-2. The test methods referred in the standard EN 61190-1-2 will be given in the standard IEC 61189-5 “Test methods for electrical materials, interconnection structures and assemblies – Part 5: Test methods for printed board assemblies”, which is still under consideration at present. An official English translation of the German standard DIN IEC 61189-5 (2002) “Test methods for electrical materials, interconnection structures and assemblies - Part 5: Test methods for printed board assemblies (IEC 91/310/CD:2002)” is available at AUD$ 196 in the website
http://www.standards.com.au/catalogue/Script/Details.asp?DocN=DIN00000012896

At present, possibilities to test fluxes according to the standards IEC 61190-1-1 “Attachment materials for electronic assembly – Part 1-1: Requirements for soldering fluxes for high-quality interconnections in electronics assembly” and ISO 9455 “Soft soldering fluxes – test methods” in the ISSP UL are under evaluation in accordance with D3.1 “Catalogue of available services for quality testing” of the “GreenRoSE” project. A report is being prepared.

ACTIVITIES FOR IMPLEMENTATION OF THE “PERCERAMICS” PROJECT ON SORPTION OF HEAVY METALS

A.Vītiņs

In order to select priority heavy metals for sorption studies, data about heavy metal emissions within industrial wastewaters and wastewater treatment sludge produced in Riga and Latvia in the years 2001 - 2004 was collected and analysed from the following available sources: the State Statistics Survey – Water 2, which is an official annual report made by the Latvian Environmental, Geological and Meteorological Agency (www.lvagma.gov.lv) and is fully available at the web page http://vdc2.vdc.lv:8998/udens.html hosted by the Latvian Environmental Agency, the report of the Inspection of Water Resources for the year 2002 by A. Ļutinska and the report “Sustainable development indicators in Latvia 2003” by the Latvian Environment Agency (2004). The following trend in the amount of heavy metal emissions may be concluded from the data (the metals have been arranged in the order of descending (>) or approximately equal (≈) levels of emissions): Zn>Cu>Pb≈Cr≈Ni>Cd. Latvian Environment Agency data reflects that emissions of Pb, Cr, Ni and Cd are not increasing and have stabilized during the recent years (2001-2003). A significant increase in the total emission of Zn and Cu was observed particularly in Riga. That can be explained with a considerable increase in business activities related to the utilization of Zn and Cu and their compounds (manufacture of textile products, metal processing, manufacture of timber preservatives, some kinds of construction materials, manufacture and utilization of sanitary materials).

Experiments on sorption of Cr(VI), Ni and Pb with intact brewery yeast biomass and dehydrated yeast, hydroxylapatite ceramics and yeasts immobilized on hydroxylapatite ceramics were carried out. Experimental solutions containing Cr(VI), Ni or Pb and industrial wastewater samples containing Cr(VI) or Ni from the joint stock company “Kurzemes atslega 1” were used for experiments. Concentrations of Cr(VI), Ni and Pb were determined by means of a “MERCK” photometer SQ 118. Sorption effects were determined. Techniques of sorption experiments were developed and elaborated during preliminary studies. The research studies still have an ongoing status. Conclusions about sorption activity of yeasts, hydroxylapatite ceramics and yeasts immobilized on hydroxylapatite ceramics in regard to heavy metals will be made in future. Two master’s theses were worked out by students Līga Ersta (the University of Latvia) and Ivars Ozoliņš (the Riga Technical University).

ANALYSIS OF PM10 MONITORING RESULTS IN RIGA IN CONNECTION WITH ORIGINATION SOURCES

J. Kleperis, A. Osite[1], A. Viksna[1], E. Vītola[2], D. Danilāne[2]
1 - University of Latvia, Chemical Faculty, Kr.Valdemara Str. 48, Riga, LV-1013, Latvia
2 - Environmental Department of Riga City Council, Basteja Blv. 1, Riga, LV-1050, Latvia;

Streets and traffic are main source of particles in Riga, but not loner. Database of air polluters in Riga collected during more than 10 years includes also different point sources with plenty emissions of particles. Particle PM10 monitoring in Riga started only from 2000, but most reliable data are from 2003, when two street monitoring stations were established with two different PM10 monitors (SM200 and ESM FH62). Results from ESM instrument are with 30 min distinction ability and are analyzed together with traffic flow and meteorological data. Higher particle concentrations are registered in the spring months, but there is high number of days during all the year too, when value used as European Common Indicator towards a Local Sustainability Profile (50 mg/m3 for 24h averages of PM10) is exceeded. Road traffic emissions are calculated from detailed information on traffic volumes, vehicle compositions and driving conditions. The database of air polluters in Riga, hosted by Riga City Council, includes emissions from burning of different fuels in district and residential heating, emissions from industry that allow to estimate background concentrations of PM10 in Riga. Very approximate estimations were made about there-suspension of particulate matter from road dust, which is very important in springtime. The most uncertain emission data for particulate matter are combustion in private sector and off-road vehicles (in Riga the private houses which burns wood, oil, etc covers about 15% of territory) .

Furthermore, black carbon concentrations are analyzed from street canyon emissions by optical detection of the blackness of filters and characteristic metal concentrations determined as well. Black carbon collection directly from exhausts of different transport units demonstrated that not only class of transport and fuel used, but also average agedness is responsible for the concentrations of particles.

PEDAGOGIC TRIPLET PHENOMENON OF ACADEMIC ACHIEVEMENTS IN THE CASE OF PART TIME STUDENTS

U.Kanders, J.Kļaviņš

Statistical analysis of part time students' academic achievements has revealed the pedagogic triplet „5-7-9" phenomenon in percent frequency of grading marks. One can explain this phenomenon by influence at least of 2 factors – the first one is using a logarithmic level scale in the students' knowledge assessment procedure, the other one – dividing obviously part time students' into 3 categories, namely, "5"- "7-" un "9-"category.

Scientific Publications

Papers

1. A. Lūsis, J. Kleperis, E. Pentjušs. Amorphous thin films of tungsten oxide as a model of nanostructured mixed electron-ion conductors. Proceedings of the 1st Latvian conference "Nanomaterials and Nanotechnologies" (NENAMAT Mobilization Workshop), March 30-31, Riga (Latvia), p.30-33.

2. L. Grinberga, J. Kleperis, Metal alloys and composites for hydrogen storage: problems and solutions. Proceedings of the 1st Latvian conference "Nanomaterials and Nanotechnologies" (NENAMAT Mobilization Workshop), March 30-31, Riga (Latvia), p. 14-19.

3. J. Gaidelene, A. Kuzmin, J. Purans and C. Guéry, Influence of hydrogen intercalation on the local structure around Re ions in perovskite-type ReO_3, Phys. stat. sol. (c) 2 (2005) 149-152.

4. A. Kuzmin, R. Kalendarev, J. Purans, J.P. Itié, F. Baudelet, A. Congeduti and P. Munsch, EXAFS study of pressure-induced phase transition in $SrWO_4$, Physica Scripta T115 (2005) 556-558.

5. 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 T115 (2005) 149-151.

6. E. Avendaño, A. Kuzmin, J. Purans, A. Azens, G. A. Niklasson and C.G. Granqvist, Changes in the local structure of nanocrystalline electrochromic films of hydrated nickel vanadium oxide upon ozone-induced coloration, Physica Scripta T115 (2005) 464-466.

7. J. Purans, G. Heisbourg, N. Dacheux, Ph. Moisy and S. Hubert, XAFS study of local structure with picometer accuracy: $Th_{1-x}U_xO_2$ and $Th_{1-x}Pu_xO_2$ solid solutions, Physica Scripta T115 (2005) 925-927.

8. A. Kuzmin, J. Purans and R. Kalendarev, Ab initio calculations of the Ni K-edge XANES in $Ni_cMg_{1-c}O$ solid solutions, Phys. stat. sol. (c) 2 (2005) 665-668.

9. 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) 2 (2005) 704–707.

10. 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) 2 (2005) 708-711.

11. J. Purans, B. Fourest, C. Cannes, V. Sladkov, F. David, L. Venault, and M. Lecomte, Structural investigation of Pd(II) in concentrated nitric and perchloric acid solutions by XAFS, J. Phys. Chem. B 109 (2005) 11074-11082.

12. E. Cazzanelli, A. Kuzmin, G. Mariotto and N. Mironova-Ulmane, Behavior of one-magnon frequency in antiferromagnetic $Ni_cMg_{1-c}O$ solid solutions solid solutions, Phys. Rev. B 71 (2005) 134415:1-5.

13. N. Mironova-Ulmane, V. Skvortsova, A. Kuzmin and I. Sildos, Influence of radiation defects on exciton-magnon interactions in nickel oxide, Proc. SPIE 5946 (2005) 59460D:1-5.

14. 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 47 (2005) 1459-1464 [In Russian]; Phys. Solid State 47 (2005) 1516-1522.

15. G.P. Karwasz, A. Miotello, E. Zomer, R.S. Brusa, B. Koscielska, C. Armellini and A. Kuzmin, Structural studies of titanium oxide multilayers, Acta Phys. Polonica A 107 (2005) 977-982.

16. P. Fornasini, S. a Beccara, G. Dalba, R. Grisenti, J. Purans, A. Sanson, F. Rocca, D. Diop, EXAFS and local thermal expansion, Physica Scripta T115 (2005) 143–145.

17. G. Kizāne, J. Tīliks, A. Vītiņš, J. Tīliks Jr., J. Rudzītis. Behaviour of tritium in breeding materials. – Fusion Engineering and Design. November 2005. Vols. 75-79. Pp. 879-901.
18. L. Grinberga, J. Kleperis, The perspectives of Hydrogen energy in Latvia. Proceedings of the Local Conference: "Energetics and Environment in Baltics", University of Latvia, Faculty of Economics and Management, "Latvenergo Projekts" branch, Riga 2005, p. 21-32.
19. A. Osite, I. Steinberga, J. Kleperis, A. Viksna. Analysis of PM10 monitoring results in Riga in connection with origination sources. Proceedings of International Conference "Transport and Urban Polution", May 28-31, 2005, Graz (Austria).
20. J. Kleperis, L. Grinberga, A.D`Amico (Editors). Special Issue Papers: ISOEN 2003, Riga, Latvia, June 25-28 2005. Special Issue of *Sensors and Actuators*, vol. B106, issue 1, 2005, 186 p.
21. Vorohobovs V., Kleperis J. Negative Resistance and Temperature Stabilisation of Small Objects. "Information Technologies, Management and Society". Proceedings of the 2nd International Conference, 2004, April 15-16, Riga, Latvia. ISA (Informācijas Sistēmu Augstskola), Riga, 2004, lpp. 145-151.
22. В.Г. Ворохобов, Я. Клеперис, Некоторые аспекты конструктивных решений генератора озона и сенсора озона. Some aspects of engineering solutions of ozonizer and ozone sensor. Материалы конференции на CD. Первая всероссийская конференция «Озон и другие экологически чистые окислители. Наука и технологии», Москва, 7 – 9 июня 2005 г., 5 lpp.
23. J. Kleperis, V. Vorohobovs, S. Cesnieks, A. Vilde, A. Cesnieks. Application of Ozone and Environmental Monitoring Methods in Grain Drying. Applied for International Scientific Conference "Agricultural engineering problems", Jelgava, Latvia, June 2 - 3, 2005.
24. Kleperis, V. Vorohobovs, A. Vilde, S. Cesnieks, A. Cesnieks. Application of ozone and modern environmental monitoring methods in agriculture. 10th International Conference „New technological processes and investigation methods for agricultural engineering", September 8-9, Kaunas, Lithuania, 2005
25. J. Kleperis, A. Plate, A. Laurs, Requirements of Latvian environmental legislation: odour assessment and recommendations for reduction of odour nuisance from agriculture". Book, published by BEF (Baltic Environmental Forum), Riga, Latvia, October 2005, 23 pages.

Lectures on Conference

21st Scientific Conference of Institute of Solid State Physics of University of Latvia, Febr.7-9, 2005, Latvia, Riga, 2005

1) J.Gabrusenoks, Amplitude of thermal vibrations of the ionic crystals, Abstracts, p.19 (oral)

2) L.Grinberga, J. Kleperis, Hydrogen absorption and desorption researches in metalhydrides. Book of abstract p. 43 (oral)

3) G. Ķizāne, J. Tīliks, A. Vītiņš, E. Kolodinska. Tritium retention and release from beryllium metal (the BERYLLIUM experiment). –p. 78. (Oral)

4) J. Tīliks, G. Ķizāne, A. Vītiņš, J. Tīliks jr. Problems of tritium breeding in fusion facilities, p. 79. (Oral presentation.)

5) Ē. Pentjušs, G. Bajārs, A. Vītiņš, A. Lūsis. Lead-free soldering quality laboratory – current resources and requirements. p. 81. (Oral presentation.)

A. Lūsis, G. Bajārs, Ē. Pentjušs, A. Vītiņš. Lead free soldering quality problems in electronics, p. 82., (oral)

6) U.Kanders, J.Kļaviņš, Analysis of monthly energy use of buildings in order to improve their energy efficiency, p.85., (oral);

7) U.Kanders, J.Kļaviņš, Pedagogic triplet phenomenon of academic achievments in the case of part time students, p.86., (oral).

8) Julija Hodakovska. Researches of the sensor recovery time reduction facilities, p.83., (oral).

9) Vladimirs Vorohobovs, Ozone sensors and application examples, p.84., (oral).

3rd Annual Meeting of the Graduate School Denmark, National Laboratory, Risø,December 8th, 2005:

L. Grinberga, J. Kleperis, A.S. Pedersen, F.W. Poulsen, Investigations of the Influence of Glass Phase to the Lanthanum Rich Mischmetal. (oral and poster).

XVII International School-Seminar 'Spectroscopy of molecules and crystals', 20.09-26.09.2005, Beregove, Crimea, Ucraine,

J.Gabrusenoks Lattice dynamic properties of ReO3 (Poster, Abstracts, p.118).

Nanomaterials and nanotechnologies (NENAMAT), March 30-31, 2005, Riga, Latvia

1) A.Kuzmin, J.Purans, European "X-TIP" project: new nano-scale spectro-microscopy (oral).
2) L. Grinberga, J. Kleperis, Metal alloys and composites for hydrogen storage: problems and solutions (oral, abstract p. 21)
3) A. Lūsis, J. Kleperis, E. Pentjušs. Amorphous thin films of tungsten oxide as a model of nanostructured mixed electron-ion conductors (oral, abstract p.30-33.

International student conference on Development in Optics and Photonics 2005 (DOP), 30 April - 1 May, 2005, Riga, Latvia

J. Gaidelene, EXAFS spectroscopy of octahedrally coordinated oxide compounds (oral).

E-MRS Spring Meeting, May 31-June 3, 2005, Strasbourg, France:

1) N.D. Afify, R. Grisenti, G.Dalba, C. Armellini, M. Ferrari, S. Larcheri, F. Rocca, A. Kuzmin, Short range order around Er^{3+} in silica waveguides containing aluminium, titanium and hafnium. (poster)

2) S. Larcheri, C. Armellini, F. Rocca, A. Kuzmin, R. Kalendarev, G. Dalba, R. Graziola, J. Purans, D. Pailharey, F. Jandard, X-ray studies on optical properties of ZnO nanostructured thin fillms. (poster).

15th International Conference on Solid State Ionics (SSI-15), July 17-22, 2005, Baden Baden, Germany:

1) J. Purans, A. Kuzmin, R. Kalendarev, E. Cazzanelli, M. Castriota, Structural characterization of mixed Ta-Re oxide films (poster);

2) J. Purans, R. Merkle, A. Kuzmin, E. Kotomin, O. Mathon, M. Vracar, and J. Maier, XAFS study with subpicometer accuracy: Local structure of Fe in $SrFe_xTi_{1-x}O_{3-\delta}$. (poster).

29th International Conference on Solution Chemistry (ICSC), August 21-25, 2005, Portoroz, Slovenia.

J. Purans, A. Kuzmin, F. Rocca, XAFS study of Ln(iii) aqua-ions and ligand exchange rate of water molecules. (poster)

E-MRS 2005 Fall Meeting, September 5-9, 2005, Warsaw, Poland:

L.Grigorjeva, D.Millers, A.Kuzmin, R.Kalendarev,W.Łojkowski, A.Tomaszewska-Grzeda, Time-resolved luminescence of nanostructured ZnO (oral)

18th International Conference on X-ray Optics and Microanalysis (ICXOM), September 25-30, 2005, Frascati, Italy.

1) J. Purans, F. Comin, D. Pailharey, A. Kuzmin, O. Dhez, R. Felici, J. Chevrier, G. Dalba, S. Larcheri, F. Rocca, Element-Specific Contrast in Local Probe Microscopy via X-Ray Spectroscopy: Present Status and Future Perspectives. (oral)

2) D. Chen, J. Zhong, Z.Y. Wu, A. Kuzmin, A. Marcelli, Oxygen K-edge Investigation of $Ni_cMg_{1-c}O$ Solid Solutions. (poster)

Study of Matter at Extreme Conditions (SMEC), April 17-21, 2005, USA.

1) V. Efimov, E. Efimova, K. Iakoubovskii, S. Khasanov, D.I. Kochubey, V.V. Kriventsov, A. Kuzmin, B.N. Mavrin, M. Sakharov, V. Sikolenko, A.N. Shmakov, S.I. Tiutiunnikov, EXAFS, X-ray diffraction and Raman studies of $(Pb_{1-x}La_x)(Zr_{0.65}Ti_{0.35})O_3$ (x = 0.04 and 0.09) ceramics irradiated by high-current pulsed electron beam. (oral)

2) V.V.Efimov, E.A.Efimova, S.S.Khasanov, D.I.Kochubey, V.V.Kriventsov, A.Kuzmin, B.N.Mavrin, N.N.Novikova, V.V.Sikolenko, S.I.Tiutiunnikov, M.Tovar, I.O.Troyanchuk, V.A.Yakovlev, Y.Zubavichus, EXAFS, X-ray diffraction and raman studies of $La_{0.7}Sr_{0.3}CoO_3$ irradiated by high-current pulsed electron beam. (poster)

Workshop on the Coupling of Synchrotron Radiation IR and X-rays with Tip based Scanning Probe Microscopies, November 16-18, 2005, Grenoble, France. (1 oral, 2 posters):

1) J. Purans, F. Comin, D. Pailharey, F. Jandard, A. Kuzmin, O. Dhez, R. Felici, J. Chevrier, G. Dalba, S. Larcheri, F. Rocca, Element-Specific Contrast in Local Probe Microscopy via X-Ray Spectroscopy: Present Status and Future Perspectives. (oral)

2) A. Kuzmin, J. Purans, R. Kalendarev, L. Grigorjeva, K. Kundzins, V. Zauls, F. Jandard, D. Pailharey, X-TIP: Development of Laboratory Setup for X-Ray/AFM Experiments. (poster)

3) D. Pailharey, Y. Mathey, F. Jandard, S. Larcheri, C. Armellini, F. Rocca, A. Kuzmin, R. Kalendarev, G. Dalba, R. Graziola, J. Purans, V. Sammelselg, Nano-XEOL in near-field detection. (poster)

NORSTORE conference/workshop, June 2-5 2005, Hveragerði (Iceland);

1) J. Kleperis “Nano-phase versus bulk hydrogen storage materials – oral
2) L.Grinberga “Electrochemical and physical properties of LaMm and LaMm composites”

International conference “Theodor Grotthus Electrochemistry Conference, June 8-10 2005, Vilnius (Lithuania):

J. Kleperis “Researches of electrodes for hydrogen evolution/absorption” - poster

Latvijas fizikas biedrības 9. zinātniskā konference, 15.-16. septembris, 2005. Daugavpils, Latvija:

L. Grīnberga, J. Kleperis. Materiāli ūdeņraža enerģētikai – izaicinājums un iespējas. - oral

International conference “EcoBalt 2005”, May 5-6, 2005, Riga (Latvia):

1) L. Grinberga, J. Kleperis, L. Ribickis, Why the hydrogen energy is necessary for Latvia. (oral, Abstracts 43-45).
2) J. Kleperis, L. Osis. European common indicator no .5 “Air Quality” applying to Riga (oral).
3) J. Kleperis, J. Hodakovska, V. Vorohobovs, A.Cesnieks. From pesticides and domestic chemicals to ozone (oral).
4) E. Ratnieks, J. Kleperis. Traffic caused air pollution in urban environment and reduction activities (oral).

International Conference «Озон и другие, экологически чистые окислители. Наука и технологии» 7-9 июня 2005 года , Maskava (Krievija),

В.Г. Ворохобов, Я. Клеперис. Некоторые аспекты конструктивных решений генератора озона и сенсора озона (oral, abstract p. 41).

ICHMS`05 „Hydrogen Materials Science & Chemistry of Carbon Nanomaterials”

L. Grinberga, J. Kleperis, G. Vaivars, A. Nechaev, F.W. Poulsen, A.S. Pedersen, Investigations of the Influence of Different Additives to the Lanthanum Rich Mischmetal. Extended Abstracts of, Sevastopol (Ukraine), 2005, p. 244-245.

2nd International Conference "Information Technologies, Management and Society", 2004, April 15-16, Riga, Latvia. ISA (Informācijas Sistēmu Augstskola), Riga, 2004,

Vorohobovs V., Kleperis J. Negative Resistance and Temperature Stabilisation of Small Objects (oral, proceedings p.145-151).

Applied for International Scientific Conference "Agricultural engineering problems", Jelgava, Latvia, June 2 - 3, 2005;

J. Kleperis, V. Vorohobovs, S. Cesnieks, A. Vilde, A. Cesnieks Application of Ozone and Environmental Monitoring Methods in Grain Drying. (oral).

10th International Conference „New technological processes and investigation methods for agricultural engineering”, September 8-9, Kaunas, Lithuania, 2005:

J. Kleperis, V. Vorohobovs, A. Vilde, S. Cesnieks, A. Cesnieks. Application of ozone and modern environmental monitoring methods in agriculture (oral).

International conference EcoBalt 2005. Riga, May 5-6, 2005. – Riga, "Intego Plus", 2005:

R. Bendere, L. Ersta, A. Vītiņš. Heavy metal biosorption application for industrial waste water treatment. –. (Oral, p.140.)

13th International Workshop on Ceramic Breeder Blanket Interactions, Nov. 30 – Dec. 2, 2005. – University of California, Los Angeles, California, USA, 2005:

1) J. Tīliks, G. Ķizāne, A. Vītiņš, B. Leščinskis. Nanostructured ceramic blanket materials. (Oral, P. E1.)

2) J. Tiliks, G. Kizane, A. Vitins, E. Kolodinska, E. Rabaglino. Magnetic field effects on the tritium release from neutron-irradiated beryllium pebbles. (Oral, P. 33.)

Starptaut. zin. konf. "SABIEDRĪBA, INTEGRĀCIJA, IZGLĪTĪBA", Rēzeknes Augstskola, Rēzekne, 25.-26.02.2005:

1) Kanders U. Akadēmisko zināšanu vērtēšanas naturālā skala un tās atvasinājumi, 56.-68.lpp.

2) Trule I., Kanders U. Elektronisko studiju materiālu izmantošana tradicionālajā pedagoģijā, 325.-336.lpp.

NONLINEAR PROCESSES IN SOLIDS

Head of Laboratory *Dr. hab. phys.* Eugene A. Kotomin

Research Area and Main Problems

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

(i) kinetics of diffusion-controlled processes, with emphasis on pattern formation and catalytic surface reactions;
(ii) stochastization of magnetic field lines in magnetized fusion plasma;
(iii) gyrotron development;
(iv) the atomic and electronic structure of numerous advanced materials, with emphasis on calculations of properties of defects, surfaces, metal/insulator interfaces and nanostructures.

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

Scientific staff

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

PhD students

10. D. Gryaznov
11. V. Kashcheyevs
12. Yu. Mastrikov

Graduate students

13. D. Bocharov

Visitors from abroad

1. Prof. D.E. Ellis, Northwestern University, Evanston, Illinois, USA (1 week).

Our scientific visits abroad

1. Dr. hab. E. Kotomin, Max Planck Institute for Solid State Physics, Stuttgart, Germany (5.5 months), EU Institute of Transuranium Elements, Karlsruhe, Germany (4.5 months), Northwestern University, Evanston, USA (1 month)
2. Dr. hab. V. Kuzovkov, Braunschweig University of Technology, Germany (3 months)
3. Dr. O. Dumbrajs, Max Planck Institute for Plasma Physics, Garching, Germany (3 months)
4. Dr. Yu. Zhukovskii, Northwestern University, Evanston, USA (4 months), Max Planck Institute for Solid State Physics, Stuttgart, Germany (1 month), National Laboratory of Frascati, Italy (3 weeks), St. Petersburg University, Russia (3 weeks)
5. Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (10 months), National Laboratory of Frascati, Italy (3 weeks)
6. Dr. R. Eglitis, University of Osnabrück, Germany (11 months)
7. Dr. G. Zvejnieks, Institute of Semiconductor Physics, Vilnius, Lithuania (2.5 months), Max Planck Institute for Plasma Physics, Garching, Germany (1 month)

8. Dr. S. Piskunov, Northwestern University, Evanston, USA (5 months)
9. D. Gryaznov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (11 months)
10. V. Kashcheyevs, Tel Aviv University, Israel (11 months)
11. Yu. Mastrikov, Max Planck Institute for Solid State Physics, Stuttgart, Germany (11 months)

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 (Dr. T.M.J. Ikonen)
France	Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre) EU Institute of Transuranium Elements, Karlsruhe (Dr. R. Konings),
Germany	Institut für Hochleistungsimpuls&Mikrowellentechnik, Karlsruhe (Dr. B. Piosczyk) Max Planck Institut (MPI) für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) Max Planck Institut (MPI) für Plasmaphysik, Garching (Prof. Dr. H. Zohm) Technische Universität Braunschweig (Prof. Dr. W. von Niessen) Universität Osnabrück (Prof. Dr. G. Borstel)
Greece	School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. Y. Kominis)
Israel	School of Physics and Astronomy, Tel Aviv University (Prof. A. Aharony) Ben Gurion University of the Negev, Ber Sheeva (Prof. D. Fuks)
Italy	Laboratori Nazionali di Frascati (Prof. S. Bellucci)
Lithuania	Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Romania	University of Craiova (Dr. D. Constantinescu)
Russia	St. Petersburg University (SpbU) (Prof. R.A. Evarestov)
Spain	University of Barcelona (Prof. F. Illas)
Sweden	Uppsala University (Prof. K. Hermansson)
UK	King's College London (Prof. L. Kantorovich) University College London (Profs. A.M. Stoneham and A. Shluger)
USA	Northwestern University, Evanston, Illinois (Prof. D.E. Ellis) University of Maryland, College Park (Dr. G.S. Nusinovich) California Institute of Technology, Pasadena (Dr. E. Heifets)

Main Results

MONTE-CARLO MODELING OF ADSORPTION AND REACTION KINETICS OF OXYGEN AND CARBON MONOXIDE ON Pd(111) SURFACE

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

In collaboration with the *Semiconductor Physics Institute, Vilnius,* we have proposed the model for numerical simulation of the reaction O + CO $\rightarrow$ CO_2 and occurring phase transitions on the Pd(111) surface. We have calculated the phase diagram for this system using kinetic Monte Carlo method. It shows appearance of two phase transitions: $p(2\times2)_O \rightarrow \sqrt{3}\times\sqrt{3}R30^o{}_O$ and $\sqrt{3}\times\sqrt{3}R30_O \rightarrow p(2\times1)_O$ with increase of CO coverage for

room and intermediate temperatures, respectively. For the low temperature limit, the direct phase transition $p(2\times2)_O \rightarrow p(2\times1)_O$ is observed. We demonstrate that the reaction rate is the crucial factor determining the occurrence of the $p(2\times1)_O$ phase and vanishing of the $\sqrt{3}\times\sqrt{3}R30^o{}_O$ with decrease of temperature. The results of correlation function analysis indicate that the reaction proceeds either inside both the $p(2\times2)_O$ and $\sqrt{3}\times\sqrt{3}R30^o{}_O$ phases, or on the perimeter of the domains of $p(2\times1)_O$ structure.

CALCULATIONS OF THE EFFECTIVE DIFFUSION COEFFICIENT AND CONDUCTIVITY IN HETEROGENEOUS SOLIDS

J.R. Kalnin and E. Kotomin,J. Maier
(*MPI for Solid State Research, Stuttgart, Germany*)

Diffusion in heterogeneous solids is a very relevant topic in many fields of science and technology, ranging from ceramics to biology. This is also relevant for polycrystalline nanomaterials and composites in which the grain boundary exhibits transport coefficients different from the bulk. In order to suggest interpretation to numerous experimental studies of the diffusion and conductivity in nanomaterials performed in collaboration with *Max Planck Institute, Stuttgart*, we have performed the joint theoretical study of this problem. Briefly, we have analyzed results suggested in numerous papers on this subject in the framework of the effective medium approach, analyzed their limitations and suggested new equations. Correctness of our theoretical approach has been confirmed by Monte Carlo (MC) computer calculations.

STOCHASTIC PROCESSES IN GYROTRONS

O. Dumbrajs,
H. Kalis, and A. Reinfelds (*Institute of Mathematics, University of Latvia, Riga*)
G.S. Nusinovich (*University of Maryland, College Park, USA*)

In collaboration with *Institute of Mathematics of University of Latvia,* limits on the power generated by coaxial gyrotrons are investigated. It is shown that among all the operating modes suggested recently for coaxial super power gyrotrons only modes with azimuthal index m lower than about 44 pass the spatial stochasticity test. Modes with higher azimuthal indices cannot be used as operating modes because gyrotron oscillations become chaotic in the azimuthal direction and efficiency is very low. It is argued that there exists a natural upper limit on power generated by gyrotrons, which is about 4 MW

Stability of efficient operation at one of the high-order modes is of great importance for the development of megawatt-level gyrotrons intended for plasma experiments in controlled fusion reactors. Typically such gyrotrons operate at modes with large azimuthal indices, which form a rather dense spectrum of eigenfrequencies. Therefore, instead of considering interaction of electrons with a large number of such modes it is more convenient to analyze the spatial-temporal evolution of an envelope formed by a superposition of these modes with the electrons. In all previous studies of stability of such envelopes it was assumed that some kind of azimuthal non-uniformity is present in the initial condition for the wave envelope. However, the physical reason for this non-uniformity, which is apparently the non-uniformity of the electron emission, was not analyzed. In collaboration *with University of Maryland, College Park,* the relation between the emission non-uniformity and resulting non-uniformity of the wave envelope is established. Then, results of numerical simulations are given, which demonstrate various changes in the gyrotron dynamics caused by the azimuthal instability of the wave envelope. These results allow one to determine the maximum azimuthal index of

the operating mode and show that this maximum index can depend on the degree of azimuthal non-uniformity of the electron emission.

COAXIAL GYROTRON FOR ITER TOKAMAK

O. Dumbrajs,
B. Piosczyk, T. Rzesnicki, G. Dammertz, S. Illy, J. Jin, W. Leonhardt, G. Michel, M. Schmid, M. Thumm, and X. Yang (*Forschungszentrum Karlsruhe, Germany*)

ITER is the experimental step between today's studies of plasma physics and tomorrow's electricity-producing fusion power plants. In collaboration with *Forschungszentrum (Institut für Hochleistungsimpuls&Mikrowellentechnik), Karlsruhe,* the cavity has been designed for a first industrial prototype of a 2 MW, CW, 170 GHz coaxial cavity gyrotron. This gyrotron is now under fabrication, the design of critical components has been verified experimentally with a short pulse (~few ms) coaxial gyrotron. This tube utilizes the same quasi-optical (q.o.) RF-output system as designed for the industrial prototype and a very similar electron gun. The performance of the electron gun and beam has been found to be in agreement with the design. Concerning the microwave generation some discrepancy occurred between theory and experiment. In particular, the excited mode spectrum is more dense than expected. The measured pattern of the RF output beam was found to be in agreement with numerical simulations.

STOCHATIZATION AS A POSSIBLE CAUSE OF FAST RECONNECTION DURING SEVERAL MHD MODES ACTIVITY

O. Dumbrajs and G. Zvejnieks,
D. Constantinescu (*University of Craiova, Romania*),
V. Igochine and H. Zohm (*MPI for Plasma Physics, Garching, Germany*)

It was first observed at ASDEX Tokamak in 1982 that externally heated plasmas can suddenly reach an operating regime of improved confinement .In collaboration with *Max Planck Insitute, Garching* and *University of Craiova,* we have analyzed the role of stochastization of magnetic field lines in fast reconnection phenomena occurring in magnetized fusion plasma. A mapping technique has been applied to trace the field lines of toroidally confined plasma where the perturbation parameter is expressed in terms of experimental perturbation amplitudes determined from the ASDEX Upgrade Tokamak. It has been found that fast reconnection observed during amplitude drops of the neoclassical tearing mode instability in the frequently interrupted regime can be related to stochastization. It has been also shown that stochastization can explain the fast lost of confinement during the minor disruption. This demonstrates that stochastization can be regarded as a possible cause for different MHD events in ASDEX Upgrade Tokamak.

HAMILTONIAN MAP DESCRIPTION OF ELECTRON DYNAMICS

O. Dumbrajs,
Y. Kominis, K.A. Avramides, K. Hizanidis, and J.L. Vomvoridis
(*National Technical University of Athens, Greece*)

In collaboration with *National Technical University of Athens*, electron dynamics in gyrotron resonators are described in terms of a Hamiltonian map. This map incorporates the dependency of electron dynamics on the parameters of the interacting rf field and it can be used for trajectory calculations through successive iteration, resulting in a symplectic integration scheme. The direct relation of the map to the physics of the

model, along with its canonical form (phase space volume preserving) and the significant reduction of the number of iteration steps required for acceptable accuracy, are the main advantages of this method in comparison with standard methods such as Runge-Kutta. The general form of the Hamiltonian map allows for wide applications as a part of several numerical algorithms, which incorporate CPU-consuming electron trajectories calculations.

ANALYTICAL TECHNIQUES FOR CORRELATION EFFECTS IN LOW DIMENSIONAL NANOSTRUCTURES

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

In collaboration with *Tel Aviv University*, we have explored new analytical methods for the description of strong quantum correlations in the electronic nanostructures (quantum dots). When the electrons are confined in a low-dimensional structure, the single particle description becomes inadequate at low temperatures. One of the typical manifestations of the associated many-body effects is the Kondo screening of the spin of a quantum dot with an odd number of electrons. Such systems can be successfully described by model Hamiltonians that derive from a single impurity Anderson model. The latter includes the Coulomb (Hubbard) interaction term only for the impurity site (the quantum dot). Nevertheless, the associated physical quantities (conductance, charge and spin accumulation etc.) are extremely difficult to calculate due to the many-body nature of the problem. Exact solution for some thermodynamic quantities is known in several limiting cases, but obtaining a valid expression for the single-particle Green function in a wide parameter range remains a great challenge. We have applied a method of equations-of-motion to the quantum dot systems, and truncated the well-known hierarchy of exact equations for the electronic Green's functions at high order.

The resulting coupled non-linear integral equations have been solved self-consistently and analytically, using the theory of functions of the complex variable. The resulting expression for the electron Green function has been check against various exact theorems (Fermi liquid relations), and the exact solution (Bethe *ansatz*) in the corresponding limits. We have established that the proposed approximation is very accurate in all regimes except the low-temperature phase dominated by the Kondo screening. For the latter regime, the method gives a correct qualitative picture (e.g. singlet ground state, exponential increase in the spin susceptibility with lowering temperature), but underestimates the Kondo temperature, and more importantly, violates the celebrated Friedel sum rule by up to 30%. A simpler version of the equations-of-motion decoupling which omits the self-consistency and which has been widely used in the recent studies of the Kondo effect in unconventional settings is shown to be incorrect even on the qualitative level. Thus our method provides a necessary improvement for the studies of strongly correlated nanosystems. We continue investigation of the correlation effects in non-equilibrium settings using the model system of resonant quantum pumping.

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

E. Kotomin, Yu Zhukovskii, **S. Piskunov, D. Gryaznov, and Yu. Mastrikov**
R.A. Evarestov (*St. Petersburg University, Russia*),
F. Illas, N. Lopez, and J. Carrasco (*University of Barcelona, Spain*)
D.E. Ellis (*Northwestern University, Evanston, Illinois, USA*)
E. Heifets (*California Institute of Technology, Pasadena, USA*),
D. Fuks (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
J. Maier (*MPI for Solid State Research, Stuttgart, Germany*)

In collaboration with *St. Petersburg University, University of Barcelona,* and *Max Planck Institute for Solid State Research, Stuttgart,* we have studied *F* centers (O vacancies) in $SrTiO_3$ perovskite (both bulk and (001) surface of cubic phase stable at room temperature). For first principles calculations on the defective structures of cubic $SrTiO_3$, we have used both *CRYSTAL-03* 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 of oxygen vacancies is accompanied by noticeable relaxation of the first and second nearest neighbors. The lattice relaxation around the *F* center has been found to be sensitive to both shape and size of supercell as well as calculation method. The larger is supercell, the closer *defect energy level* in the band gap lies to the conduction band bottom, approaching the optical ionization energy of 0.49 eV for 270- and 320-atomic supercells, where the distance between neighboring defects is as large as four lattice constants. For these supercells, the defect bandwidth decreases down to 0.02-0.03 eV, *i.e.* the defect-defect interaction becomes negligible.

In collaboration with *Max Planck Institute for Solid State Research, Stuttgart, St. Petersburg University, and California Institute of Technology, Pasadena,* we have performed detailed *ab initio* calculations on technologically important material used as a cathode of the solid oxide fuel cells, *i.e.* $LaMnO_3$ bulk (both high temperature cubic and low temperature orthorhombic phases) and its (100) and (110) surfaces (with emphasis on the surface energies and polarization). We have compared two density functional theory formalisms: DFT-LCAO (as implemented in *CRYSTAL-03* code) and DFT with plane waves (*VASP code*). When comparing results of our calculations with those available in the literature, we have showed that only the hybrid exchange-correlation functional (B3PW) allows us to reproduce the experimental magnetic coupling constants and optical gap. Keeping in mind the fuel cell applications, we have treated the orthorhombic cells with Mn-terminated stoichiometric slabs in the 001 direction. We have found that the surface containing cubic cells is energetically more favorable. Moreover, the (001) surface possesses a lower energy than that of the (110) surface. In these large scale modeling we have increased the slab thickness from 4 to 14 planes. Different spin configurations on Mn have been used and compared. We also relaxed those surfaces and analyzed the charge density redistribution near the surface indicating the chemical bond covalency.

In collaboration with *Ben Gurion University, Ber Sheeva,* a special thermodynamic approach has been developed, to predict material properties as the temperature changes, *i.e.* to analyze order-disorder transitions. Ground state energies of different Sr-doped $LaMnO_3$ ordered structures have been calculated using first principles method and later used in the thermodynamic approach. This allowed us to conclude that disordering of a technologically important 12.5% Sr-doped $LaMnO_3$ phase with respect to the

decomposition into the heterogeneous mixture can occur only at temperatures above the melting point. Along with the thermodynamic analysis, we could also compare two realizations of DFT method for calculation of the properties of Sr-doped $LaMnO_3$, using the packages *WIEN-2k* and *CRYSTAL-03*. Both methods give similar tendencies for predicting the material behavior, however, DFT-LCAO method overestimates temperature of the order-disorder transition as compared to plane wave DFT. Based on *CRYSTAL-03* calculations for a number of the $Ba_cSr_{1-c}TiO_3$ (BST) superlattices, we have also developed a thermodynamic approach to these solid solutions. In particular, we have calculated the BST phase diagram and showed that at relatively low temperatures (below 400 K for c=0.5 and 300 K for c=0.1) the spinodal decomposition of the solid solution occurs. As a result, we predict for small Ba concentrations formation of $BaTiO_3$ nanoregions in a predominantly $SrTiO_3$ matrix and vice versa, which is confirmed by the Raman, polarization, ultrasonic, neutron diffraction, and diffusion experiments.

Adsorption of gas-phase oxygen on the ABO_3 perovskite surfaces is important for high temperature oxygen sensors, in photocatalysis, and fuel cell applications. In close cooperation with *Northwestern University, Evanston*, we have performed *ab initio* calculations of the energetics, geometry of fully relaxed structure, electronic charge redistribution, and density of states for adsorbed atomic and molecular oxygen on defectless unreconstructed SrO- and TiO_2-terminated $SrTiO_3$(001) surfaces. We have found substantial binding energies for *atomic O adsorption*: (*i*) atop surface oxygen ion (up to 1.8 eV) and (*ii*) at bridge sites, ***i.e.*** positions between the two adjacent metal and oxygen surface ions on both SrO- and TiO_2-terminated surface (over 2.0 eV). In both cases the strong bonding is rather caused by formation of surface molecular peroxide ion O_2^{2-} which ground state is a singlet. *For molecular adsorption*, different adsorption sites and orientations of O_2 molecule have been studied, however, adsorption energy never exceeded 0.1 eV. Adsorption of oxygen on strontium titanate has been found to depend significantly on temperature and partial pressures in the gas phase.

FIRST PRINCIPLES MODELING AND THERMODYNAMIC STUDY OF THIN METAL FILMS ON METAL OXIDES AND PEROVSKITES

Yu. Zhukovskii and E. Kotomin,
A.M. Stoneham (*University College London, UK*),
D. Fuks (*Ben Gurion University of the Negev, Ber Sheeva, Israel*),
D.E. Ellis (*Northwestern University, Evanston, Illinois, USA*)
P. Balaya and J. Maier (*MPI for Solid State Research, Stuttgart, Germany*),

In collaboration with *Northwestern University, Evanston, Ben Gurion University Ber Sheeva,* and *University College London,* we have continued *ab initio* calculations (using hybrid B3LYP method) and thermodynamic study of copper and silver adhesion onto both perfect and defective magnesia substrate. For a defectless magnesia surface, we confirm the experimentally observed submonolayer growth of 3D metallic islands (Ag possesses a higher trend than Cu). Their shapes have been found to be pyramid-like. Formation of O vacancies on the substrate markedly enhances metal atom adsorption as compared to physisorption over regular sites on a defect-free substrate. For the first time, we predict that the presence of these surface defects (beginning with concentrations of 5 per cent for Cu and 22 per cent for Ag) can stimulate the growth of uniform 2D metallic sublayers.

In collaboration with *Northwestern University, Evanston,* we have continued *CRYSTAL-03* calculations for copper adsorption on a regular, defect-free TiO_2- and BaO-terminated (001) surfaces of a cubic $BaTiO_3$, using the hybrid B3PW method (instead of

a posteriori HF-CC used earlier). 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 binding energy (*per* adatom) and enhances the interatomic interactions inside growing metallic film. For mostly ionic BaO-terminated substrate we compare our results with earlier obtained data for the perfect Cu/MgO(001) interface.

In collaboration with *Max Planck Institute for Solid State Research, Stuttgart,* we present theoretical support for experimentally observed storage anomaly for nanocomposites in the context of lithium batteries. According to experimental investigations on Ru/Li_2O nanocomposite (2-5 nm), an extra Li storage is possible resulting in a capacitive voltage-charge behavior, which is neither due to homogeneous (insertion) nor heterogeneous (conversion) reactions. The low potential (1.2-0.02 V *vs.* Li^+/Li) extra capacity, obtained in metal/Li_2O nanocomposite can be explained by an "interfacial storage mechanism". *Ab initio* calculations on the atomic and electronic structure of Ti(0001)/Li_2O(111) model interface performed using hybrid B3PW method, both indicate the validity of the phenomenological model of the interfacial Li storage mechanism and predicts conditions of its realization. Compared to a pure Li_2O, a Ti/Li_2O(111) interface can store at least a monolayer of additional Li per interface with electrons being transferred largely to the titanium adatoms. In addition it highlights the occurrence of a varied stoichiometry of nanosized solids compared to massive phases.

FIRST PRINCIPLES SIMULATION OF ELECTRONIC STRUCTURE OF PERFECT AND DEFECTIVE CaF_2

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

In collaboration with *Osnabrück University,* we have performed *ab initio* calculations on technologically important calcium fluoride (perfect and defective bulk and densely-packed surfaces), using hybrid B3PW method as implemented in *CRYSTAL'03* code, which provides the best agreement with experiment for the band gap width (11.0 *vs.* 12.1 eV, respectively). When comparing results of calculations on CaF_2 (111), (110), and (100) surfaces, we confirm that the CaF_2(111) surface is the most stable one, in agreement with the experiment. The characterization of *F* centers in CaF_2 is still a question of debate. We found, that the vacancy formation energy in CaF_2 is 7.87 eV. The charge-density map of the *F* center in CaF_2 shows that the charge is well localized inside the vacancy. The spin density in *F* center has been found to be 0.716 *e*. The relaxation of atoms around the *F* center is rather small. *F* center level within band gap suggests a possible mechanism for explanation of the optical absorption observed experimentally in CaF_2 at 3.3 eV.

EXPERIMENTAL AND THEORETICAL STUDIES OF NANOSTRUCTURED ALUMINIUM NITRIDE

A. Popov and Yu. Zhukovskii
C. Balasubramanian and S. Bellucci (*National Laboratory of Frascati, Italy*),
A. Ivanov and H. Schober (*Institut Laue Langevin, Grenoble, France)*
V. Savchyn, N. Krutyak, and I. Karbovnyk (*National University of Lviv, Ukraine*)

AlN nanotubes (NTs) and nanoparticles (NPs) have been synthesized by using a highly nonequilibrium direct-current (DC) arc plasma method. The nanotubes sample contained around 80% NTs (~25-30 nm in diameter, ~700 nm length) and the rest NPs. The nanoparticles sample contained more than 95% NPs, with diameter varying between 40–60 nm, and the rest were NTs. In collaboration with *National Laboratory of Frascati* we have studied cathodoluminescence (CL) spectra of powder samples containing mostly AlN NTs, and of powder samples consisting mostly of AlN NPs, in comparison to that of the commercially available aluminum nitride powder. A clear difference between emission spectra of commercial AlN, AlN NPs and AlN NTs has been found. Commercial AlN emits light at 3.5 eV. For the sample, containing AlN NPs, this peak is slightly shifted to higher energies. It is well known that the position of this emission band depends on oxygen content in the sample. We suggest that the slight difference in the band positions might be due to the different concentration of oxygen impurities in the investigated samples. The CL spectrum of aluminum nitride NTs shows an additional emission peak near 2.25 eV.

In collaboration with *Institut Laue Langevin, Grenoble,* we have performed the neutron scattering study of synthesized AlN NTs. We discuss the generalized density of phonon states G(ω) for the NTs in comparison with bulk AlN. *G*(ω) for the bulk features two main bands at low (~30 meV) and high (~80 meV) frequencies. Both bands are completely smeared out in the nanomaterial indicating a broad distribution of force constants induced by structural disorder. Apart from the smearing out of the vibrational bands we observe enhanced intensities at low frequencies (< 10 meV) as usually found in disordered systems. The observed changes in the microscopic dynamics must lead to appreciable differences in the thermal and transport properties of the NTs with respect to the bulk material.

Theoretical simulations serve as the effective tool for a study of both the atomic and electronic structure of AlN nanotubes and can complement the corresponding experiments for the comprehensive development of nanotube engineering. In collaboration with *National Laboratory of Frascati,* we have constructed single-walled models of AlN nanotubes with two different chiralities: armchair- and zigzag-type. To analyze dependence of their electronic structure on the thickness of AlN NT, we have considered two different diameters for both NT types: 1 nm and 6 nm. It allows us to analyze how a curvature of NT changes their properties as compared to both AlN bulk and n-type densely packed surfaces (with either wurtzite or zincblende structures). We have found, the smaller diameter of AlN NT, the closer its total density of one-electron states to that for bulk material, and *vice versa*, the properties of thick nanotubes approach to surface. Our periodic 1D calculations performed using *CRYSTAL-03* code show that various configurations of AlN NTs are energetically stable with a smooth tubular single wall and a uniform diameter. The larger NT diameter, the closer its properties to AlN(0001) surface and smaller dependence of NTs on their chirality, *i.e.* their armchair- and zigzag-structures become energetically closer.

Scientific papers published in 2005

1. D. Fuks, S. Dorfman, S. Piskunov, and E.A. Kotomin, *Ab initio* thermodynamics of $Ba_cSr_{1-c}TiO_3$ solid solutions. - *Physical Review B*, 2005, **71**, 014111, (p. 1-9).
2. H. Shi, R.I. Eglitis, and G. Borstel, *Ab initio* calculations of the CaF_2 electronic structure and *F* centers. - *Physical Review B*, 2005, **72**, 045109, (p. 1-9).
3. R.A. Evarestov, E.A. Kotomin, Yu.A. Mastrikov, D. Gryaznov, E. Heifets, and J. Maier, Comparative density-functional LCAO and plane-wave calculations of $LaMnO_3$ surfaces. - *Physical Review B*, 2005, **72**, 214411, (p. 1-12).
4. S. Piskunov, E. Heifets, E.A. Kotomin, J. Maier, R.I. Eglitis, and G. Borstel, Hybrid DFT calculations of the atomic and electronic structure for ABO_3 perovskite (001) surfaces. - *Surface Science*, 2005, **575**, p. 75-88.
5. V.N. Kuzovkov and W. von Niessen, The phase diagram of the multi-dimensional Anderson localization *via* analytic determination of Lyapunov exponents. - *European Physics Journal B*, 2004, **42**, p. 529-542.
6. R.I. Eglitis and G. Borstel, Towards a practical rechargeable 5 V Li ion battery. - *Physica Status Solidi (a)*, 2005, **202**, p. R13-R15.
7. R.A. Evarestov, A.V. Bandura, V.E. Alexandrov, and E.A. Kotomin, DFT LCAO and plane wave calculations of $SrZrO_3$. - *Physica Status Solidi (b)*, 2005, **242**, p. R11-R13.
8. E.M. Fernandez, R.I. Eglitis, G. Borstel, and L.C. Balbos, Adsorption and dissociation of water on relaxed alumina clusters: a first principles study. - *Physica Status Solidi (b)*, 2005, **242**, p. 807-809.
9. H. Shi, R.I. Eglitis, and G. Borstel, First-principles calculations of the CaF_2 bulk and surface electronic structure. - *Physica Status Solidi (b)*, 2005, **242**, p. 2041-2050.
10. Y. Kominis, O. Dumbrajs, K.A. Avramides, K. Hizanidis, J.L. Vomvoridis, Chaotic electron dynamics in gyrotron resonators. – *Physics of Plasmas*, 2005, **12**, 043104 (p. 1-9).
11. O. Dumbrajs and G.S. Nusinovich, Azimuthal instability of radiation in gyrotrons with overmoded resonators. – *Physics of Plasmas*, 2005, **12**, 053106 (p. 1-9).
12. O. Dumbrajs, V. Igochine, D. Constantinescu, and H. Zohm, Stochastization as a possible cause of fast reconnection in the frequently interrupted regime of neoclassical tearing modes. - *Physics of Plasmas*, 2005, **12**, 110704 (p. 1-4).
13. Y. Kominis, O. Dumbrajs, K.A. Avramides, K. Hizanidis, J.L. Vomvoridis, Canonical perturbation theory for complex electron dynamics in gyrotron resonators. – *Physics of Plasmas*, 2005, **12**, 113102 (p. 1-12).
14. E.A. Kotomin, R.A. Evarestov, Yu.A. Mastrikov, and J. Maier, DFT plane wave calculations of the atomic and electronic structure of $LaMnO_3$ (001) surface. - *Physical Chemistry & Chemical Physics*, 2005, **7**, p. 2346–2350.
15. Yu.F. Zhukovskii, E.A. Kotomin, Yu. Mastrikov, and J. Maier, *Ab initio* simulations on AgCl(111) surface and AgCl(111)/*a*-Al_2O_3(0001) interface. - *Computational Materials Science*, 2005, **33**, p. 276-281.
16. T.M.J. Ikonen and O. Dumbrajs, Search for deterministic chaos in ELM time series of ASDEX Upgrade tokamak. - *IEEE Transactions on Plasma Science*, 2005, **33**, p. 1115-1122.
17. O. Dumbrajs, H. Kalis, and A. Reinfelds. "Are coaxial super power gyrotrons feasible?" - *International Journal of Infrared Millimeter Waves*, 2005, **26**, p.787-805.

18. R.I. Eglitis, E.A. Kotomin, and G. Borstel, Large scale computer modeling of point defects in ABO_3 perovskites. - *Physica Status Solidi (c) (Proceedings of ICDIM'04, Riga, 2004)*, 2005, **2**, p. 113-119.

19. V.S. Vikhnin, S.E. Kapphan, R.I. Eglitis, and R.M. Pirc, Charge transfer vibronic excitons. - *Physica Status Solidi (c) (Proceedings of ICDIM'04, Riga, 2004)*, 2005, **2**, p. 120-123.

20. J. Carrasco, F. Illas, N. Lopez, E.A. Kotomin, Yu.F. Zhukovskii, S. Piskunov, J. Maier, and K. Hermansson, First principles simulations of *F* center in $SrTiO_3$ perovskite. - *Physica Status Solidi (c) (Proceedings of ICDIM'04, Riga, 2004)*, 2005, **2**, p. 153-158.

21. Yu.F. Zhukovskii and E.A. Kotomin, Coin metal adsorption on defective MgO(001) surface: *ab initio* study. - *Physica Status Solidi (c) (Proceedings of ICDIM'04, Riga, 2004)*, 2005, **2**, p. 347-350.

22. S. Piskunov, E.A. Kotomin, D. Fuks, and S. Dorfman, *Ab initio* calculations of the atomic and electronic structure of layered $Ba_{0.5}Sr_{0.5}TiO_3$ structures. - *Materials Science & Engineering B (Proceedings of Spring EMRS, Strasbourg, 2004)*, 2005, **118**, p. 15-18.

23. Yu.F. Zhukovskii, D. Fuks, E.A. Kotomin, and S. Dorfman, *Ab initio* thermodynamics for the growth of ultra-thin Cu film on a perfect MgO(001) surface". *Materials Science & Engineering C (Proceedings of Spring EMRS, Strasbourg, 2004)*, 2005, **25**, p. 713-717.

24. S. Dorfman, S. Piskunov, E.A. Kotomin, and D. Fuks, Electronic properties of layered $Ba_{0.5}Sr_{0.5}TiO_3$ heterostructure: *ab initio* hybrid density functional calculations. - *Physica Scripta (Proceedings of International Meeting on Applied Physics, Badajos, 2003)*, 2005, **T118**, p. 276–279.

25. D. Gryaznov, J. Fleig, and J. Maier, Numerical study of grain boundary diffusion in nanocrystalline Materials. - *Defect & Diffusion Forum (Proceedings of 6th International Conference DIMAT'04, Cracow, 2004)*, 2005, **237-240**, p. 1043-1048.

26. Yu.F. Zhukovskii, S. Piskunov, E.A. Kotomin, O. Sychev, and G. Borstel, *Ab initio* modeling of copper adhesion on regular $BaTiO_3$(001) surfaces. - *Microelectronic Engineering, (Proceedings of Nano and Giga Challenges Microelectronics Symposium, Cracow, 2004)*, **81**, 2005, p. 467-471

27. 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. - *Microelectronic Engineering, (Proceedings of Nano and Giga Challenges Microelectronics Symposium, Cracow, 2004)*, 2005, p. 472-477.

28. S. Piskunov, S. Dorfman, D. Fuks, and E.A. Kotomin, $Ba_cSr_{1-c}TiO_3$ perovskite solid solutions: Thermodynamics from *ab initio* electronic structure calculations. – *Microelectronic Engineering, (Proceedings of Nano and Giga Challenges Microelectronics Symposium, Cracow, 2004)*, 2005, p. 478-484.

29. E.A. Kotomin, Yu.A. Mastrikov, D. Gryaznov, and Yu.N. Shunin, First principles calculations of the atomic and electronic structure of $LaMnO_3$ surface. – *Proceedings of 3^d International Conference "Information Technologies and Management" (IT&M, Riga, 2005)*, 2005, p. 7-22.

30. Yu.F. Zhukovskii, R.A. Evarestov, E.A. Kotomin, Yu.A. Mastrikov, S.N. Piskunov, and Yu.N. Shunin, The simplest defect in perovskite $SrTiO_3$ crystals: atomic and electronic structure of a single *F*-center. - *Proceedings of 3^d International Conference "Information Technologies and Management" (IT&M, Riga, 2005)*, 2005, p. 23-39.

Popular scientific articles

31. J.R. Kalnin and G. Ozolinsh, Integrated framework for social, economic or business system modelling. - *Proceedings of 3d International Conference "Information Technologies and Management" (IT&M, Riga, 2005),*, 2005, p. 40-48.
32. V.I. Florovs, A. Cebers, D. Bocharov, V. Kashcheyevs, and D. Docenko, The 30th Open Olympiad of Latvia in Physics. - *The Starry Sky*, 2005, **190**, p. 63-70.

Presentations at Conferences

I. 21st ISSP Conference (Riga, Latvia, February, 2005).

1. D. Bocharov and A. Kuzmin, "Quantum chemistry interpretation of X-Ray spectra". Abstracts: p. 21.
2. G. Zvejnieks and V.N. Kuzovkov, "Analysis of JET ELMy time series". Abstracts: p. 73.

II. The 3rd International Conference "Information Technologies and Management", IT&M'05 (Riga, Latvia, April, 2005).

1. E.A. Kotomin, E. Heifets, Yu. Mastrikov, D. Gryaznov, and Yu.N. Shunin, "*Ab initio* calculations of the atomic and electronic structure of ABO_3 perovskite surfaces". Abstracts: p. 15-16.
2. Yu.F. Zhukovskii, R.A. Evarestov, E.A. Kotomin, S. Piskunov, and Yu.N. Shunin, "The simplest defect in perovskite $SrTiO_3$ crystals: atomic and electronic structure of a single *F*-center". Abstracts: p. 17-18.
3. O. Dumbrajs, "Stochastic processes in gyrotrons". Abstracts: p. 19.
4. J.R. Kalnin, "Fostering creativity". Abstracts: p. 63.
5. J.R. Kalnin and G. Ozolinsh, "Integrated framework for social, economic or business system modeling". Abstracts: p. 64-65.

III. The 9th V.A. Fock Meeting on Quantum and Computational Chemistry (Velikiy Novgorod, Russia, May, 2005).

1. R.A. Evarestov, E.A. Kotomin, and Yu.F. Zhukovskii, "DFT study of a single *F* center in cubic $SrTiO_3$ perovskite: periodic model of *aperiodic* system". Abstracts: p. 26.

IV. Lithium Batteries Discussion (LiBD-2005) "Electrode Materials" (Arcachon, France, May, 2005).

1. P. Balaya, M. Dolle, H. Li, Y. Hu, J. Jamnik, Yu.F. Zhukovskii, E.A. Kotomin, and J. Maier, "Nanocrystallinity effects in lithium battery electrodes with RuO_2 as a model material". Abstracts: p. 72-73.

V. 36th Lithuanian National Physical Conference (Vilnius, Lithuania, June, 2005).

1. V. Petrauskas, E.E. Tornau, G. Zvejnieks, and V.N. Kuzovkov, "Monte-Carlo modelling of adsorption and reaction kinetics of oxygen and carbon monoxide on Pd(111) surface". Abstracts: S2-50.

VI. 13th International Congress on Thin Films/8th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures ICTF13/ACSIN8 (Stockholm, Sweden, June 2005).

1. G. Zvejnieks, V.N. Kuzovkov, V. Petrauskas, and E.E. Tornau, "Modelling of phase transitions and reaction at CO adsorption on oxygen precovered Pd (111)".

VII. 3rd International Conference on Materials for Advanced Technologies ICMAT-2005 (Singapore, July 2005).

1. P. Balaya, A. Bhattacharyya, J. Jamnik, and E.A. Kotomin, "Nano-ionics in the context of Li Batteries". Abstracts: p. 4.
2. R.I. Eglitis, H. Shi, and G. Borstel, "*Ab initio* calculations of the CaF_2 bulk and surface electronic and band structure". Abstracts: p. 235.
3. R.I. Eglitis, G. Borstel, E. Heifets, S. Piskunov, and E.A. Kotomin, "*Ab initio* calculations of the $SrTiO_3$, $PbTiO_3$, $BaTiO_3$ (001) and $BaTiO_3$ (110) surfaces". Abstracts: p. 142.

VIII. 15th International Conference on Solid State Ionics (Baden-Baden, Germany, July, 2005).

1. P. Balaya, Y.F. Zhukovskii, M. Dolle, E.A. Kotomin, H. Li, and J. Maier, "Experimental and theoretical evidence for novel interfacial mechanism for lithium storage in nanocomposites". Abstracts: 164.
2. D. Gryaznov, J. Fleig, and J. Maier, "Numerical study of grain boundary diffusion in nanocrystalline solid state ionics". Abstracts: P-258.
3. D. Fuks, J. Felsteiner, L. Bakaleinikov, A. Gordon, E.A. Kotomin, J. Maier, and J. Fleig, "Thermodynamic stability and chemical bonding in $(La_{7/8}Sr_{1/8})MnO_3$". Abstracts: P-257.
4. J. Purans, R. Merkle, A. Kuzmin, E.A. Kotomin, O. Mathon, M. Vracar, and J. Maier, "XAFS study with subpicometer accuracy: local structure of Fe in $SrFe_xTi_{1-x}O_{3-y}$". Abstracts: P-489.

IX. 8th International Conference on the Structure of Surfaces (Munich, Germany, July, 2005).

1. Yu.F. Zhukovskii, E.A. Kotomin, and D. Ellis, "First principles simulation on the defect-free $Cu/BaTiO_3(001)$ cubic interfaces". Abstracts: p. 155.
2. D. Fuks, Yu.F. Zhukovskii, E.A. Kotomin, and D. Ellis, "Coin metal adsorbtion on perfect and defective MgO(001) surfaces: the electronic structure calculations and film growth thermodynamics". Abstracts: p. 227.
3. Yu.F. Zhukovskii, E.A. Kotomin, S. Krischok, O. Hőfft, and V. Kempter, "A comparative analysys of electron spectroscopy and *ab initio* studies on Cu adsorbtion on MgO". Abstracts: p. 228.

X. 6th International Workshop "Strong Microwaves in Plasmas" (Nizhniy Novgorod, Russia, July, 2005).

1. B. Piosczyk, S. Alberti, D. Bariou , P. Benin, T. Bonicelli, G. Dammertz, O. Dumbrajs, *et al.*, "Progress in the development of the 170 GHz Coaxial cavity gyrotron for ITER". - Abstract: S9.
2. O. Dumbrajs and G.S. Nusinovich, "Are coaxial super power gyrotrons feasible?". - Abstract: S16.

XI. 7th International Working Session "Statistical Physics for Anomalous Transport in Plasmas" (Craiova, Romania, August, 2005).

1. O. Dumbrajs, Y. Kominis, K.A. Avramides, K. Hizanidis, J.L. Vomvoridis, "Hamiltonian map description of electron dynamics in gyrotrons".

XII. 23rd European Conference on Surface Science, ECOSS'23, (Berlin, Germany, September 2005).

1. Yu.F. Zhukovskii, E.A. Kotomin, S. Krischok, P. Stracke, O.Höfft, and V. Kempter, "A comparative analysis of electron spectroscopy and *ab initio* studies on Cu adsorption on MgO". - Abstract: p. 191-192.

XIII. 9th Conference of Latvian Physical Society (Daugavpils, Latvia, September 2005).

1. J. Tambergs, A. Andrejevs, D. Bocharov, and J. Ruzha, "Albert Einstein's heritage". Abstracts: p. 31.

XIV. The Ψ_k Conference 2005 (Schwäbisch Gmünd, Germany, September, 2005).

1. Yu.F. Zhukovskii, E.A. Kotomin, Yu.A Mastrikov, and J. Maier, "*Ab initio* study of ionic conductivity on AgCl/*a*-Al_2O_3 (0001) interface". Abstracts: p. 472.
2. Yu.F. Zhukovskii, E.A. Kotomin, P. Balaya, and J. Maier, "First principles modelling of interfacial Li storage". Abstracts: p. 473.

XV. International Conference on Diffusion Fundamentals (Leipzig, Germany, September, 2005).

1. J.R. Kalnin, E.A. Kotomin, J. Maier, and V.N. Kuzovkov. "Calculation of the effective diffusion coefficient for heterogeneous media". Abstracts: p. 142-143.
2. V.N. Kuzovkov and W. von Niessen. "Anderson localization and generalized diffusion". Abstracts: p. 152-153.
3. V.N. Kuzovkov, G. Zvejnieks, O. Kortlüke, and W. von Niessen. "Forced oscillations in self-oscillating surface reaction models." Abstracts: p. 154-155
4. V.N. Kuzovkov, E.A. Kotomin, and G. Zvejnieks. "Modelling of diffusion-controlled pattern formation in thin metallic film growth on crystalline substrates." Abstracts: p. 156-157.
5. D.Gryaznov, J. Fleig, and J. Maier, "Numerical study of grain boundary diffusion: size effects". Abstracts: p. 266-267.

XVI. GLOBAL 2005 International Conference "Nuclear Energy Systems for Future Generation and Global Sustainability" (Tsukuba, Japan, October, 2005).

1. C. Ronchi, P.V. Uffelen, A. Schubert, C. Bruynooghe, J.V. Laar, E.A. Kotomin, *et al.*, "The new nuclear fuel R&D plan of the JRC-ITU on uranium-plutonium-americium nitrides and carbides". - Abstracts: 5B-II, 391.

XVII. 47th Annual Meeting of the Division of Plasma Physics (Denver, CO, USA, October, 2005).

1. O. Dumbrajs, V. Igochine, D. Constantinescu, and H. Zohm, "Stochastization as a possible cause of fast reconnection during several MHD modes activity". Abstracts: FO2.00009

XVIII. 10th Workshop on Active Control of MHD Stability (Madison, WI, USA, October-November, 2005).

1. O. Dumbrajs, V. Igochine, D. Constantinescu, and H. Zohm, "Stochastization as a possible cause of fast reconnection in the frequently interrupted regime of neoclassical tearing modes". Abstracts: 1-NTM.3.

XIX. Nanoscience & Nanotechnology (Frascati, Italy, November, 2005).

1. E.A. Kotomin and A.I. Popov, "Point defect aggregation and metallic colloid formation in ionic solids". Abstracts: p. 58.
2. Yu.F. Zhukovskii, A.I. Popov, C. Balasubramanian, P. Onorato, and S. Bellucci, "Structural and electronic properties of single-walled AlN nanotubes of different chiralities and sizes". Abstracts: p. 71.
3. S. Bellucci, A.I. Popov, C. Balasubramanian, V. Savchyn, N. Krutyak, and I. Karbovnyk, "Cathodoluminescence of nanostructured aluminum nitride". Abstracts: p. 85-86.

XX. Materials Models and Simulations for Nuclear Fuels (Washington DC, USA, November, 2005).

1. E.A. Kotomin, P. Van Uffelen, and C. Ronchi, "Atomistic modeling of radiation and impurity defects in UN nuclear fuels".

XXI. 2005 MRS Fall Meeting (Boston, MA, USA, November-December, 2005).

1. S. Piskunov, E.A. Kotomin, Yu.F. Zhukovskii, and D.E. Ellis, "Adsorption of atomic and molecular oxygen on the $SrTiO_3$(001) surfaces: Computer simulations by means of hybrid density functional calculations and *ab initio* thermodynamics. Abstracts: LL8.5.

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 are studied. The main task was RTD of high sensitive photoresists in the visible region for holography and lithoghraphy for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed. 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

Technical Staff

1. J.Gurovs
2. D.Popele

PhD Students

1. O.Balcers

Students

1. T.Bernots
2. U.Gertners
3. A.Zeipiņš

Scientific visits abroad

1. Dr. K.Jefimovs, University of Joensuu, Finland (5 months).
2. Dr. P.Stradins, National Renewable Energy Laboratory, Colorado, USA (12 months).
3. Dr. K.Jefimovs, post-doc researcher, Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, Switzerland (7 months).

Cooperation

Latvia

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

Finland

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

USA

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

Lithuania

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

Main Results

PHASE CONJUGATION PROPERTIES OF As-S-Se FILMS

A.Ozols, K.Ozols, M.Reinfelde

Light wavefront inversion (phase conjugation) in a-As-S-Se films has been studied experimentally. Phase conjugation (PC) of plane and spherical waves is carried out in a-$As_{40}S_{15}Se_{45}$ films using degenerate four-wave-mixing (DFWM) geometry at 633 nm. In the plane wave case simultaneous PC efficiency and DE measurements have been made versus exposure time, light intensity and holographic grating period. The maximal PC efficiency was 2.3% and the minimal PC specific recording energy was 2 J/(cm^2%) whereas the maximal DE was 0.9% and the minimal specific hologram recording energy was 10 J/(cm^2%). The optimal grating period was 2 μm. When compared to a-Se films a-As-S-Se films exhibit lower PC efficiency but higher photosensitivity. The advantages of a PC setup for the investigation of photoinduced processes in comparison with a usual holographic setup are observed. The PC setup was optimized using "Matlab"program.

METHOD FOR THE INTERFERENCE PATTERN PERIOD MEASUREMENT BY A MICROOBJECTIVE

A.Ozols

A simple experimental method is derived for the measurement of the period of the light interference pattern created by two intersecting laser beams. Such measurements are needed in holography especially when light beams are transformed inside a nonlinear medium. The interfering beams are directed to the microobjective whose focal length is known. A system of bright light hyperboloids (interference maxima) arises after the microobjective. Their intersection with the screen gives a system of corresponding fringes whose spacing is measured directly at the sufficiently large distance. After that the interference pattern period is calculated according to formula including the wavelength, the microobjective focal length, distance between microobjective and fringes and their spacing. The method was experimentally proven.

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.

IMMERSION HOLOGRAPHIC RECORDING IN AMORPHOUS CHALCOGENIDE THIN FILMS

Teteris J. and M.Reinfelde

The recording of the surface-relief and refractive index modulated gratings with a period of 0.15 – 1.0 μm was performed by solid immersion holographic method. The grating period for two intersecting light beams in a coupling prism with refractive index n can be expressed as $\Lambda=\lambda_0/2\ n\ \sin\theta$, 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.

Scientific Publications

1. A.Ozols, M.Reinfelde, V.Kampars and V.Kokars. *Structure optimization of azobenzene oligomers for holography*, Physica Status Solidi (c), 2005, vol.2, issue 1, pp.673-6.
2. A.Ozols and M.Reinfelde. *Angular selectivity of thin gratings*. Proc. SPIE, 2005, vol.5946, pp.59461H-(1–12).
3. A.Ozols, V.Kampars, M.Reinfelde and V.Kokars. *Effect of chromophore groups on the holographic characteristics of azobenzene oligomers.* Scientific Proc. of RTU: Material Science and Applied Chemistry, 2004, vol.9, pp.1123 – 30.
4. J.Teteris. *Application of amorphous chalcogenide thin films in optical recording technologies.* Proc. SPIE, 2005, vol.5946, pp.59461K-(1–12).
5. M.Reinfelde and J.Teteris. *Holographic recording of subwavelength structures in amorphous chalcogenide thin films.* Proc. SPIE, 2005, vol.5946, pp.59461J-(1–8).
6. I.Kuzmina and J.Teteris. *Bragg and asymmetric relief reflection gratings in As-S-Se thin films.* Proc. SPIE, 2005, vol.5946, pp.59461G-(1– 6).
7. M.Kuwata-Gonokami, N.Saito, Yu.Ino, M.Kauranen, **K.Jefimovs**, T.Vallius, J.Turunen, and Yu.Svirko, *Giant optical activity in quasi two-dimensional planar nanostructures,* PRL **95**, 227401.1-4, 2005.
8. **K.Jefimovs**, N.Saito, Yu.Ino, T.Vallius, P.Vahimaa, J.Turunen, R.Shimano, M. Kauranen, Yu.Svirko, and M.Kuwata-Gonokami, *Optical activity in chiral gold nanogratings*, Microelectron. Eng. **78-79**, 448-51, 2005.
9. B.K.Canfield, S.Kujala, **K.Jefimovs**, T.Vallius, J.Turunen and M.Kauranen, *Remarkable polarization sensitivity of gold nanoparticle arrays*, Appl. Phys. Lett. **86**, 183109.1-3, 2005.
10. B.K.Canfield, S.Kujala, **K.Jefimovs**, T.Vallius, J.Turunen and M.Kauranen, *Polarization effects in the linear and nonlinear optical responses of metal nanoparticles*, J. Opt. A: Pure Appl. Opt. **7**, S110-S117, 2005.

11. D.A.Lyashenko, A.N.Obraztsov, F.Simon, H.Kuzmany, E.D.Obraztsova, Yu.P.Svirko, and **K.Jefimovs**, *A comparative study of field emission from single- and double-wall carbon nanotubes and carbon peapods,* AIP Conf. Proc. **786**, 301 (2005).
12. J.Teteris, I.Kuzmina and M.Reinfelde, *Application of amorphous chalcogenide thin films in optical recording technologies,* Physica Status Solidi (c), 2005, vol.2, issue 1, pp.677-80.

Lectures on Conferences

21th Scientific Meeting of Institute of Solid State Physics, University of Latvia, Riga, February 7-9, 2005.

1..A.Ozols, K.Ozols, Ģ.Ivanovs. *Phase conjugation in a-As-S-Se films.* Abstracts, p.50.

2. Dm.Saharovs, A.Ozols, M.Reinfelde.*Holographic recording in amorphous As_2S_3 films by He-Ne laser at 633 nm.* Abstracts, p.51.

3. J.Teteris. *Immersion holographic recording in amorphous chalcogenides.* Abstracts, p.48.

4. J.Teteris. *Lāzeru izmantošana informācijas tehnoloģijās.* Abstracts, p.97.

5. M.Reinfelde and J.Teteris. *Transmisijas hologrammu ieraksts $As_{55}Se_{45}$ kārtiņās.* Abstracts, p.49.

6. O.Balcers and J.Teteris. *Optiskie ķīmiskie vielu sensori.* Abstracts, p.53.

The 1st Latvian Conference on Nanomaterials and Nanotechnologies, Riga, March 30-31, 2005.

7. J.Teteris. *Application of holography in nanotehcnology.* Abstracts.

International Conference on Holography, Optical Recording and Processing of Information *Holography 2005*, Varna, Bulgaria, May 21-25, 2005.

8. J.Teteris. *Amorphous Chalcogenide Thin Films as Media for Holographic Data Storage.* Abstracts p.91.
9. M.Reinfelde and J.Teteris. *Holographic Recording in Amorphous As-Se Thin Films.* Abstracts p.36.

The 5th Int.Conf. on Photonics, Devices and Systems, June 8-11, 2005, Prague, Czech Republic.

10. A.Ozols, K.Ozols and Ģ.Ivanovs. *Phase conjugation properties of a-As-S-Se films.* Abstracts, p.89.

The 3rd International Symposium on *Irradiation-induced Phenomena Chalcogenide, Oxide and Organic Thin Films*, Tryavna, Bulgaria, 15-19 June, 2005.

11. J. Teteris. *Holographic recording in amorphous chalcogenide thin films.* Abstracts p.12.
12. J.Teteris, M.Reinfelde and I.Kuzmina. *Immersion holographic recording of subwavelength gratings in amorphous chalcogenide films.* Abstracts p.54.

The 2nd International Workshop on Amorphous and Nanostructured Chalcogenides, ANC-2,Fundamentals and Applications, Sinaia, Romania, June 20-24, 2005

13. J.Teteris. *Holographic Data Storage in Amorphous Chalcogenide Thin Films.* Abstracts p.56.

The 21st International Conference on Amorphous and Noncrystalline Semiconductors, Lisbon, Portugal, 4-9 September, 2005.

14. O.Balcers, M.Reinfelde. and J.Teteris. *Holographic Recording in Amorphous As-Se Thin Films.* Abstracts p.344.
15. J.Teteris. *Holographic Data Storage in Amorphous Chalcogenide Thin Films.* Abstracts p.408.

The 1st Conference on Advances in Optical Materials, October 12 – 15, 2005, Tucson, Arizona, USA.

16. Dm.Saharovs, A.Ozols and M.Reinfelde. *Holographic recording in amorphous As_2S_3 films at 633 nm.* Abstracts, P47.
17. J.Teteris. *Amorphous chalcogenide thin films as media for holographic data storage.* Abstracts O64.

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. G. Krūmiņa
4. Dr. J.Dzenis

PhD Students

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

Graduate Students

1. B.Sc. S. Fomins
2. B.Sc. V. Karitāns

Scientific visits

M.Sc. A. Švede
Institut fur Arbeitsphysiologie an der Universität Dortmund - (Dec. 2005).

B.Sc. V. Karitāns
Colour Research Laboratotry, University of Joensuu (Jan.-May, 2005)

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)
Finland	Colour Research Laboratotry, University of Joensuu (Prof. J.Parkkinen)
Germany	Institut 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)

MAIN RESULTS

COLOUR VISION EXPERIMENTAL STUDIES IN TEACHING OF OPTOMETRY

Maris Ozolinsh, Gatis Ikaunieks[1] and Sergejs Fomins[1]
[1]Department of Optometry and Vision Science, University of Latvia

Following aspects related to human colour vision are included in experimental lessons for optometry students of University of Latvia. Characteristics of coloured stimuli (emitting and reflective), determination their coordinates in different colour spaces. Objective characteristics of transmitting of colour stimuli through the optical system of eye together with various types of appliances (lenses, prisms, Fresnel prisms). Psychophysical determination of mono- and polychromatic stimuli perception taking into account physiology of eye, retinal colour photoreceptor topography and spectral sensitivity, spatial and temporal characteristics of retinal receptive fields. Ergonomics of visual perception, influence of illumination and glare effects, testing of colour vision deficiencies.

PASSIVE AND ACTIVE LIGHT SCATTERING OBSTACLES

Maris Ozolinsh, Juan M. Bueno[1], Varis Karitans[2], and Gatis Ikaunieks[2]
[1]Laboratorio de Óptica (Dpto. Física), Universidad de Murcia, SPAIN
[2]Department of Optometry and Vision Science, University of Latvia

Simulation of vision pathologies and adverse viewing conditions in laboratory conditions requires optical phantoms with different level of light scattering. Such obstacles can be designed as passive or active elements applying several technologies. We have used for such purposes two kinds of solid state smart materials with electrically controllable light scattering – electrooptic PLZT ceramics, polymer dispersed liquid crystals PDLC and obstacles with fixed light scattering - composite of polymer methylmethaacrilat PMMA together with ground glass microparticles.

PLDC cells used in experiments as eye obstacles consist of two glass plates with transparent ITO electrodes forming a 10 microns gap of a composite polymer (PN393 *MerckKgaA*) with dispersed liquid crystal (BL035 *MerckKgaA*) droplets of micrometers size. Values of the refractive index were – for polymer n = 1.473 (at 589nm) and for birefringent liquid crystal n_o = 1.528 and n_e same as for polymer. Applying the AC voltage aligns directors of liquid crystal droplets along the direction of the electric field *E* in the layer - light passing the cell does not meet refractive index variations, and no scattering takes place. At absence of an external influence droplets are randomly oriented causing local optical non-homogeneities and light scattering. As the birefringence is much higher as compared with PLZT ceramics the thickness of the scattering layer for similar scattering degrees is within a micrometer range. Thus the voltage U needed maximally to align liquid crystal droplet directors along the transmitted light beam does not override 30-40 V. In such PDLC plate Mie light scattering takes place opposite to PLZT ceramics that due to smaller size of light scattering birefringent domains can be characterized with Rayleigh scattering. However also for Mie scattering in PDLC the noticeable wavelength dependence is observed. Figure 1shows the attenuation of the collimated directly transmitted light beams at three wavelengths (red, green and blue) of the RGB laser.

Another way to obtain graded step-by-step light scattering is using of composite – matrix of less refractive glue monomer of methaacrilate PMMA (refractive index n = 1.45) mixed together with dispersed small glass particles (n = 1.5). A gap between two glass plates of thickness 0.06-0.5 microns are filled with such mixture (glass powder concentration 100-200 mg/ml) thus obtaining pairs of obstacles with fixed but graded degrees of the light scattering. A picture of an interference contrast microscopy is depicted in Fig.2. Besides intensity and spectral dependencies the scattered light produced by such obstacles reveals also noticeable polarization dependencies. Figure 3

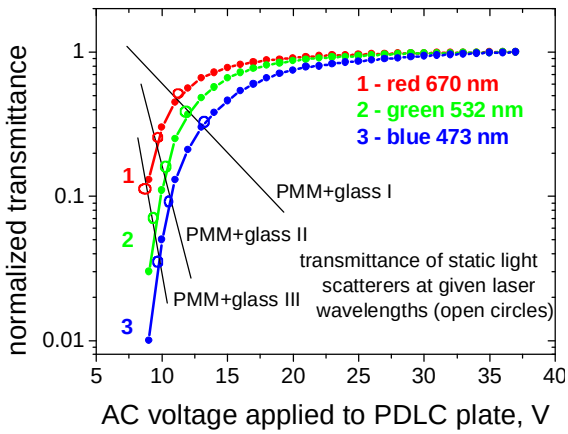
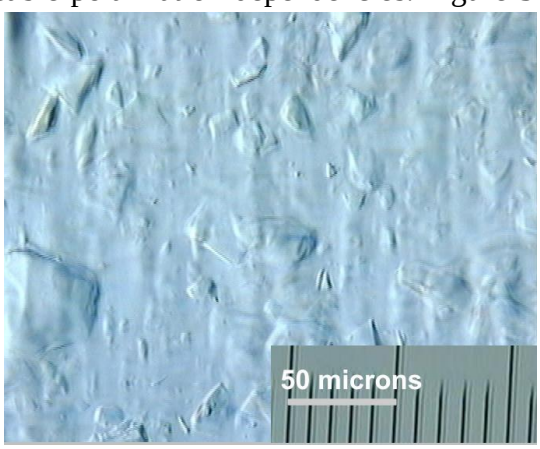


Fig.1. Transmittance of PLDC cell with AC voltage applied at three RGB laser wavelengths 670 nm (upper curve), 532 nm (middle) and 473 nm (lower curve).



. Interference contrast microscopy of glass
les in PMMA matrix.

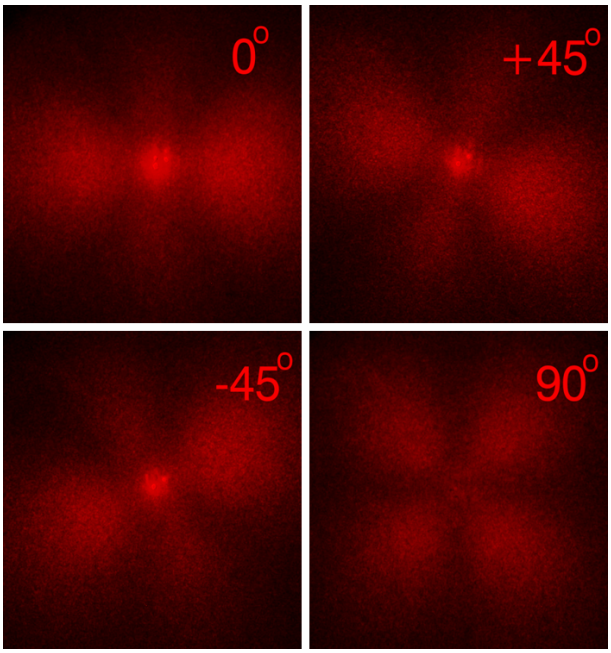


Fig.3. Indicatrices of the scattered light by PDLC light scattering obstacles analysing it with a rotating polarizer. Orientation of analyser corresponding to the polarization plane of the initial 633 nm laser beam is shown at the right upper part of images.

shows polarimetry analysis of the scattered by PDLC cell linear polarized 633 nm laser light applying the rotating analyzer. Obtained pictures allow to analyze polarimetry of the scattered light for angles much larger as those determining normal visual acuity. However previously Bueno at all. have analysed light scattering in human eyes and have revealed similarity of changes of the depolarization degree produced by such scatterers (PLZT ceramics) comparing it with the depolarization degree of the scattered light in elder cataract eye patients at smaller angles - below 1 arc degree.

All kind of such light scattering obstacles have been used for determination of various visual performance characteristics. Visual acuity looking through such obstacles with graded scattering drops down from standard VA=1.0 to zero for black-white and black-red, black-green and black-blue stimuli (for black-blue the most drastic between all listed optotypes). Scattering obstacles are used in vision research also for studies of colour contrast sensitivity, stimuli recognition search time and diminishing of objective optical characteristics of the model eye in presence of scattering. Studies of visual performance of observers without any vision pathologies however using obstacles capable to induce different degrees of light scattering allow to simulate a decrease of visual functions for cataract persons and also decrease of recognition of colour stimuli in adverse weather conditions.

VISUAL ACUITY WITH ISOLUMINANT COLOURED STIMULI FOR AMBLYOPIC EYE AND DEFOCUSED EYE

G. Krumina[1], G. Ikaunieks[1], and M. Ozolinsh
[1]Department of Optometry and Vision science, University of Latvia

In real eye examination the visual acuity usually is determined using standard charts with black letters on a white background. At the same time Westheimer et al (2003) have applied the reversed-contrast chart (white letters on a black background) to show improving of visual acuity for older subjects. Visual acuity established by colour stimuli should be worse comparing to black-white stimuli, due to lowering of the chart luminance contrast. We estimated difference in visual acuity with coloured stimuli comparing to that for high contrast black-white stimuli for real amblyopia and blurring cases. Tests were generated on computer screen. Visual acuity was detected using different charts in two ways: standard achromatic stimuli (black symbols on a white background) and isoluminant coloured stimuli (white symbols on a yellow background, grey symbols on blue, green or red background). Thus isoluminant tests had colour contrast only but hadn‘t luminance contrast. Visual acuity evaluated with the standard method and colour tests were studied for subjects with good visual acuity, if necessary using the best vision correction. The same was performed for subjects with induced blurring and real amblyopia. Blurring was realized with optical lenses placed in front of

the good seen eye or in front of the best vision correction. Experiments were performed when eyes were adapted to dark room conditions and in the normal lightened room (approximately 200-300 lx). The obtained results applying the isoluminant colour charts revealed worsening of the visual acuity comparing with the visual acuity estimated with a standard high contrast method (black symbols on a white background): 2.4 ± 0.8 times decrease for defocusing, however only 1.7 ± 0.3 times for real amblyopia.

DIFFERENT COLOUR CONTRAST STIMULI PERCEPTION IN FOG

M. Ozolinsh, M. Colomb[1], G. Ikaunieks[2] andV. Karitans[2]
[1]Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand, FRANCE
[2]Department of Optometry and Vision science, University of Latvia

Colour stimuli visual acuity VA and colour contrast sensitivity CS as the main visual performance parameters were determined in Clermont-Ferrand artificial fog chamber for fog density of visibility range 6-15 m. Red, green, blue and yellow on white background Landolt-C optotypes served as stimuli for visual acuity studies. Stimuli for colour contrast sensitivity were red, green, and blue Gabor gratings with spatial frequencies 5-30 cycles/deg. Two factors were taken as main occasions for different behaviour of the fog influence on visual perception. First, different distribution of "blue", "green" and "red" cone photorecptors within eye retina in the central vision area and retina periphery. Secondly, the stronger short wavelength (blue) light scattering in fog. The lowest contrast sensitivity was determined for blue gratings (CS decreasing in fog from 50 to 2 comparing to the decrease for red: 100 to 15). However visual acuity in fog for blue Landolt-C optotypes was the highest as compared to red and green optotypes. The colour intensity of Landolt-C optotypes presented on LCD screen was chosen corresponding to the blue, green and red colour contributions in achromatic white stimulus. Thus the blue stimuli had the greatest intensity contrast, and besides: blue stimuli on white background correspond to uniform stimuli blue distribution within all stimuli area either within white background or within stimuli C optotype area and sequentlly, the greater shorter wavelength scattering does not alter blue stimuli perception. Search time of different colour stimuli and dynamic visual acuity (up to stimuli speed 30 degree/sec) also were determined in simulated fog conditions using scattering obstacles with controllable degree of light scattering. These experiments also revealed the smallest increase of visual search times and better dynamic visual acuity in fog for blue-white colour contrast stimuli comparing with red-white and green-white - combinations used in road and traffic signs.

LIGHT SCATTERING EFFECT ON CONTRAST SENSITIVITY OF DIFFERENT COLOUR GABOR GRATINGS

G. Ikaunieks[1], M. Colomb[2], M. Ozolinsh, and G.Krumina[1]
[1]Department of Optometry and Vision Science, University of Latvia, Latvia
[2]Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand, France

To asses the effect of light scattering on perception of colour stimuli with different contrast level, we have measured contrast sensitivity in fog using different colour Gabor gratings. Gratings were red, green, and blue with spatial frequencies 8, 13 and 23 cycles/deg. Experiments were performed in an artificial fog camera at visibility 6, 8 and 11m. Additional indoor experiments were carried out using light scattering PDLC polymer dispersed liquid crystal eye occluders that allowed to control the level of light scattering. The Gabor gratings with different contrast were displayed on LCD monitor. Contrast sensitivity was determined from psychophysical curves. Test subjects should recognize horizontal or vertical orientation of gratings using a 2-alternative

forced-choice method. Due to the stronger short wavelength light scattering in fog the most reduction of contrast sensitivity was expected for blue colour gratings. Light scattering decreased contrast sensitivity of all three colour stimuli. Results showed better contrast sensitivity for green and red comparing to blue colour stimuli at all used spatial frequencies. Results for blue colour stimuli showed the most abrupt decrease of contrast sensitivity toward higher spatial frequencies. Additional ERG and VEP studies using reversal monochromatic (red, green, blue) stimuli of different Weber contrast together with scattering induced by PDLC obstacles are in progress.
G. Ikaunieks is thankful to the European Social Fund (ESF) for the support of this study.

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

Maris Ozolinsh and Gatis Ikaunieks

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

Scientific publications

Published in 2005

1. M. Ozolinsh, K. Anisko, G. Ikaunieks and G. Krumina, "Assessment of ocular stereovision prevalence and eye dominance stability," In: "Optical Materials and Applications ," *Proc. SPIE*, **5946**, pp.510-515 (2005).
2. G. Krumina, M. Ozolinsh, I. Lacis, and V Lyakhovetskii, "Assessment of ocular stereovision prevalence and eye dominance stability," In: "Optical Materials and Applications ," *Proc. SPIE*, **5946**, pp.481-490 (2005).
3. R.van Ee, G.Krumina, S. Pont, and S.van der Ven, "Voluntarily controlled bi-stable slant perception of real trapezoidal surfaces and their photographed counterparts", *Proc.of the Royal Society **B***, 272, pp.141-148 (2005).
4. M. Ozolinsh, G. Ikaunieks, and S. Fomins, „Colour vision experimental studies in teaching of optometry." Proc. „*Education and Training in Optics and Photonics*." Pôle Optique et Photonique, Marseille, pp.295-297 (2005).
5. M. Ozolinsh, G. Ikaunieks, and D. Fridrihsone, „Dynamics of eye aberration detected by high-speed Hartmann-Shack aberrometer." Proc. „*Optical Complex Systems*." Pôle Optique et Photonique, Marseille, pp.51-54 (2005).

Lectures on Conferences

1. Int. Student conference on Development in Optics and Photonics 2005, May, Riga.

G.Ikaunieks, M.Ozolinsh, M. Colomb, "Effects of blurring on spectral sensitivity of the human eye."

R.Paeglis, I.Lacis, N.Sjakste"Speed Matters:Grasping Rapid Vision by Saccadic Eye Movements."

V. Karitans, "Assessment of visual perception dynamics of polychromatic stimuli with different contrast level."

2. The 18th Symp. of the International Colour Vision Society, July, Lyon, France.

G. Ikaunieks, M. Colomb, M. Ozolinsh, and G. Krumina, "Light scattering effect on contrast sensitivity of different colour Gabor gratings."

M. Ozolinsh, M. Colomb, G. Ikaunieks, and V. Karitans , "Colour stimuli perception in presence of light scattering."

G. Krumina, G. Ikaunieks, and M. Ozolinsh, "Visual acuity with isoluminant coloured stimuli for amblyopic eye and defocused eye."

3. Eur. Conference on Visual Perception 2005, August,A Coruña, Spain.

M.Ozolinsh, M.Colomb, G.Ikaunieks, V.Karitans, 'Different colour contrast stimuli perception in fog."

4. Palanga International summer conference-school, August,Lithuania, 2005

G. Ikaunieks, V. Karitans, M. Ozolinsh & G. Krumina, "Differences in retinal and visual cortex response percepting stimuli of different colour."

5. Conference on Education and Training in Optics and Photonics ETOP-2005, October Marseille.

M. Ozolinsh, G. Ikaunieks & S. Fomins, "Colour vision experimental studies in teaching of optometry."

6. Conference "Optical Complex Systems", October, Marseille.

M. Ozolinsh, G. Ikaunieks & D. Fridrihsone, "Dynamics of eye aberration detected by high-speed Hartmann-Shack aberrometer."

WIDE BAND GAP MATERIALS

Head of Division *Dr. hab. 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 such as AlN, BN, diamond, and other related materials are promising for various applications including optoelectronics and dosimetry. Besides the well-known bulk materials composed by single and polycrystals, currently the interests of scientists working in material sciences are focused especially on synthesis of different types of nanomaterials displaying the new prospective features, which are promising for different applications. The properties of each material strongly depend on defects presented in it and forming their energy levels within the energy band gap. Therefore, the spectral investigation of material can give essential information about its defects.

The field of interests include studies of light-induced processes in materials, revealing luminescence properties, mechanisms and defect structures involved in these processes; studies of energy accumulation and its release mechanisms; studies of new optical properties characterizing materials when their size transforms from macroscale to nanoscale, as well as evaluation of possible applications of material.

During this year the laboratory of Wide band gap materials worked on investigation of spectral characteristics and light-induced energy accumulation in bulk materials: AlN ceramics, AlN powder, h-BN powder, as well as in h-BN nanotubes, AlN nanotips and AlN nanopowder. Part of investigations was performed together with the collaboration partners from abroad.

Scientific Staff

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

Students

1. R.Krutohvostov.
2. V.Korsaks

Visitors from abroad

1. Prof. Richard Williams, Wake Forest University, USA (2 weaks).
2. Dr. Burak Ucer, Wake Forest University, USA (2 weaks).

Scientific Visits Abroad

1. L.Trinkler, Wake Forest University, USA . (10 days).
2. B.Berzina, Wake Forest University, USA (14 days).
3. B.Berzina, National Taiwan University, Taiwan (10 days)
4. J.Sils, University of Osnabrik, Germany (11 month)

Collaborations

Latvia

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

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

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

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

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

Main results

SPECTRAL CHARACTERISTICS OF h-BN NT/h-BN MIXED MATERIAL

B. Berzina, L.Trinkler, R.Krutohvostov, V.Korsak, R.T.Williams[1], B.Ucer[1], D.Carroll[2]
[1] *Department of Physics, Wake Forest University, USA*
[2] *Center of Nanotechnologies, Wake Forest University, USA*

A nanomaterial - nt-BN/hBN mixed material formed by BN nanotubes (mixture of single-walled and multi-walled tubes) containing a small part of h-BN powder impurity synthesized in Center of Nanotechnologies, Wake Forest University, USA and a macromaterial - hBN powder from Belarus were used for investigations. Photoluminescence (PL) spectra and photoluminescence excitation (PLE) spectra have been studied at room temperature (RT) and liquid nitrogen temperature (LNT). In hBN powder (macromaterial) two types of luminescence bands originated from different luminescence centers were found. One of them forms a well-resolved and isolated phonon structure in both the PL and PLE spectra located at 300 nm and 290 nm, respectively. It is the classic absorption-emission spectrum of a defect from the bulk material weakly coupled to the lattice. In hBN powder that luminescence is predominant. The second type of luminescence forms a broad band at ~395 nm with PLE at 270 nm. In hBN powder this luminescence is weak.

In nt-BN/hBN nanomaterial the second type luminescence becomes predominant. Analysis and comparison of PL and PLE spectra obtained at RT and LNT allow us conclude that the luminescence centers responsible for 395 nm luminescence are inherent to the material surface. Therefore, in a case of nanomaterial the role of surface defects are predominant. In a case of bulk material – hBN powder - the same type of surface defects is also formed, when neighboring or near-neighbor sheet edges bond with each other to form nano-arches, i.e. half-nanotubes. Thus, h-BN surfaces (other than the sheet-face [0001]) naturally contain half-nanotubes. A luminescence mechanism in nt-BN is proposed and discussed.

OPTICAL PROPERTIES OF AlN NANOTIPS AS GROWN AND TREATED BY IMPLANTATION OF OXYGEN IONS.

L.Trinkler, B.Berzina, A.Auzina, L.C. Chen[1], S.C.Shi[1]
[1] *Center of Condensed Matter Sciences, National Taiwan University, Taiwan*

UV light induced luminescence properties have been studied for AlN nanotips synthesized in National Taiwan University, Center of Condensed Matter Sciences, Taiwan and compared with those for AlN ceramics made in Latvia. Characteristics of photoluminescence (PL) and optically stimulated luminescence (OSL) were investigated. In AlN nanotips the well-pronounced 480 nm luminescence with its own photo excitation at 280 nm appears beside the well-known luminescence at 400 nm being predominant in bulk material (AlN ceramics) and caused by oxygen-related defects. According to our present suggestions the 480 nm luminescence could be probably related to some types of surface defects. The main excitation for both luminescence types in AlN nanotips are observed at 200 nm situated at the long wavelength edge of fundamental absorption corresponding to the band-to-band transitions or exciton generation. The spectrum of OSL is composed by the same two luminescence bands.

Implantation of the oxygen in AlN nanotips does not lead to cardinal changes in PL and OSL spectra. However in PL spectra the 480 nm band seems to be better pronounced comparing with the spectra obtained from AlN nanotips before oxygen implantation. It allows us to conclude that a process of ion implantation promotes the surface defect creation probably responsive for the 480 nm luminescence formation.

SPECTRAL CHARACTERISTICS OF AlN POWDES - MACROSIZED AND NANOPOWDERS

L.Trinkler, B.Berzina, J.Grabis[1], I.Šteins[1]
[1] *Institute of Inorganic Chemistry, RTU, Latvia*

Photoluminescence (PL) and its excitation spectra (PLE) were studied at room temperature and compared for macrosized (1000 nm) and nanosized (10 nm – 100 nm) AlN powders synthesized in Institute of Inorganic Chemistry, RTU, Latvia. The complex luminescence spectrum was observed consisting of two main bands at 400 nm and 480 nm. The 400 nm luminescence is predominant in macromaterial – ceramics. At present it is known that 400 nm luminescence is caused by oxygen-related defects and luminescence mechanisms is also proposed. In AlN ceramics beside the main 400 nm band a weak 480 nm luminescence is also observed forming an asymmetric shoulder at the long wavelength side of the main band.

In macrosized AlN powder the PL spectra are also complex consisting of both the 400 nm and 480 nm bands, but now the 480 nm band is predominant with its own excitation band at 280 nm. In AlN nanopowder no new luminescence band is observed, but the 480 nm band is the main luminescence, nevertheless, a weak luminescence traces are also seen around the 400 nm. The results observed allow us ascribe the 480 nm luminescence band to surface defects of AlN, since relative yield of this band into the total luminescence rises with diminishing of material size, and hence, increase of surface area .

Scientific Publications

1. 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.

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,* phys. stat. sol. (c) **2**, No.1, (2005) 334-338.

3. M.Benabdesselam, P.Iacconi, L. Trinkler, B. Berzina. *Potential application of some wide band gap materils for UV dosimetry.* phys. stat. sol. (c) **2**, No.1, (2005) 539-542.

Lectures on Conferences

21. LU CFI Zinātniskā konference (Scientific Conference in Riga): Rīga. 7.-9. februāris, 2005.

1. A.Auzina, L. Trinkler, B.Berzina. *Spectral Characteristics of Oxygen-Related Defects.* (Book of Abstracts, p.13).
2. R.Krutohvostov, L.Trinkler, B.Berzina. *The Spectral Characteristics of Hxagonal Boron Nitride.* (Book of abstracts, p. 14).
3. B.Berzina, L.Trinkler, R.Krutohnostov, A.Auzina. *Spectral Characterization of Some Wide Band Gap Materials Formed From III-V Group Elements.* (Book of Abstracts, p. 15).

Invited Lectures

1. B.Berzina. *Spectral Characterization of Some III-V Group Nitrides.* National Taiwan University, Center of Condensed Matter Sciences, Taipei. (Invited Lecture) 21.12.2005.
2. B.Berzina. *Spectral Characterization of AlN (Macrosized and Naniomaterials).* National Tsing-Hwa University, Chiao-Tung, Taiwan (Invited Lecture) 27.12.2005.

SURFACE PHYSICS

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

Research Area and Main Problems

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

- micromechanical properties of surfaces, interfaces and thin films;
- adhesion and related processes on phase boundaries and interfaces in heterogeneous and
  nanostructured materials;
- modification of surfaces by different treatments (e.g. light- and ion- irradiations, environmental effects).

Scientific staff

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

Technical staff

1. A.Petersons

Students

1. G.Bakradze

Visitors from abroad

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

Scientific Visits Abroad

1. Dr.F.Muktepavela, St.Petersburg, Russia (1 week).
2. Dr.I.Manika, Darmstadt, Germany (1 week).

Cooperation

Latvia

1. Institute of Physical Energetics, Latvian Academy of Sciences (Dr.J.Kalnacs).
2. Riga Technical University (Prof.V.Mironovs).
3. Daugavpils University (Dr. E.Tamanis).
4. Institute of Physics, University of Latvia (Dr.A.Shishko).

Germany
GSI, Darmstadt (Prof.K.Schwartz).

Israel
Technion, Haifa (Dr.S.Stolyarova).

Russia
Institute of Solid State Physics RAN, Chernogolovka (Prof.B.Straumal)
Participation in PHANTOMS -IST Nanoelectronic network.

Main Results

ADHESION AND INTERFACIAL REACTIONS ON METAL/OXIDE INTERFACE DURING PLASTIC DEFORMATION AT ROOM TEMPERATURE

F. Muktepavela, G. Bakradze, V. Skvortsova, E. Tamanis[1], S. Stolyarova[2]

[1]Daugavpils University, Latvia
[2]Technion, Solid State Institute, Haifa, Israel

Metal/oxide interfaces play a crucial role in different technological applications including optoelectronic systems, nanocomposites, dispersion-strengthened materials, etc. The present study is focused on adhesion and related properties of metal/oxide interfaces (Al/SiO_2, Al/MgO, In/glass, Mg/SiO_2, etc.). The solid-state joints were obtained at room temperature, when the contribution of thermoactivation in adhesion is negligible. The interfaces were formed under the conditions of plastic flow of metal on the oxide surface in high vacuum (10^{-6}Pa) and in air at 293K. The structure and composition of contact surfaces were studied by AFM, X-ray diffraction, SIMS, and optical microscopy methods. The micromechanical properties were determined using light load (from 0.12 mN) indentation tests.

Results show a strong chemical bonding at the metal/oxide interface for metals with low oxide formation energy. The bonding occurs in the regions of maximum shear stress. The AFM studies demonstrate that the metal transferred to oxide surface has a non-homogeneous nanostructure with the grain size of 30 to 100 nm. The chemical composition of the transferred metal was experimentally traced level-by-level using the SIMS method. The Me-MeO reaction zone with a gradient of oxygen concentration was detected in the interfacial layer of 0.5-1mm. The microhardness and brittleness of the reaction zone were found to be higher compared to bulk metal. Thus, the enhancement of the oxygen diffusion in the zones of maximum shear stress is observed. The role of deformation-induced defects (dislocations and point defects in oxide and grain boundaries in metal) in diffusion processes on In/MgO and Pb/MgO interfaces was investigated. The effect of dislocations was found to be insignificant, while a high concentration of point defects on oxide surface and the nanostructured state of the metal can be the primary factors promoting interfacial chemical interaction.

ION-INDUCED HARDENING IN LiF: ENERGY LOSS AND FLUENCE EFFECTS

I.Manika, J.Maniks, K.Schwartz[1], C.Trautmann[1] and M.Toulemonde[2]
[1] Gesellschaft für Schwerionenforschung (GSI), Darmstadt, Germany
[2] CIRIL, Caen, France

Fast ions are suitable means for the modification of mechanical properties of solids. In the present study, the behavior of hardening of LiF crystals irradiated with different ion species (Au, Pb, Bi, Bi, Kr, Ni, Ti and S) at a specific energy of 10 MeV/u is compared. For all projectiles, a pronounced increase in hardness is observed, which scales with the ion range and depends on the fluence and energy loss. Heavy ions (Bi, Pb and Au) create higher and more uniform hardening in the irradiated layer compared to lighter Kr, Ni, Ti and S ions. The hardening effect increases with increasing the fluence and above 10^{12} ions/cm^2 bends towards saturation at an upper limit of 3.5-3.7 GPa that exceeds the hardness of non-irradiated crystals by a factor of about 2.5.

The ion-induced hardening is related mainly to impeding of dislocations by ion tracks. At moderate fluences, the magnitude of the hardening effect is inversely related to the distance between tracks in agreement with the Orovan's dispersion strengthening model. The pinning efficiency of tracks depends on track structure determined mainly by ion energy loss. The highest pinning efficiency exhibit tracks created by swift heavy ions, for which the energy loss noticeably exceeds the threshold of about 10 keV/nm for severe track core damage. Markedly lower core damage and efficiency of dislocation impeding exhibit tracks created by lighter ions. It follows from annealing experiments, that the defect aggregates in track core (possibly small Li colloids, vacancy clusters and bubbles of molecular fluorine) play a dominant role in hardening while the contribution of single defects is found to be comparatively small (few percent).

HARDENING IN LiF INDUCED BY FAST Kr AND Ni IONS AND RECOVERY OF STRUCTURE AND PROPERTIES UNDER ANNEALING

I.Manika, J.Maniks, P.Kulis, L.Gailite

The recovery of optical and mechanical properties of LiF crystals irradiated with 790 MeV ^{78}Kr and 640 MeV ^{58}Ni ions at 10^{12} ions/cm^2 under annealing at temperatures up to 810 K was investigated. Marked softening of irradiated crystals was initiated at temperatures above 520 - 530 K, where a transition from a complex absorption spectrum to a spectrum with only one broad peak at 275 nm occurs. Full recovery of mechanical and optical properties was reached after annealing at 810K. Activation energy of $0.13\ \text{eV} \pm 0.02\text{eV}$, which is close to that of the migration of H-centers, is obtained from the Arrhenius-type plots. The result is indicative of possible contribution of the H-center aggregates in the ion-induced hardening. The thermally most stable radiation defects responsible for hardening are found to be located around the Bragg maximum at the depth of about 70μm from irradiated surface, where the ion-induced hardening displays a maximum

Scientific publications

1. 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.
2. 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.
3. 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.
4. F.Muktepavela, G.Bakradze, E.Tamanis, V.Skvortsova, S.Stolyarova. *Adhesion and interfacial reactions on metal/oxide interface during plastic deformation at room temperature.* Materialwissenschaft und Werkstofftechnik, 2005, vol.36, No10, pp.513-517.
5. F.Muktepavela. *The role of diffusion in superplasticity and brittleness of fine-grained binary eutectics*. Defects and Diffusion Forum, 2005, vol.237-240, pp.745-752.
6. M.Šilinskas, A.Grigonis, Ž.Rutkūniene, J.Maniks, V.Kulikauskas. *The Mechanical and Optical Properties of A-C:H Films Deposited from Acetylene*

Using Direct Ion Beam Deposition Method. Physics and Chemistry of Solid State, 2005, vol.6, No3, pp.394-397.

7. F.Muktepavela, G.Bakradze, V.Skvortsova, E.Tamanis, S.Stolyarova. *Effect of mechanoactivation on interfacial interaction in metal/oxide systems*, Latvian Journal of Physics and Technical Sciences 2005, No1, pp.3–9.
8. 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*. Proc.SPIE, Optical Materials and Applications; Arnold Rosental; Ed., 2005, vol.5946, pp.81-86.
9. 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*. Proc.SPIE, Optical Materials and Applications; Arnold Rosental; Ed., 2005, vol.5946, pp.73-80.
10. F.Muktepavela, G.Bakradze, E.Tamanis, V.Skvortsova, S.Stolyarova. *Adhesion and interfacial reactions on metal/oxide interface during plastic deformation at room temperature.* Proceedings of the 1st International Conference on Diffusion in Solids and Liquids (DSL-2005), University of Aveiro, Portugal, 2005, pp.499-504.
11. I.Bucenieks, R.Krishbergs, E.Platacis, G.Lipsbergs, A.Shishko, A.Zik, F.Muktepavela. *Investigation of corrosion effects of EUROFER steel in Pb-17Li flow in the magnetic field*. Proc.of the Joint15th Riga and 6th PAMIR International Conferences of Fundamental and Applied MHD, Riga-Jurmala, Latvia, June 27-July 1, 2005, vol.1, pp.255-258.
12. F.Muktepavela, G.Bakradze, S.Stolyarova. *Investigation of the role of metal deformation and nanostructure state in solid-state adhesion between s-p metals and oxides at 293K*. Proc. Riga Technical University: Materials Science and Applied Chemistry, 2005, vol.10, pp.133-142.

Lectures on Conferences

21th Scientific Conference of Institute of Solid State Physics, University of Latvia, February 6-9, 2005, Riga, Latvia

1. I.Manika, O.Janchenko. *Energy loss and dose dependency of hardening in LiF induced by irradiation with swift ^{50}Ti ions*. Abstracts, p.28 (oral).
2. F.Muktepavela, G.Bakradze, A.Misnovs, S.Stoyarova, E.Tamanis. *Metal-oxide nanostructured coatings obtained by microtribological method.* Abstracts, p.41 (oral).

The Sixth International Symposium on Swift Heavy Ions in Matter (SHIM 2005), May 28 - 31, 2005, Aschaffenburg, Germany

1. I.Manika, J.Maniks. Ion-induced hardening in LiF: energy loss and fluence effects. Book of Abstracts, p.93 (poster).
2.

1st International Conference on Diffusion in Solids and Liquids, July 6-8, 2005, Aveiro, Portugal

1. F.Muktepavela, G.Bakradze, E.Tamanis, V.Skvortsova, S.Stolyarova. *Adhesion and interfacial reactions on metal/oxide interface during plastic deformation at room temperature* (poster).

The 7-th International Conference-School "Advanced Materials and Technologies", August 27 – 31, 2005, Palanga, Lithuania

1. F.Muktepavela, G.Bakradze, E.Tamanis. *Structure formation and adhesion processes on metal/oxide interfaces.* (poster).

Joint15th Riga and 6th PAMIR International Conferences of Fundamental and Applied MHD, June 27-July 1, 2005, Riga-Jurmala, Latvia

1. I.Bucenieks, R.Krishbergs, E.Platacis, G.Lipsbergs, A.Shishko, A.Zik, F.Muktepavela. *Investigation of corrosion effects of EUROFER steel in Pb-17Li flow in the magnetic field* (poster).

1st Latvian conference "Nanomaterials and Nanotechnologies", March 30-31, 2005, Riga, Latvia

1. F.Muktepavela, G.Bakradze, S.Stolyarova, E.Tamanis. *Nanostructured metal-oxide coatings obtained by microtribological method* (oral).

International Conference on Diffusion in Solids: Past, Present and Future (DiSo-05), May 23-27, 2005, Moscow, Russia

1. F.Muktepavela, G.Bakradze, S.Stolyarova, E.Tamanis. *Effect of mechanoactivation on interfacial reactions in metal/oxide systems*. Abstracts, p.2. (oral)
2. F.Muktepavela, N.Zaporina. *Segregation, self-healing and grain boundary phase transitions in Pb-Sn and Al-Sn eutectics during severe plastic deformation*. Abstracts, p.39 (poster).

44 International Conference on Actual Problems of Strength, October 3-7, 2005, Vologda, Russia

1. F.Muktepavela, G.Bakradze, S.Stolyarova. *Solid-state interfacial reaction in metal/oxide systems during plastic deformation of metals*. Abstracts, p.170 (oral).

46-th International Scientific Conference of Riga Technical University, October 13 – 15, 2005, Riga, Latvia.

1. F.Muktepavela, G.Bakradze, S.Stolyarova. *Investigation of the role of metal deformation processes and nanostructured state in Al/glass solid-state adhesion at 293°K* (oral).

4th International Conference on Joining and Powder Metallurgy, April 28-29, 2005, Jurmala, Latvia

1. V.Mironovs, F.Muktepavela, G.Bakradze, *Investigation of structure homogenities and micromechanical properties of complex shaped machnes parts from Fe-C-Cu powders*. (oral)

9th Conference of Latvian Physical Society September 15-16, 2005, Daugavpils, Latvia

1. *E.Tamanis, F.Muktepavela.* Carbon interlayers for ensuring the stability of nanostructured coatings *(poster).*

46th Scientific Student Conference of Riga Technical University, April 28, 2005, Riga, Latvia

1. G.Bakradze, F.Muktepavela. *Investigations of the structure and mechanical properties of metal/oxide nanocomposites*.(oral)

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 liquid scintillation methods for monitoring tritium content in surface and underground waters;
- the magnetic ions exchange interaction in the antiferromagnetic oxides MeO - MgO solid solutions were studied using of optical absorption, luminescence, EPR and Raman spectroscopies;
- exchange interaction between radiation defects and transition metals ions in the dielectric crystals with the transition metals ions;
- develop electron paramagnetic resonance (EPR) dosimetry to measure accumulated doses of ionising radiation absorbed by individuals;
- physical, structural and magnetic properties of solid state fine particles.

International projects:

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
17. Mag. sc.A.Pavlenko
18. Mag. sc. J. Proskurins

Technical Staff :

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

Students

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

Visitors from abroad

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

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).
Dr. hab. J. Berzins Institute Laue Langevin, Grenoble France (6 days).
Dr. hab. M. Balodis Institute Laue Langevin, Grenoble France (6 days).
Mag.sc. J.Proskurins, June 28 – July 1, 2005. Conference "Frontiers in the Physics of Nucleus", St.Petersburgh, Russia
Dr. D.Riekstina, X. European Ecological Congress, Turkey, Kusadasi (1 week),
Dr. D.Riekstina, LSC 2005 Conference Advances in Liquid Scintillation Spectrometry, Poland, Katowice (5 days),
Dr. D.Riekstina, 20. Seminar Aktivierungsanalyse, Germany, Munchen (3 days),
Dr. hab. N.Mironova-Ulmane 25-29 October Institute of solid state physics and semiconductor,of National Academy of Science of Belorus
Dr. hab. N.Mironova-Ulmane, Institute of Physics Tartu Estonia (3 weeks)
Dr. hab. N.Mironova-Ulmane, Eurasian national university, Astana, Kazahstan (1 weeks)
Dr. hab. N. Mironova-Ulmane, 4-10 September Poland

Cooperation

Latvia

1. Medical Academy of Latvia (Dr. hab., Prof. M.Eglite, Dr. hab. Prof. I. Cema, Dr.T.Zvagule).
2. VA "BAPA".
3. Radiation Safety Center (A.Skujina)
4. Riga Technical University, Institute of Inorganic Chemistry(Dr. I.Vitina,).
5. University of Latvia, Chemical faculty (Dr. A.Viksna,)
6. Instityute of Wood Chemistry (Dr. hab. G. Dobele Dr.hab. G. Telesheva, Dr.hab.T.Dizbit)
7. Riga Technical University, Faculty of Material Science and Applied Chemistry (Prof. J.Dehtjar,).

USA

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

Brasil

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

Lithuania

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

Canada

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

Germany
1. Technische Universität Műnchen (Prof. T von Egidy, Dr. H.-F. Wirth)

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

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

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

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)

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

Main Results

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

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

The level structure of ^{185}W has been studied using the prompt and delayed gamma-gamma coincidences from thermal neutron capture in ^{184}W accompanied with the one-nucleon transfer reactions (d,p) and (d,t) with polarized beams. From these data and those of previous studies a total of 183 levels has been established for energies below 3 MeV. Many of these states have been grouped into rotational bands built on 28 intrinsic states of quasiparticle and quasiparticle-plus phonon character. Although the DWBA analysis permitted definite spin-parity assignments for most of states a large number of particle transitions have 'anomalous' angular and asymmetry shapes with respect to the DWBA which indicate an influence of strong mixing between particle and hole states. The extra exchange of phonons and the significance of configurational mixing that embraces N=5,7 shells together with N=4,6 shells across the Fermi surface lead to a fine structure in the fragmentation of most single particle strengths and at the same time has the effect of breakdown of the individual properties of Nilsson states. The accumulated total spectroscopic (d,p) strength is about a factor two smaller than the equivalent (d,t) strength. Thus, the previously observed loss of the (d,p) strength in the W nuclei with A=184,185 is presumably because of their redistribution amongst particle- and hole-type states. The observation of hole states in the (d,p) reaction also might indicate that inner shells are only partially occupied.

The observed states below 2 MeV are compared with predictions of the Nilsson plus quasiparticle-phonon nuclear model. A large number of observed levels was interpreted in terms of rotational bands associated with Nilsson configurations that reflects the validity of the concept of axially symmetric deformation in this transitional nucleus. Lowest levels below 1 MeV were assigned to rather pure quadrupole and octupole vibrations coupled to the quasiparticle states closest to the Fermi level. Other states established around and slightly higher 1 MeV offer an example of structures with mixed one-quasiparticle and vibrational components. The established band structures above this region indicate a progressively greater degree of mixing. 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.

*Nuclear Physics Institute, 250 68 Řež, Czech Republic,
**Physik-Department, Technische Universität München, D-85748 Garching, Germany,
$Joint Institute for Nuclear Research, Dubna, 141980, Russia,
+Sektion Physik, Ludwig-Maximilians-Universität München, D-85748 Garching, Germany,
#Institute of Chemical Technology, Technická 5, CZ-166 28 Prague 6, Czech Republic

STRUCTURE OF ^{194}Ir VIA GEOMETRIC AND ALGEBRAIC MODELS

M.Balodis, H.-F.Wirth[1], G.Graw[1], R.Hertenberger[1], J.Bērziņš, N.Krāmere, J.Jolie[2], S.Christen[2], O.Moeller[2], D.Tonev[2], and T.von Egidy[1]

Model interpretation needed for a complete picture of the studied ^{194}Ir nuclear structure is shortly described.

Recently, a revised interpretation via Nilsson configurations (see our earlier publications) and associated rotational bands is obtained. New rotational levels is an important result.. Most low energy levels belong to negative parity, and they are grouped into nine bands: three with K=0, three – K=1, two – K=2, one – K=3. The high spin isomer K=11- also is a band head. Positive parity levels are interpreted via four bands resp. band heads with K=2, 3, 4, and 5.

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

Today's interpretation is thought to be essentially better, although an approach is traditional. One should note that ^{194}Ir is the heaviest rare earth region nucleus interpreted in detail via prolate-deformed nuclear shape. Main configurations are attributed for generally highly mixed band structures.

Algebraic model of supersymmetry for ^{194}Ir and the neighbouring nuclei is analyzed by our coauthors Jan Jolie et al. (Univ.Koeln (Cologne)) in their recent conference reports. These results should be soon added to the manuscript being prepared for the publication.

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

2. Istitute of physics,University of Kőln, Germany.

STUDIES OF ^{188}Re STRUCTURE

V. Bondarenko, l. Simonova

^{188}Re has been studied using the prompt γ-γ coincidences from thermal neutron capture in ^{187}Re(n,γ)^{188}Re reaction at the LWR-15 reactor in Rež (Czech Republic). Secondary gamma transitions were recorded in the energy range 60 – 2230 keV. 37 new levels were established in the the energy range 700 – 2150 keV. The data evaluation is in progress.

STUDIES OF PHASE TRANSITIONS AND QUANTUM CHAOS RELATIONSHIPS FOR THE EXTENDED CASTEN TRIANGLE OF THE INTERACTING BOSON MODEL (IBM-1)

A.Andrejevs, T.Krasta, J.Proskurins, J.Tambergs

It has been shown that the minimum problem for the classical energy functional E(N,η,χ;β) of IBM-1 two-dimensional parametrization (η,χ) in the framework of simplified Casten's version of the standard interacting boson model (IBM-1) Hamiltonian can be solved exactly with respect to deformation parameter β via a precise cubic equation. The features of three roots of this equation have been analyzed in a whole area of extended Casten's triangle. The characteristics of the first order phase transition lines E(5)-O(6), X(5)-E(5)-X(5) and the critical point E(5) have been studied, basing on obtained solutions without referring to Landau theory of phase transitions. Dynamical criterions of quantum chaos – the fragmentation width of basis states and the wave function entropy, have been evaluated for the (η,χ) parameter space of extended Casten's triangle, using the diagonalization of corresponding quantum Hamiltonian matrix. Possible relationships between these criterions and phase transition lines have been considered.

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

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

According to Latvian law, the permissible level of tritium in drinking water should not exceed 100 Bq/L. Therefore, it is important to monitor tritium in groundwater around potentially polluted zones, such as those surrounding a waste repository and an inactive nuclear reactor.

In order to perform the tritium monitoring in groundwater, the method of liquid scintillation spectrometry was used along with optimised modes of using the scintillation liquid OptiPhase HiSafe 3™. We used Packard TRI-CARB® and Wallac liquid scintillation spectrometers. Samples were gathered from 19 wells, at depths ranging between 2.5 and 9 m. Water samples were gathered 4 times a year. In specific wells, where the higher level of pollution was detected, samples were gathered every month.

In some of the wells, the tritium monitoring was carried out over a period of 7 yr. The tritium content in groundwater in certain wells varies within a wide range of concentration, and seasonal changes are recognisable. The maximum concentration of tritium in the same well in severally years changes different. The results obtained made it possible to estimate changes and the migration of tritium pollution and to forecast future changes.

INVESTIGATION OF RADIOECOLOGICAL SITUATION IN THE AREAS OF SHUT DOWN NUCLEAR REACTOR AND RADIOACTIVE WASTE REPOSITORY OF LATVIA

D. Riekstina, J. Berzins, O. Veveris, J. Alksnis, G. Smilskalne, A. Skujina

The aim of presented work was to provide an assessment of the accumulation of artificial radionuclides: Cs-137, Sr-90 and tritium, as well as the migration of them in the soil and ground-waters of the potentially most polluted regions of Latvia: the areas of the shut-down (1998) Salaspils research nuclear reactor (within 3 x 3 km zone) and the radioactive waste repository. Measurements of Cs-137 and tritium were included in the Environmental Radioactivity monitoring program.

It was found that the concentration of Cs-137 in soils varies in the range from 20 to 1940 Bq/m^2, whereas in groundwater it was below the minimal detectable activity level – 0.3 Bq/l). In any of the checkpoints it doesn't exceed the average value (262 Bq/kg) in Latvia according to our previous results.

The concentration of tritium in the wells outside reactor's territory and in the waste repository during last 5 years was below the permitted level for drinking water in Latvia.

The concentration of Sr-90 in the soils of reactor's and waste repository territories was in the range from 0.06 to 7.4 Bq/kg, which corresponds to the average level for soils in Latvia.

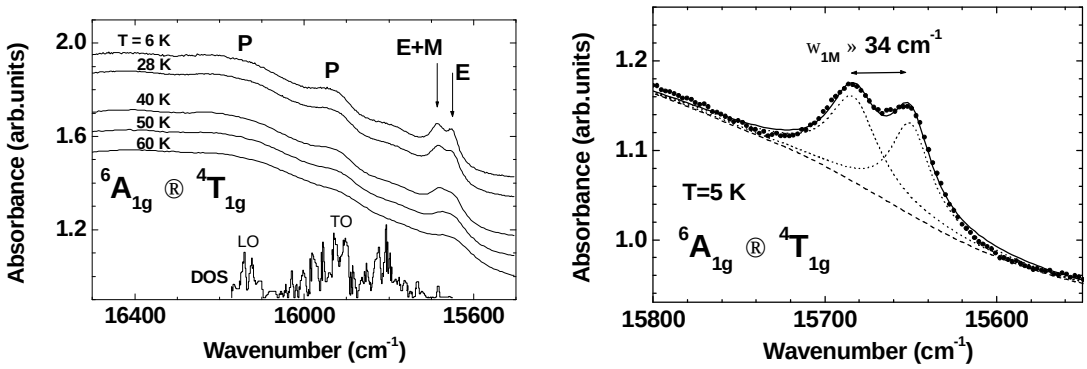
Obtained data allow one to assess the quality of the environment in these specific places.

PHONON AND MAGNETIC EXCITATIONS IN ANTIFERROMAGNETIC OXIDES

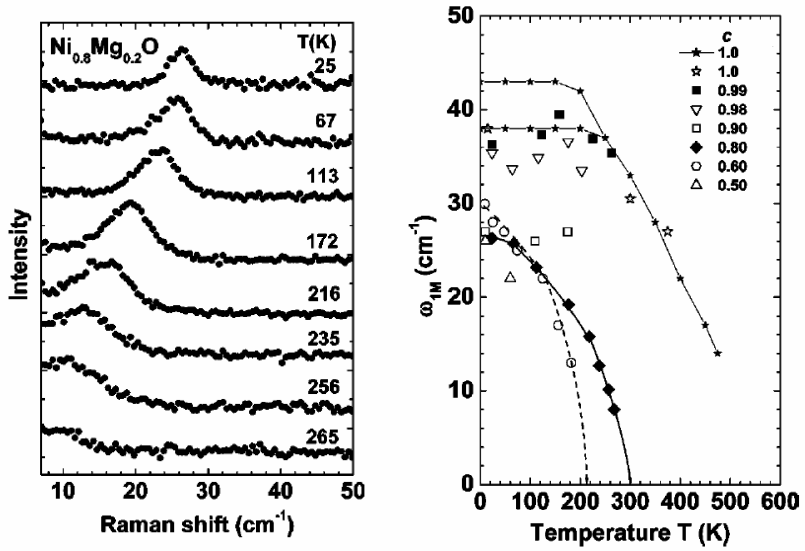
N. Mironova-Ulmane, V. Skvortsova, A. Kuzmin, U. Ulmanis

High-resolution optical absorption spectra of MnO were studied in the temperature range from 6 K to 60 K, corresponding to antiferromagnetic state region. The fine structure consisting of three main peaks at 15680, 15950 and 16150 cm^{-1} was well observed at 6 K, and the first peak (at 15680 cm^{-1}) splitting into two components, separated by about 34 cm^{-1}, was detected as well.

We attribute the two peaks at 15680 cm^{-1} to pure exciton transition (E) and exciton–one-magnon excitation (E+M). The separation between two peaks gives the one-magnon frequency of about 34 cm^{-1}: this value is in good agreement with high-frequency magnon mode found by neutron scattering.



The fine structure at higher energies is attributed to the phonon side-bands. The theoretically calculated phonon density of states (PDOS) for MnO indicates the location of the TO and LO phonon modes exactly under the two observed peaks at 15950 and 16150 cm^{-1}. Moreover, recent high-resolution inelastic neutron scattering study of the TO mode in the temperature interval from 4.3 to 300 K found the TO mode splitting by about 25 cm^{-1} below 100 K due to the magnetic-order induced phonon anisotropy. Therefore, this fact could explain large sensitivity of the peak at 15950 cm^{-1} to the temperature change.



The one-magnon scattering was studied in antiferromagnetic $Ni_cMg_{1-c}O$ solid solutions. The unpredicted behavior of both temperature and composition dependences

of one-magnon excitation energies (ω_{1M}) was observed. We found that the abrupt change of the one-magnon frequency by 7–8 cm^{-1} occurs between c=0.98 and c=0.90 in the limit of T→0 K. Besides, upon increasing temperature, the one-magnon energy for highly diluted nickel oxide vanishes significantly below the Néel temperature.

ELECTRON PARAMAGNETIC RESONANCE FOR ACCUMULATED DOSE MEASUREMENT

N. Mironova-Ulmane, A. Pavlenko

The EPR method is selected as appropriate technique for retrospective dose for group of Chernobyl Nuclear Power Pant (NPP) accident clean-up workers from Latvia. estimation with description of equipment, measurement modes, uncertainties budget.
The EPR dosimetry system has been calibrated by the other method, internationally proved Thermoluminescence Dosimetry (TLD) method. The uncertainty analysis for EPR and TLD methods is performed. The doses from internally incorporated nuclides given in some cases more then half of the total dose are estimated. The contribution to the total dose form internal irradiation, and external exposure is estimated.
Accuracy in the measurement of small dose values may be increased by physical and chemical processing of the enamel to achieve a weakening of the background signal. One possible approach is meticulous removal of dentine from the enamel and removal of areas of the enamel damaged by caries and pigmentation, as well as the removal of protein and its degreasing.
When dose values are relatively high, the accuracy is limited by differences in the radiation yield of the paramagnetic centres in the enamel. These differences are due to individual variations in the chemical composition and microstructure of the enamel.
Since the adjustment of the background signal is effected manually in its deduction from the total EPR spectrum, the subjective element makes a large contribution to the measurement uncertainty.

GADOLINIUM CONTAINING FERRITES AND SUPERCONDUCTORS AFTER THERMAL NEUTRON IRRADIATION

A.E.Petrov, I.V.Kudrenitskis.

Magnetic and structural properties of ceramic samples $R_3Fe_5O_{12}$ and additionally superconducting ones of ceramic $RBa_2Cu_3O_{7-}$, (R - natural mixture of Gd isotopes, ^{155}Gd, ^{157}Gd, ^{160}Gd) irradiated to fluences $F_{thermal}=10^{19}$ cm^{-2} (ratio $F_{th}/F_{fast(E>0.1\ MeV)}$ was approximately 5:1) were investigated and compared [1,2]. Gd recoil nuclei may become interstitials due to very large (~10^5 brn) neutron-capture cross-section of ^{155}Gd and ^{157}Gd and their large enough recoil energy. There are no macroscopic disordered regions and the defects of this type should be interpreted as a microscopic point defect having the size of a few lattice cell units.
Main results are following: 1) The temperature of magnetic sublattices compensation linearly depends on thermal neutron fluence and may serve as the method of measuring this fluence [3].
2) The dependence of the volume fraction of the disordered state C_t upon the irradiation fluence of the thermal neutrons F_{th} was:

$$C_t=1-\exp(-\beta_t F_{th}),$$

where $\beta_t=2{,}5*10^{-20}$ cm^2.

3) The decrease in T_c was caused by the increase of the lattice parameter "a" for $Gd_3Fe_5O_{12}$ ferrite, the fact has been described as the linear relation:

$$\Delta T_c = -1250K^* Å^{-1} * \Delta a.$$

4) The X-ray analysis had provided for the possibility to separate the contribution of the thermal and fast neutrons irradiated $Gd_3Fe_5O_{12}$ samples surface from their intrinsic part, irradiated solely by fast neutrons.

5) The discussion of several possible superconductivity supressing mechanisms connected with (i) oxygen variations, (ii) arising pressure, (iii) magnetic moments of Gd^{+3} rons in irregular positions of 123 structure was given. The last mechanism is the most preferable.

6) The recoil Gd atom spectra obtained after Monte-Carlo simulation have enabled to compute the displacement probabilities for different threshold energies [4].

1) M.M.Brezgunov, A.E.Petrov. Ukrainskij Fizicheskij Zhurnal, 33(4) (1988), p.616

2) S.V.Belogurov, M.M.Brezgunov, A.E.Petrov, I.V.Polikarpov, A.J.Yakubovsky. Superconductivity 5(12) (1992), p.2242

3) M.M.Brezgunov, A.E.Petrov. Certificate for Invention N4215825 from 8.07.1988, USSR

4) A.A.Makletsov, A.E.Petrov, V.V.Gann. Nuclear Instruments and Methods in Physics Research B94 (1994), p.203.

5) A.E.Petrov, I.V.Kudrenitskis. PHYSICS OF ELEKTRONIC MATERIALS, 2nd International Conference Proceedings, Kaluga, Russia, May 24-27, 2005; volume 2, page 130-131

Scientific Publications

1. J.A.Castilho Alcaras, J.Tambergs, T.Krasta, J.Ruža, O.Katkevičius. A dimension formula for reduced plethysms. Journal of Physics A: Mathematics and General, Vol.38 (2005), p.7501-7508.
2. V. Bondarenko, J. Honzatko, I. Tomandl, T. von Egidy, H.-F. Wirth, A. M. Sukhovoj,
3. L.Simonova, P. Alexa, J. Berzins, R. Hertenberg, Y. Eisermann, G. Graw, Low-spin mixed particle-hole structure in ^{185}W, Nucl. Phys. A762 (2005) 167-215.
4. A. V. Afanasjev**,** P. Ring and M. Wiescher, Pycnonuclear reaction rates between neutron- rich nuclei, Nuclear Physics A 758 (2005) 134c-137c.
5. A. V. Afanasjev and S. Frauendorf, Description of rotating N=Z nuclei in terms of isovector pairing, Physical Review C 71 (2005) 064318: 1-17.
6. A. V. Afanasjev and S. Frauendorf, Central depression in nuclear density and its consequences for the shell structure of superheavy nuclei, Physical Review C 71 (2005) 024308: 1-5.
7. P. Reiter, T. L. Khoo, I. Ahmad, … A. V. Afanasjev et al, Structure of the Odd-A, Shell-Stabilized Nucleus $^{253}_{102}No$, Physical Review Letters 95 (2005) 032501: 1-4.
8. L. R. Gasques, A. V. Afanasjev, E. F. Aguilera, M. Beard, L. C. Chamon, P. Ring, M. Wiescher and D. G. Yakovlev, Nuclear fusion in dense matter: Reaction rate and carbon burning, Physical Review C 72 (2005) 025806: 1-14.
9. A. V. Afanasjev and S. Frauendorf, Superdeformation and hyperdeformation in ^{108}Cd Physical Review C72, 031301(R) (2005): 1-5.
10. J. J. Valiente-Dobon, T. Steinhardt, C. E. Svensson, A. V. Afanasjev et al, Evidence for non-termination of rotational bands in ^{74}Kr, Phys. Review Letters, 95 , 232501 (2005): 1-5.
11. 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) 2 (2005) 704-707.

12. D. Riekstina, O. Veveris, A. Skujina, A.Zalkalne, Application of liquid scintillation spectrometric method for monitoring tritium in ground waters , Proceedings of the LSC 2005 Conference "Advances in Liquid Scintillation Spectrometry", Katowice, Poland, October 17-21 2005, 76, pp. 1-4.
13. D. Riekstina, O. Veveris, A. Skujina, A.Zalkalne, Application of liquid scintillation spectrometric method for monitoring tritium in ground waters ,Mining and Environment, Special edit. Central Mining Institute, Katowice, 2005, p. 57.
14. I. Taure, D. Riekstina, O. Veveris: *Neutron activation analysis.* Scientific Papers University of Latvia, 661, pp. 51-60.
15. E. Cazzanelli, A. Kuzmin, G. Mariotto and N. Mironova-Ulmane, Behavior of one-magnon frequency in antiferromagnetic $Ni_cMg_{1-c}O$ solid solutions. Phys. Rev. B 71 (2005) 134415:1-5.
16. U. Ulmanis and N. Mironova-Ulmane, Radiation induced conductivity in inorganic dielectric materials. Latv. J. Phys. Tech. Sci. 1 (2005) 10-18.
17. F. Muktepavela, G. Bakradze, V. Skvortsova, E. Tamanis and S. Stolyarova, Effect of mechanoactivation on interfacial interaction in metal/oxide systems, Latv. J.Phys. Tech. Sci. 1 (2005) 3-9.
18. N. Mironova-Ulmane, V. Skvortsova, A. Kuzmin and I. Sildos, Influence of radiation defects on exciton-magnon interactions in nickel oxide, Proc. SPIE 5946 (2005) 93-97
19. 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 47 (2005) 1459-1464 [In Russian]; Phys. Solid State 47 (2005) 1516-1522.
20. A.E.Petrov, I.V.Kudrenitskis. PHYSICS OF ELEKTRONIC MATERIALS, 2nd International Conference Abstracts, Kaluga, Russia, May 24-27, 2005; page 98
21. A.E.Petrov, I.V.Kudrenitskis. PHYSICS OF ELEKTRONIC MATERIALS, 2nd International Conference Proceedings, Kaluga, Russia, May 24-27, 2005; volume 2, page 130-131

Lectures on Conferences

21th Scientific Meeting of Institute of Solid state Physics, University of Latvia, dedicated to the Int. Year of Physics Riga, February 7.-9., 2005.

1J. Bērziņš, U. Ulmanis, Full member of LAS Peteris Prokofjevs, p.65-68.
2. J. Berzins, National multipurpose cyclotron center in Latvia, p. 69.
3. M. Balodis, J. Berzins, Enlarged study of the ^{194}Ir nuclear structure, using the (n,γ), (n,e$^-$), (d,p) and (d,α)reaction data, p.70.
4. A. Andrejevs, J. Tambergs, Studies of phase transitionsin the framework of interacting boson model, p.71.
5. D. Riekstina, J. Berzins, O. Veveris, Applied gamma spectrometric methods for estimation of local soils pollution, p. 72.
6.N. Mironova-Ulmane. The role of phonons and magnons in formation of optical absorption fine structure in MnO.
7.N. Mironova-Ulmane, The optical and EPR spectra of Fe^{2+} and Fe^{3+} ions in the haemoglobin

LV National Conference of Nuclear Physics, Frontiers in the Physics of Nucleus, June 28 – July 1, 2005, Saint-Petersburg, Russia

1. M. Balodis, J. Berzins, N. Kramere, H. F. Wirth, G. Graw, R. Hertenberg, J. Jolie, T. von Egidy, Transfer and neutron capture reactions to ^{194}Ir, p.61.

2. V. Bondarenko, J.Honzatko, I. Tomandl, T. von Egidy, H. F. Wirth, A. M. Sukhovoj, L.A. Malov, L. I. Simonova, J. Berzins, P. Aleksa, G. Graw, R. Hertenberg, Y. Eisermann, Low-spin mixed particle-hole structures in ^{185}W, p.78.
3. V. Bondarenko, J.Honzatko, V. A. Khitrov, A. M. Sukhovoj,I. Tomandl, Two-cascades of the 187W compound state gamma-decay, p. 79.
4. J. Proskurins, A. Andrejevs, T. Krasta, J.Tambergs, Studies of phase transitions and quantum chaos relationships in extendedcasten ctriangle of IBM-1, p.95.

International conference "Actual problems of solid state physics-2005" 25-29 October 25-29, 2005, Minsk Belarus
1.N. Mironova-Ulmane, The role of phonons and magnons in formation of optical absorption fine structure in MnO.
2.N. Mironova-Ulmane. Optical properties of solid solution $Ni_cMg_{1-c}O$.
3.N. Mironova-Ulmane. Defects in gadolinium gallium garnet single crystals irradiated by neutrons.

The 1st International Laser Ceramic Symposium which is organized as a satellite event at 2005 E-MRS Fall Meeting (5-9 of September 2005 Warsaw, Poland).
1. N. Mironova-Ulmane. Concentration dependence of Ni^{2+} luminescence in MgO.

20. Seminar Aktivierungsanalyse, Munchen, 23-25 Februar 2005

1. D. Riekstina**,** I. Taure, N. Mironova-Ulmane, R. Denisova, Applied of INAA method for human bones and teeth analysis, S. 2.

LSC 2005 Conference "Advances in Liquid Scintillation Spectrometry", Katowice, Poland, **17-21 Oktober 2005**
1. D. Riekstina, O. Veveris, A. Skujina, A.Zalkalne, Application of liquid scintillation spectrometric method for monitoring tritium in ground waters, p.76.

X. European Ecological Congress, Kusadasi, Turkey, November 08-13, 2005

1. D. Riekstina, O. Veveris, A. Skujina, A.Zalkalne, Investigations of radiological situation in areas of shut down nuclear reactor and radioactive waste repository of Latvia, p. 568.

9th scientific conference of the Latvian Physics Society, Daugavpils, 15-16 September, 2005
1. Tambergs, A.Andrejevs, D.Bočarovs, J.Ruža. Einšteina mantojums [Einstein's Heritage]. Daugavpils: "Saule" (2005), 31.lpp.

2nd International Conference Proceedings, Kaluga, Russia, May 24-27, 2005
1. A.E.Petrov, I.V.Kudrenitskis. PHYSICS OF ELEKTRONIC MATERIALS, volume 2, page 130-131.

Popular scientific papers

1. J. Tambergs, Lejup pa pasaules uzbūves kāpnēm (J.Tamberga intervija Zandai Garančai un Līgai Timšai par 2004.gada Nobela prēmiju fizikā). "Terra", Nr.35, janvāris-februāris 2005.g., 14.-17., 38.-39.lpp. [Downwards the stairs of Universe

construction (the interview about the 2004 year Nobel prize in physics, given by J.Tambergs to Zanda Garanča and Līga Timša),
2. Kvantu mehānikas un teoloģijas dialoga problēmas. “Zvaigžņotā debess”, Nr.185, 2004.gada rudens, 3.-10.lpp.; “Zvaigžņotā debess”, Nr.186, 2004/05.gada ziema, 3-10. (The problems of dialogue between quantum mechanics and theology).

Lectures at Universities

J. Tambergs
Latvian University, Faculty of Phycis and Mathematics: 1) Basic principles of nuclear and particle physics; 2) Basics principles of general relativity and cosmology

Latvian University, Faculty of Theology: 1) Biblical and scientific conceptions of the Universe; 2) Dialogue between religion and science.

J. Ruza

Riga Technical University: General physics.

LABORATORY OF ORGANIC MATERIALS

Head of the Laboratory: Dr.habyl.phys. I.Muzikante

Research Area and Main Problems

The laboratory's research interests cover polar organic materials for application in optics, 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.phys. E.Fonavs
2. Dr.chem. L.Gerca
3. Dr.habil.phys. I.Muzikante
4. Dr.phys. M.Rutkis
5. Dr.phys. O.Vilitis

Students

1. R.Dobulans
2. E.Laizāne
3. J.Latvels
4. A.Vembris

Scientific visits abroad

1. Dr.h. I.Muzikante, Zurich Technical Institute, Switzerland (1 week)
2. Dr.h. I.Muzikante, Vilnius University (1 month)

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, I.Kaulačs)

Lithuania

Institute of Physics (Prof. L.Valkunas)
Institute of Material Science and Applied Research, Vilnius University, Vilnius, Lithuania (Prof. S.Juršenas)

Germany

Lehrstuhl Physik kondensierter Materie, Universität Potsdam, Potsdam (Prof. L.Brehmer, B.Stiller)

France

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)

Japan

Institute for Chemical Research, Kyoto University, (Prof. N.Sato).

Denmark

Fysisk Institut Syddansk Universitet (Prof.Dr. H-G.Rubahn)

Main results

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[1], B.Stiller[2], L.Brehmer[2], O.Neilands[3]

[1]Institute of Physical Energetics, Aizkraukles Str. 21, Riga LV 1006,(Latvia)
[2]Potsdam University, Am Neuen Palais 10, D-14415, Potsdam (Germany)
[3]Riga Technical University, Azenes Str. 4, Riga LV 1048 (Latvia)

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.

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.

OPTICALLY INDUCED SWITCHING OF DICYCLOHEXYLAMINO SUBSTITUTED AZOBENZENE DERIVATIVES IN THIN ORDERED FILMS

I.Muzikante, E.Fonavs, L.Gerca[1], B.Stiller[2], L.Brehmer[2], E.Markava[3], D.Gustina[3]

[1]Institute of Physical Energetics, LAS., Aizkraukles St 21, 1006 Riga, Latvia
[2]Institute of Physics, University Potsdam, 601553, 14415 Potsdam, Germany
[3]Latvian Institute of Organic Synthesis, Aizkraukles St 21, 1006 Riga, Latvia

During the last years there has been increasing interest in the investigation of photoinduced switching effects. Among the objects of concern, azobenzene derivatives occupy a promising position due to their capability to isomerize under UV and visible light irradiation. To understand photoresponse of these materials, their spectroscopic and

electrical properties are studied. The orientation of photoresponsive molecules and their packing in the condensed phase influence the behavior of the solid under irradiation.

We have examined a number of novel synthesized azobenzene derivatives containing a N,N-dicyclohexyl sulfonamide moiety. The derivatives with different length of alkyl chain between azobenzene moiety and SH or COOH groups were synthesized. The morphology and photoinduced surface potential switching of the self-assembled monolayers and Langmuir-Blodgett multilayers are investigated.

We have observed the fast reversible photoisomerization of the newly synthesized amphiphilic dicyclohexylamine group containing azobenzene derivatives in Langmuir-Blodgett multilayer and self-assembled monolayer on alternating irradiation with UV and visible light. The surface potential kinetics may approximate by exponential function. The time response of changes of surface potential caused by trans-to-cis isomerization last between 16s and 40s in dependence of length of alkyl chain. The spectral dependence of changes of surface potential correlates with appropriate absorption spectra with maximum at wavelengths characteristic for trans and cis-isomers. This dependence confirms, that the switching process of surface potential mainly is determined by photoisomerization reaction of azobenzene group.

ALL OPTICAL POLING STUDY THE DMABI MOLECULE IN A POLYMER MATRIX

A.Vembris, A.Apostoluk[1], M.Rutkis, A.Tokmakov, I.Muzikante, S.Dabos-Seignon[1], J-M.Nunzi[1]

[1]Laboratoire des Propriétés Optiques des Matériaux et Applications, UMR CNRS 6136, Université d'Angers, 2 Bd. Lavoisier, 49045 Angers, France

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 syndioatactic 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.

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.

PHOTOINDUCED PHENOMENA IN ORGANISED POLAR ORGANIC FILMS

I.Muzikante, E.Fonavs, B.Stiller[1], L.Brehmer[1]

Organic materials have received considerable attention because of their large dipole moments and optical nonlinearities. The optically induced switching of material properties is important for investigations of optoelectronic effects including second harmonic generation. Organic materials for photonic applications contain chromophore dipole consisting of acceptor and donor groups bridged by a delocalized π-electron system. Both calculations and experimental data show a reversible highly dipolar

photoinduced intra molecular charge transfer in betaine type molecules accompanied by change of the sign and the value of the dipole moment.

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 main advantage from the point of view of photoinduced switching effect is the fact that in the excited state molecule does not change it geometry and, to the contrary of azobenzene molecule, photoinduced change of dipole moment of betaine molecule does not need free volume in thin films. Disadvantage of investigated polymer films is slow response time up to several minutes of the changes of surface potential to irradiation at wavelength of photoinduced intramolecular charge transfer, which is of the order of femtoseconds.

The experimentally observed changes of the surface potential on irradiation is considerably higher in corona poled regions. The greatest response of the surface potential is observed polymer film with chemically attached betaine group (IPB-3).
Photoinduced change of the surface potential of poled polymer films observed in UV and visible spectral region has the maximum close to the photoinduced intramolecular electron transfer 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 this case the photogenerated charge carries may influence the density of the surface charge. In order to understand the photoinduced changes of the surface potential in polymer films with betaine derivatives the further investigations are in progress.

MOLECULAR DIODE FOR GAS SENSING

R.Dobulans[1], J.Latvels, I.Muzikante, E.Fonavs, A.Tokmakov, M.Bouvet[2]
[1]Institute of Physical Energetics LAS, 21, Aizkraukles str., Riga LV1006, Latvia.
[2]Ecole Supérieure de Physique et Chimie Industrielles - City of Paris and Laboratoire de Chimie Inorganique et Matériaux Moléculaires - CNRS UMR 7071 Université Pierre et Marie Curie - 4, place Jussieu - 75252 Paris cedex 05 – France

Organic thin films with semiconducting properties have been intensively studied in nowadays due to very promising applications in organic electronics. Among organic semiconductors metallophthalocyanines (PcMe) with their electrical properties, thermal and chemical stability and rich substitution chemistry are good candidates for use in design of novel molecular electronic devices. The well-known reversible electrical property changes on exposing to gases have already been exploited to create highly sensitive gas sensors and transducers. It has been known for a long time that oxidizing gases (for example, O_2, O_3 and NO_2) influences the electrical properties of metallophtalocyanines. Whereas fluorinated metallophtalocyanines exhibit change of conductivity on the presence of or reducing gases (for example, H_2, NH_3).

The first experiments with both pure PcNi and pure F_{16}PcNi sandwich-type samples show symmetrical current-voltage (I-U) characteristics both in vacuum and argon atmosphere. Some deviations from symmetrical case are observed due to different electrodes used in these sandwich type samples. In both interfaces metal-semiconductor two different processes are taking place. The space charge limited current (SCLC) regime for sandwich-type samples with bottom Au and top Al electrode was applied.

The energy structure of F_{16}PcNi and PcNi thin layers were investigated by space charge limited currents methods. A diode-type conductivity may also be observed in pure n- or p-type phthalocyanines. The Schottky effect corresponds to the flow of carriers a metal--semiconductor interface under reverse bias, when the dominant effect controlling the form of the current is field lowering of the Schottky barrier. However, if the voltage is applied in the opposite (or forward) direction the current density increases according to the diode equation.

In a different light the I-U characteristics of bilayer Au/F_{16}PcNi/PcNi/Al sample was observed. We got what we were expecting for – marked rectification effect was observed. The higher current level was observed when the positive voltage is applied to the bottom Au electrode and we should be able to investigate interface of PcNi and F_{16}PcNi and observe p-n junction there.

Scientific publications

1. 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), Vol. 242, No. 4, 815-818, 2005.
2. 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*, Vol. 5946, pp. 179-185, 2005
3. 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*, Vol. 5946, pp. 186-191, 2005
4. I.Muzikante, E.Fonavs, B.Stiller, L.Brehmer, Photoinduced phenomena in organised polar organic films, *Advances in Colloid and Interface Science*, Vol. 116, No.1/3, pp133-141, 2005.
5. I.Muzikante, E.Fonavs, A.Vembris, A.Tokmakov, L.Gerca, B.Stiller, L.Brehmer, Photoinduced processes in ordered organic polar thin films, Proceedings of First Latvian Conference *"Nanomaterials and Nanotechnologies"*, Riga, 2005, pp.52-60.
6. M.Rutkis, I.Muzikante, B.Stiller, A.Vembris, V.Zauls, Indandione derivatives as a chromophores for the non-linear optical applications and photonics, Proceedings of First Latvian Conference *"Nanomaterials and Nanotechnologies"*, Riga, 2005, pp. 125-129.
7. A.Tokmakov, A.Vembris, L.Gerca, I.Muzikante, E.Laizāne, Betaine type molecule guest-host system thin film preparation possibilities with spin-coating method, Proceedings of First Latvian Conference *"Nanomaterials and Nanotechnologies"*, Riga, 2005, pp. 143-147.
8. R.Dobulans, J.Latvels, I.Muzikante, E.Fonavs, A.Tokmakov, M.Bouvet, Molecular diode for gas sensing, Proceedings of First Latvian Conference *"Nanomaterials and Nanotechnologies"*, Riga, 2005, pp. 130-135.lpp.
9. I.Kaulach, E.Fonavs, I.Muzikante, A.Tokmakov, Influence of poling on charge trapping in PMMA doped with dimethylaminobenzylidene 1,3 – indandione, *Latv.J.Phys. Technical Sciences*, No.4, pp.63 - 70, 2005
7. I.Kaulach, I.Muzikante, E.Fonavs, J.Kalnacs, G.Shlihta, M.Plotniece, A.Tokmakov, P.Shipkovs, V.Kampars, Magnetic field influence on photovoltaic effect of PMMA doped with dimethylaminobenzylidene 1,3 –indandione and fullerene C_{60} derivative, *Latv.J.Phys. Technical Sciences*, No.5, pp.3-11, 2005

Lectures on Conferences

Latvijas universitātes Cietvielu fizikas institūta 21.zinātniskā konference, Rīga, Latvija, 2005.gada 7.-9.februāris
21st Scientific Conference, Institute of Solid State Physics, University of Latvia, Riga, Latvia February 7-9, 2005:

1. R.Dobulāns, E.Fonavs, I.Muzikante, A.Tokmakov, M.Bouvet, Gāzes jutīga molekulārā diode, Gas sensitive molecular diode, Abstracts, lpp.61. (oral)
2. V.Kampars, M.Utinans, P.Pastors, V.Grazulevicius, I.Muzikante, M.Rutkis, A.Vembris, Jauni DMABI atvasinājumi nelineārai optikai, New derivatives of DMABI for nonlinear optics, Abstracts, pp.63. (oral)
3. I.Kaulačs, I.Muzikante, A.Tokmakov, P.Šipkovs, Lādiņa nesēju fotoģenerācija un fotovoltaiskais efekts ar krāsvielu DMABI dopētā polimērā, Charge carrier photogeneration and photovoltaic effect of polymer doped with chromophore DMABI, Abstracts, pp.59. (oral)
4. J.Latvels, E.Fonavs, I.Muzikante, Lādiņnesēju saķeršanas centru pētījumi metāla ftalocianīna plānās kārtiņās, Studies of charge carrier traps in metal phthalocyanine thin films, Abstracts, pp.62. (oral)
5. I.Muzikante, A.Tokmakovs, B.Stiller, K.Morawetz, DMABI molekulu optiski ierosinātā pārnese polimēra kārtiņās**,** Optical induced mass transport of DMABI molecules in polymer matrix Abstracts, pp.58. (oral)
6. E.Laizāne, A.Vembris, A.Tokmakovs, L.Gerca, I.Muzikante, E.Markava, D.Gustiņa, Optiski ierosinātā pārslēgšanās process pētījumi azobenzola plānās kārtiņās, Optical switching effect of azobenzene in solution and thin films Abstracts, pp.60. (oral)
7. M.Rutkis, V.Zauls, Nelineāro optisko koeficientu d_{ij} noteikšana – metodika, problēmas un to risinājumi CFI, Determination of the nonlinear coefficients d_{ij} – methodology, problems and solution in the ISSP, Abstracts, pp.55. (oral)
8. A.Tokmakovs, A.Vembris, I.Muzikante, L.Gerca, E.Laizāne, Polimēra matricas ar betaīna tipa molekulām iegūšanas iespējas ar "spin-coating"metodi, Polymer matrix with betaine tupe molecules processing possibilities by spin-coating method, Abstracts, pp.56. (oral)
9. A.Vembris, M. Rutkis, A. Tokmakovs, DMABI saimnieka-viesu sistēmas nelineārās optiskās īpašības, Nonlinear optical properties of DMABI host-guest system, CFI, Abstracts, pp.57. (oral)

Pirmā Latvijas konference "Nanomateriāli un nanotehnoloģijas", NENAMAT Mobilization Workshop Ņanomaterials and Nanotechnologies" Riga, Latvia, March 30-31, 2005:

1. I.Muzikante, E.Fonavs, A.Vembris, A.Tokmakov, L.Gerca, B.Stiller, L.Brehmer, Fotoierosinātie procesi sakārtotās polārās organiskās plānās kārtiņās, Photoinduced processes in ordered organic polar thin films. (oral)
2. A.Vembris, M.Rutkis, V.Zauls, A.Tokamkov, E.Fonavs. N, N-dimeti-aminobenzilidēn- 1,3-indandiona nelineārās optiskās īpašības polimēra matricā, Non-linear optical properties of the N, N-dimethylaminobenzylidene 1,3-indandione molecules in the polymer matrix. (poster)
3. M.Rutkis, I.Muzikante, B.Stiller, A.Vembris, V.Zauls Indandiona atvasinājumu izmantošanas iespējas nelineārajā optikā un fotonikā, Indandione derivatives as a cromophores for the non-linear optical applications and photonics. (oral)
4. J.Latvels, I.Muzikante, E.Fonavs, Lādiņnesēju saķeršanas centru pētījumi metāla ftalocinanīna plānās kārtiņās, Studies of charge carrier trapping states in metallo-phthalocyanines thin films. (poster)

5. R.Dobulāns, E.Fonavs, I.Muzikante, A.Tokmakovs, M.Bouvet, Gāzes jutīga molekulārā diode, Molecular diode for gas sensing. (poster)
6. A.Tokmakov, A.Vembris, L.Gerca, I.Muzikante, E.Laizāne, Polimēra matricas ar betaīna tipa molekulām iegūšanas iespējas ar *spin-coating* metodi, Betaine type molecule guest-host system thin film preparation possibilities with spin-coating method. (poster)

SPIE International student conference "Developments in optics and photonics", 30 April -1 May 2005 Riga, Latvia:

A.Vembris, Nonlinear optical properties of DMABI molecules in polymer host-guest system, Abstracts, pp. 29. (oral)

Electrical and Related Properties of Organic Solids and Polymers (ERPOS-10), Cargese, France, July 10-15, 2005:

1. I.Muzikante, E.Fonavs, B.Stiller, L.Brehmer, Photoinduced phenomena in organised polar organic films, Programme Booklet, P42. (poster)
2. M.Rutkis, A.Vembris, V.Zauls, A.Tokmakov, E.Fonavs, Non-linear optical properties of polymer systems with poled indandione derivatives as a chromophores, Programme Booklet, G103. (oral)
3. R.Dobulāns, J.Latvels, I.Muzikante, E.Fonavs, A.Tokmakov, M.Bouvet, Molecular diode of metallophthalocyanines for ammonia sensing, Programme Booklet, P33. (poster)
4. A.Vembris, A.Tokmakovs, E.Laizane, I.Muzikante, Influence of the structure of azo dyes on cis- trans photoisomerization kinetics in solution, polymer matrix and LB films, Programme Booklet, A113. (oral)

Congrès SFC-EuroChem Nancy-2005, Symposia 20: Chimie et Envinnorement, Vandoeuvre-les-Nancy, France, August 28 – September1, 2005:

M.Bouvet, I.Muzikante, E.Fonavs, A.Tokmakov, R.Dobulans, Thin films of phthalocyanine derivatives for ozone and ammonia sensing, Abstracts, (poster)

The 7-th International Conference-School "Advanced Materials and Technologies", Palanga, Lithuania, August 27-31, 2005:

1. R.Dobulans, E.Fonavs, I.Muzikante, A.Tokmakov, M.Bouvet, Gas sensitive molecular diode based on metallophthalocyanines, Abstracts, pp. 48 (poster)
2. E.Laizāne, A.Vembris, A.Tokmakov, L.Gerca, I.Muzikante, E.Markava, D.Gustiņa, Optical switching effect of azobenzenes in solution and thin film, Abstracts, pp.109 (poster)
3. J.Latvels, E.Fonavs, I.Muzikante, Studies of charge carrier traps in metal phthalocyanine thin films, Abstracts, pp.110 (poster)
4. I.Muzikante, E.Fonavs, M.Rutkis, B.Stiller, Optically induced phenomena in thin organized films of polar organic molecules and polymers, Abstracts, pp.16 (oral)
5. A.Tokmakov, A.Vembris, L.Gerca, I.Muzikante, E.Laizāne, Processing possibilities of polymer matrix with betaine type molecules by spin-coating method, Abstracts, pp.108 (poster)
6. A.Vembris, M.Rutkis A.Tokmakovs, Nonlinear optical properties of DMABI molecules in polymer host-guest system, Abstracts, pp.107. (poster)

3rd International Conference on Organic Electronics and Related Phenomena (ECOER'05), Winterthur (Switzerland), September 27-30, 2005:

I.Muzikante, R.Dobulans, E.Fonavs, M.Bouvet, Molecular diode based on n-and p-type metal phthalocyanines, Book of Abstracts, pp. 72-73. (oral)

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
4. Riga Technical University
5. *Trafik* Ltd
6. IB *Biakss*
7. *GROG* Ltd
8. *Apollo AS* Ltd
9. *AlarmLat* Ltd
10. .*Mikoniks* Ltd
11. .*Energoremonts Rīga* Ltd

Denmark

DanBalt Electronics

Russia

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

Estonia

Tallinn Universiti of Technology

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";
14. SIA "Godske Latvian Textile" etc.

Lectures on Conferences

21th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2005

1. I.Gvardina, A.Kristiņš, J.Melderis, G.Pikurs, J.Tībergs, J.Zvirgzds, *Soft Start Devices for Electric Motors*. Abstracts, p.87. (Oral).
2. A.Grablevskis, D.Gusevs, A.Kristiņš, *ADMCF326 Microcontroller Using in Frequency Converters.* Abstracts, p.88. (Oral).
3. P. Annus, E. Haldre, V. Kaulio, A. Kristins, M.Min, *Multichannel Data Acquisition System.* Abstracts, p.89. (Oral).
4. D.Gusevs, V.Narnicka, E.Petersons, *WEB Node Traffic Statistical Data Analyze.* Abstracts, p.90. (Oral).

46th International Scientific Conference at the Riga Technical University (Latvia) October, 2005

1. P.Annus, V.Kaulio, M.Min, A.Kristiņš, *Delta-Sigma Data Asquisition Module with USB-Interface.* (Oral).

Symposium "Buried Sea Mines - Threat to the Security of the Baltic Sea Region" October, 2005

A.Kristiņš, D.Millers, A.Zeļenkovs, S.Zelenkovs, *Technologies and Solutions for Searching and Classifying of Mine-Type Objects Buried in Sediments Using Hidroacoustic and Radiolocation Methods* (Oral)

ORGANIZED CONFERENCES

21th Scientific Conference of the Institute of Solid State Physics, University of Latvia

Riga, February 7 – 9, 2005

The anual Scientific Conferences of the ISSP are held at the Institute of Solid State Physics in February the 7 – 9 and is a part of Scientific Conference of University of Latvia (UL).

The 21th Conference worked in 6 sections:
- non – linear optical properties and organic materials (16 reports),
- nuclear reactions and "EURATOM"projects (12 reports),
- structure and phase transitions (11 reports),
- nanomaterials and nanotechnologies (14 reports).
- defects, optical spectroscopy and luminescence (16 reports),
- materials and applications (17 reports),

Alltogether 86 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.

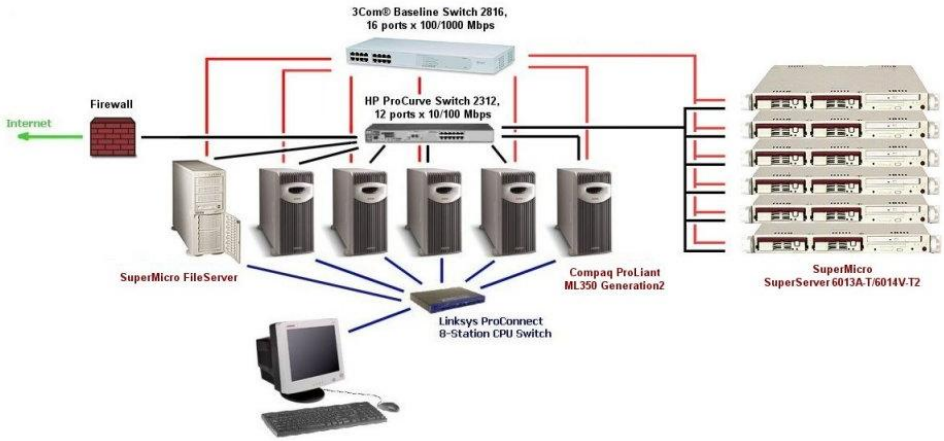
The aim of the Conference was to inform the physicists community of Latvia about the most important results obtained in the previous year.

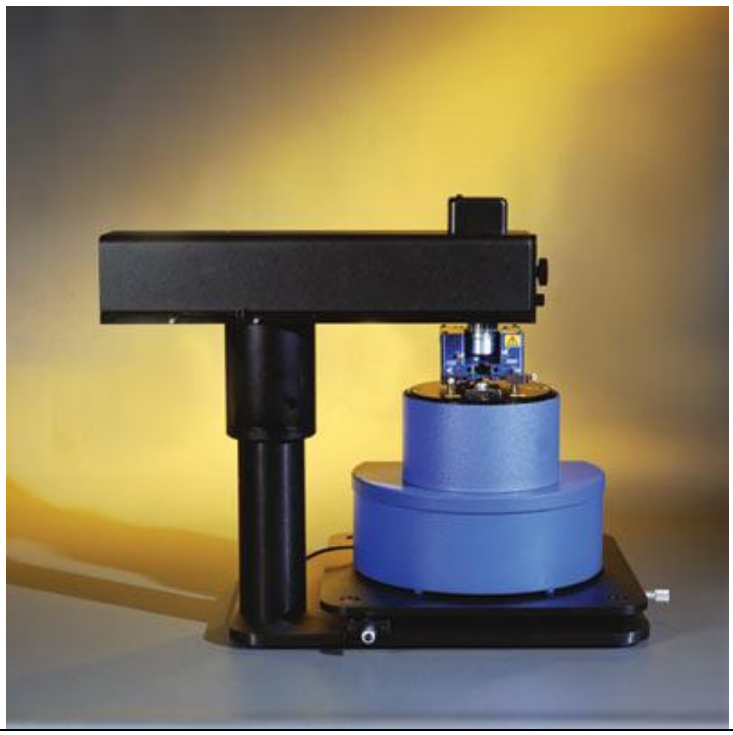
Abstracts of the scientific reports presented at the Conference were published in Latvian and English and were available to participants before the meeting.

Conference chairman
Prof. A.Krumins

Appendix 1

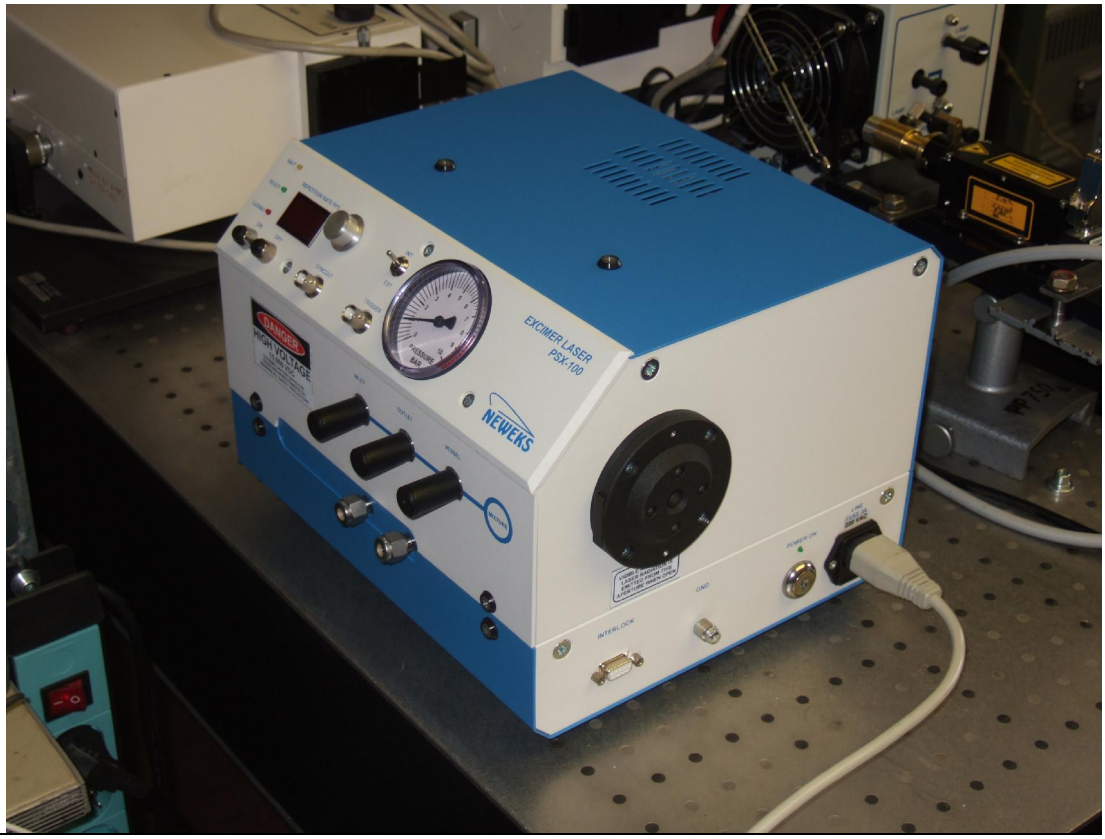
New scientific equipment, purchased at 2005

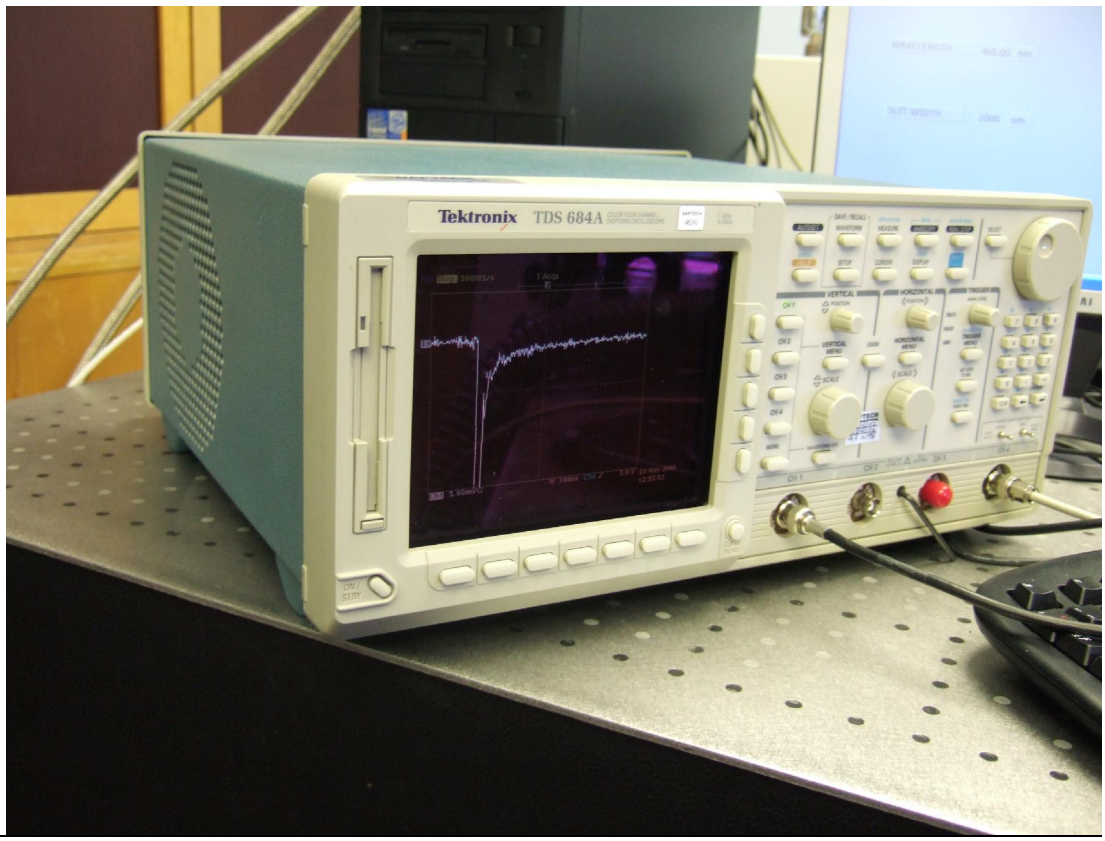
Instrument title:	**Latvian SuperCluster (LASC) - a Beowulf-type system**
Photo:	
Technical details:	• LASC is a Beowulf-type Linux/openMosix PC cluster. It consists of 12 nodes: one front-end (master) node (SuperMicro FileServer), and 11 computational nodes (5 Compaq ProLiant ML350 G2, 2 SuperMicro SuperServer 6013A-T and 4 SuperMicro SuperServer 6014V-T2 servers). The cluster is connected to the Internet through the Firewall. Each node has two Network Interface Cards (NICs), supporting the Fast (100 Mbps) or Gigabit (1000 Mbps) Ethernet connections. • The Fast Ethernet NICs are connected to a HP ProCurve 2312 (12 ports) Fast Ethernet switch and are used for file exchange and communication purposes. The Gigabit Ethernet NICs are connected to a 3COM Baseline 2816 (16 ports) Gigabit Ethernet switch and are used for data exchange during parallel computations. • The total resources available to the users are 22 CPUs, having the theoretical peak performance of about 48 GFLOPS (12.7 GFLOPS on 10 Pentium III-1.27 GHz + 18.36 GFLOPS on 6 Pentium IV XEON 3.06 GHz + 16.8 GFLOPS on 6 Pentium IV XEON 2.8 GHz), 44 GB RAM memory and 3.0 TB total hard disk space.
Application example:	**High-performance computing (HPC) in the fields of quantum chemistry, materials science and physics.**
Responsible: (name, second name, e-mail, phone, room number)	**Dr. Aleksejs Kuzmins**, E-mail: a.kuzmin@cfi.lu.lv, Phone: +371 7251691 Room number 307.

Instrument title:	**Scanning Probe Microscope CP-II** **Veeco Digital Instruments**
Photo:	
Technical details:	§ **CP-II Probe Head,** § **manual XY stage 8×8 mm, resolution 2 μm,** § **motorized Z stage,** § **optical microscope (20×) with video monitoring for tip and sample view,** § **Sample size: up to 50×50 mm,** § **Scanning by sample;** § **scanning area 100×100×7.5 μm, scanner is capable of achieving atomic resolution.** § **ProScan Software, Pentium IV computer**
Application example:	1. Imaging of surfaces of a wide range of materials with high resolution using different SPM techniques: § **Contact Mode, Tapping Mode, Force Modulation Mode, Force vs. Distance Curves,** § **Scanning Tunneling Microscopy (STM)** § **Magnetic Force Microscopy (MFM),** § **Electrostatic Force Imaging (EFM).** **2. Nanolithography by mechanical scratch.** **3. Nanoindentation (nanohardness) tests**
Responsible: (name, second name, e-mail, phone, room number)	**1. Dr. Jānis Maniks** E-mail:**manik@latent.lv** **2. Eng. Georgijs Bakradze** Phone 7261132 Room number **317**

Instrument title:	**Thermo gravimetric analyzer SHIMADZU model DTG-60**
Photo:	
Technical Deta:	Temperature range 20 – 1100 °C Measurable range ± 500 mg Readability 0.001 mg Sample quantity 1 g
Application example:	Adsorption / desorption of porous materials Determination of non volatile matter in soft soldering fluxes
Responsible: **(name, second name, e-mail, phone, room number)**	Dr.phys. Evalds Pentjušs Evalds.Pentjuss@cfi.lu.lv +371-27187817 Room 219

Instrument title:	**Multi Channel Frequency Response Analyser System for Electrochemical and Mechanical Impedances Measurments SOLARTRON model 1091**
Photo:	
Technical Deta:	Cell connections 2,3 and 4 terminal/probes DC voltage range ± 14.5 V DC current range ± 2 A Resolution 100 µV / 100 pA Frequency range 10 µHZ – 100 kHz Impedance 0.01 Ω – 1 GΩ
Application example:	Component control Potentiostatic / Galvanostatic measurements Coulometric / Ampermetric measurements Battery testing pH measurements Coatings / finishes control
Responsible: **(name, second name, e-mail, phone, room number)**	Dr.phys. Vilis Eglītis STS@cfi.lu.lv +371 -27260538 Room 216

Instrument title:	**EXCIMER LASER**
Photo:	
Technical details:	**The NEWEKS AS excimer laser Model: PSX-100** **Laser Medium: F_2** **Wavelength: 157 nm** **Maximum Repetition Rate: 100 pps** **Beam Dimensions: 2.0 x 2.0 mm** **Beam Divergence (HxV): 3.5 x 2.0 mrad** **Gas Mixture: 0.2 bar 5% F_2 in He;** **5.8 bar He 0.17% F_2;** **Total Fill Pressure: 6 Bar** **Pulse Energy: 0.5 mJ** **Maximum Average Power: 0.04 W**
Application example:	§ **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. Anatoly Truhin, (VUV spectroscopy, time-resolved spectroscopy)** **E-mail: truhins@latnet.lv; Phone +371 7260686; Room number 329.** **2. Dr. Linards Skuja, (VUV spectroscopy)** **E-mail: skuja@latnet.lv; Phone +371 7260756; Room number 327.**

Instrument title:	**Facility for Time-resolved Laser Spectroscopy**
Photo:	
Technical details:	§ **Digitizing Oscilloscope, model TDS 684A (Tektronix)** Digitizing rate, max 5 GS/s on each channel simultaneously; analog bandwidth 1 GHz; 4 channels, each with 8-bit resolution; record lengths 15K samples per channel; asquisition modes: sample, envelope, average; color display with zoom; trigger modes: edge, logic, pulse; NVRAM storage; full GPIB programmability; hardcopy output using GPIB, RS-232, or Centronics ports. § **Honeycomb Optical Table, model 1HT15-15-20 (Standa Ltd)** Surface size: 1500 x 1500 mm; surface flatness of the top skin ± 0.1 mm/m^2; top skin pattern: grid of M6 holes spaced by 25 mm with ± 0.1 mm accuracy; two H type table supports 800 – 900 mm height with rubber levelling element.
Application example:	§ **Time-resolved laser spectroscopy of wide band gap materials.** § **Luminescence decay kinetics (*5* ns – *n* ms time scale; excitation by tunable laser pulses).**
Responsible: **(name, second name, e-mail, phone, room number)**	***1.Dr. Peteris Kulis,*** *E-mail: p.kulis@cfi.lu.lv; Phone +371 7187511; Room number 331.* **2. Dr.Maris Springis,** E-mail: springis@cfi.lu.lv; Phone +371 7187471; Room number 533.

Instrument title:	**High sensitivity cooled CCD camera-based spectrograph for spectroscopic studies in deep-ultraviolet, visibel and near-infrared spectral regions**
Photo:	
Technical details:	§ **CCD camera (model Newton DU971N-UVB, Andor Technology):** Thermoelectrically cooled (-80.. -95C), 1600x400 pixels UV-enhanced back-thinned silicon CCD with on-chip electron multiplication, UV-coating and MgF_2 front window, capable of single-photon sensitivity, with USB 2.0 interface, spectral range 150-1050 nm. § **Spectrograph/monochromator (model Shamrock 303i, Andor Technology)** Czerny-Turner optical scheme with toroidal optics, focal length 303 mm, f/4 aperture f/4, Mechanical scan range 0 – 1450 nm, interchangeable 3-grating turrets with gratings (150..2400 lines/mm), fiber-optic input cables, output port switchable between spectrograph and monochromator modes, computer control of grating, grating turret, input and output slits, shutter and filter wheel through USB 2.0 interface.
Application example:	§ **Express optical absorption, reflection and luminescence measurements in UV to infrared spectral regions. High-sensitivity luminescence and Raman analysis. Studies of fiber optics and their materials.**
Responsible: **(name, second name, e-mail, phone, room number)**	***Dr. Linards Skuja*** *E-mail: ls1@cfi.lu.lv Phone +371 7260756; Room number 327.*

Instrument title:	**Spectrum / impedance / network analyser for material characterization AGILENT 4395A**
Photo:	
Technical details:	§ **Type** General purpose spectrum / impedance / network analyser for wide spectral range complex impedance § **Measurement parameters:** |Z|, |Y|, θ, R, X, G, B, C, L, D, Q, harmonic analysis § **Frequency range** 10 Hz to 500MHz, depending on measurement type § **Control and data readout** external keyboard and display or remote control by GPIB interface
Application examples:	§ **Dielectrics** resonance frequency response of piezoactuators or ultrasonic devices § **Material analysis** complex impedance analysis of materials up to 500MHz § **Radioelectronics** testing of high frequency electronic components and curcuits
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:	**Picoammeter Keithley 6487 with built-in voltage source**
Photo:	
Technical details:	§ **Type** High sensitivity multipurpose picoammeter with built-in voltage source § **Sensitivity and resolution:** full scale range from 2 nA to 20 mA with resolution from 10fA to 100nA § **Voltage source** max. Voltage up to 500V; resolution from 200 μV to 10 mV depending on range; automated voltage sweep § **Control and data readout** internal data buffer with writting speed up to 1000 readings per second, remote control by RS232 or GPIB interface
Application examples:	§ **Physics of dielectrics** dielectric polarization hysteresis and I-V characteristics § **Material testing** resistivity measurements up to 1TΩ in constant voltage or alternate voltage mode
Responsible: **(name, second name, e-mail, phone, room number)**	**Dr. Vismants Zauls** **E-mail: vism@latnet.lv** **Phone: +371-7260803** Room number **438**

Appendix 2

Systems and equipment, developed at Institute of Solid State Physics