

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



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**2001**

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# INTRODUCTION

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

In 1995 four laboratories from the Institute of Physics of the Latvian Academy of Science, working in the field of solid state physics joined our Institute. In 1999 twenty scientists from the former Nuclear Research Centre joined the ISSP establishing Laboratory of Radiation Physics

Since 1992 a new field in research and education was launched in the Laboratory of Optical Materials of the ISSP - optometry and vision science. Co-located with the Institute, the Optometry Centre was established in 1995 with facilities to provide primary eye care and serving as a technological basis for student and staff research projects.

The main subjects of research of the ISSP include:

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

The highest decision-making body of the Institute is the Council of 23 members, elected by the employees of the Institute. Dr. hab. M.Springis is presently the elected chairman of the ISSP Council. The Council appoints director and its deputy.

During the last years the ISSP has intensified its participation in teaching. Three research staff members of the Institute have been elected as professors of the University of Latvia. Post graduate and graduate curricula are offered in solid state physics, material physics, chemical physics, physics of condensed matter, semiconductor physics and experimental methods and instruments in physics.

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

The annual report summarizes research activities of the ISSP during 2000. The staff of the Institute has successfully finished the four years work at 35 scientific national grants and national program No 5 (The Synthesis, Research and Application of new Materials for Microelectronics and Photonics) with the total financing 238.3 thous. lats (Ls) (exchange rate: 1 Ls ~ 0,60 USD), see Table 1 and Fig.1.

The proposals for 31 new national scientific projects and one cooperation project (program No 5: Intelligent Materials and Structures for Microelectronics and Photonics) was successfully accepted by experts of Latvian Scientific Council. Thus, for the next four years the state funding will be 238 thous. Ls per year. Additional funding from the state budget in 2000 was 36.9 thous. Ls as a support to participation in international conferences (11.3 thous. Ls) and development of computer network (24.5 thous. Ls).

Table 1

## INCOME OF ISSP, THOUSAND Ls, FROM 1993 - 2000

Year	Total financing	Grants and programs from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Rent of space
1993	100.7	56.8	-	40.8	-	3.1
1994	211.4	127.8	-	64.2	9.6	9.8
1995	281	145.7	45	38.2	40	12.1
1996	322.5	167.1	11.7	62.4	68	13.3
1997	370	192.1	39	93	26	15.2
1998	414 + 156	205.2	26	114	42	26.5
1999	475.6+186	238.1	48.8	156.5	16.5	15.6
2000	478.8 + 77	238.3	36.9	146.3	43	14.3

Year 2000 has been successful in contract signing as well: the market oriented contracts reached 76.8 thous. Ls, contracts with Latvian companies including SMEs – 69.6 thous. Ls. The prospects of some instruments and materials developed at the ISSP due to contracts are enclosed in the Appendix.

The international funding was 43 thous. Ls. For organization of two International Conferences (LUMDETR-2000 and ECAPD-5, see chapter 15) we received 35.8 thous. Ls. The main part of this funding (27,6 thous. Ls) was from EC 5<sup>th</sup> Framework programme “High Level Scientific Conferences”. Additional funding was from EC 5<sup>th</sup> Framework program EURATOM for the project “Irradiation Effects in Ceramics for Heating and Current Drive, and Diagnostic Systems”.

The Institute has obtained 14.3 thous. Ls from leasing part of its space. The rent money decreases since more space is being used by the Institute for its own activities. 77 thous. Ls from the state budget have been invested in thermal insulation and improvement of more efficient energy conservation of the building.

In order to improve the energy efficiency of the building and to diminish the loss of the heat, as well as to reduce the funding necessary for energy, a large – scale reconstruction work in the framework of the state investment project *ED 15 Energy Efficiency in Higher Education and Science Institutions*, comprising the total sum of 418 thous. Ls, has been carried out in the laboratory part of the building during the last three years. A double-pitch roof has been built, thermal insulation of outer walls and windows have been changed, as well as a partial renovation of the interior is carried out. Since 1993 an energy monitoring is carried out for the building in order to evaluate the effect of improved insulation and to work out general recommendations for heat insulation of other buildings in Latvia.

ISSP income dynamics for 1993-1999 are given in Table 1 and Figure 1.

Due to the increased rent (from 1.30 Ls/m<sup>2</sup> per month to 1.40 Ls/m<sup>2</sup> per month) the deduction % from the grants and the projects of infrastructure has increased up to 18.2% in 2000 (see Figure 2).

The interdisciplinary character of research at the ISSP is reflected by the highly qualified staff (see Figure 3). At present there are 172 employees working at the Institute, 34 of

98 research staff hold Dr. hab. degrees, 47 hold Dr. or PhD. At the end of 2000 there were 8 post-graduates and 32 undergraduate and graduate students from physics and optometry programmes working at the ISSP. Educational activities of the Institute were continued and extended in 2000.

Main achievements in 2000:

- in a large competition the ISSP obtained the status of the Centre of Excellence with European Commissions' funding: 703 000 EUR per 3 years (2001-2004). The contract with EC was signed in December 2000 (See chapter1);
- successful organization of two Euroconferences: LUMDETR-2000 and ECAPD-5 (see Chapter 15);
- two books in NATO Science Series have been prepared in cooperation with NATO Scientific Affairs Division:
  - “Defects and Surface-Induced Effects in Advanced Perovskites”, edited by G.Borstel, A.Krumins and D.Millers, Kluwer Academic Publishers, Series 3. High Technology – Vol 77, pp.492.
  - “Defects in SiO<sub>2</sub> and Related Dielectrics: Science and Technology”, edited by G.Pacchioni, L.Skuja and D.L.Griscom; II Mathematics, Physics and Chemistry, Vol. 2, pp.624.

Many thanks to everybody who contributed to this report as well as to the organizations that supported the Institute financially: Latvian Council of Science, Science Department of the Latvian Ministry of Education and Science, EC 5<sup>th</sup> Framework Programme, European Community Council Program COST 514, NATO Scientific Affairs Division as well as to many foreign Universities and institutions.

Prof. Dr. A.Krumins

## Centre of Excellence: New Challenge for ISSP

At the end of 1999 the 5<sup>th</sup> European Commission Framework Programme announced the competition to establish 34 Excellence Centres in Eastern and Central European countries. European Commission allocated 30 milj. EUR for this three- years long program.

Main tasks of the Centre of Excellence:

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

The Centre of Excellence is defined here as scientific institution having its own specific research agenda with multidisciplinary approach and preferably distinct organisational and administrative boundaries.

The ISSP named its project: *Centre of Excellence for Advanced Material Research and Technologies CAMART*. In the framework of this project it is intended to promote and develop our national/international research topics by stressing the applied research and cooperation. For two months the leading scientists of the institute worked on the preparation of the project (approx 500 pages in English).

In the competition of 185 projects from 12 countries our project was highly valued: by gaining 48 points out of 50 possible it took the 5-8 position and the absolute first position among the material science projects.

Six institutes from Latvia took part in the competition. Good results showed also Biomedicine Research and Studies Center of Latvian University (40 points out of 50), Atom Physics and Spectroscopy Institute of Latvian University (37 points) as well as Wood Chemistry Institute (37 points). Still, the Institute of Solid State Physics was the only one to get the financing from Latvia. In Estonia where the science gets more support on the national scale, two institutes got the Excellence Centre funding, while in Lithuania only one institute received it.

After the contract preparation negotiations with European Commission in Brussels in the mid 2000 the contract for 703 000 EUR or 400 000 Ls for three years was signed in December, 2000. This EC's distributed funding should be spent on:

- funding of extended visits (more than of 1 month duration) by foreign colleagues at the ISSP (31%);
- ISSP employees visits abroad, the conference attendance included (35%);
- purchase of the equipment and materials if it is necessary for foreing colleagues during their visits (9%);
- overhead expenses (25%)

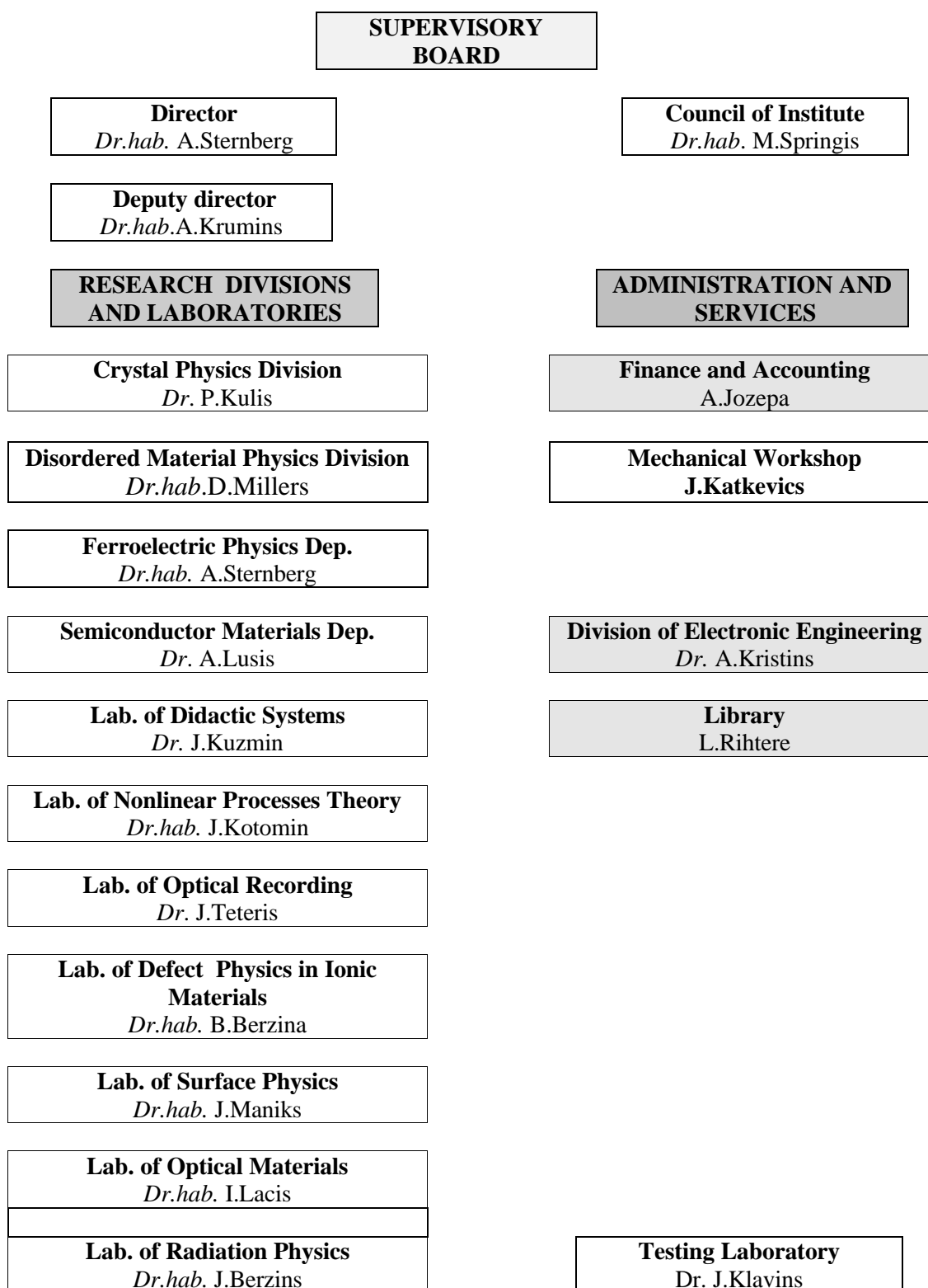
Already in January 2001 the first scientists from Europe came to the Institute in the framework of this project. One of the most painful tasks is to provide them with modern scientific working conditions. As during the last decade the science in Latvia has been on a strong diet (almost no raise in state funding has been experienced since 1995) the scientific equipment (apart from computers) has not been upgraded. We are happy that in state budget for 2001 there is allocated additional funding for the

improvement of infrastructure. We do hope that with additional state support the ISSP will be able to successfully contribute to European Excellence Centres network.

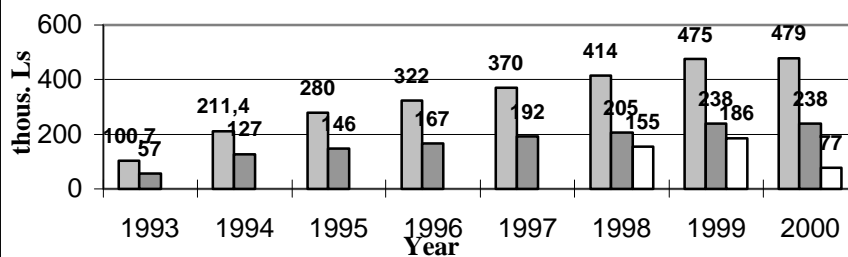
Prof. Dr. A. Krumins  
Scientific coordinator of CAMART



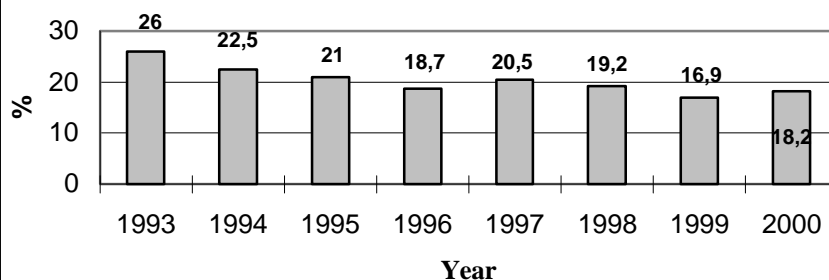
## Organizational structure of the ISSP in 2000



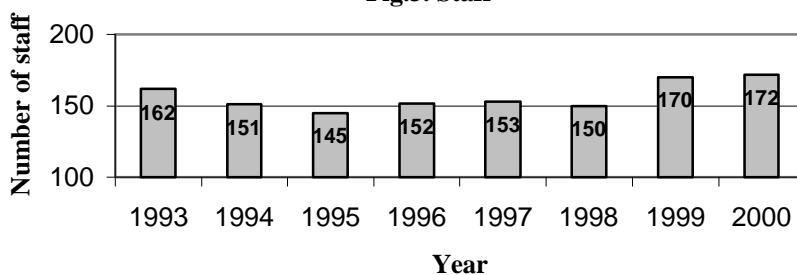
**Fig.1. Grants, investments in reconstruction and total budget financing of the ISSP**



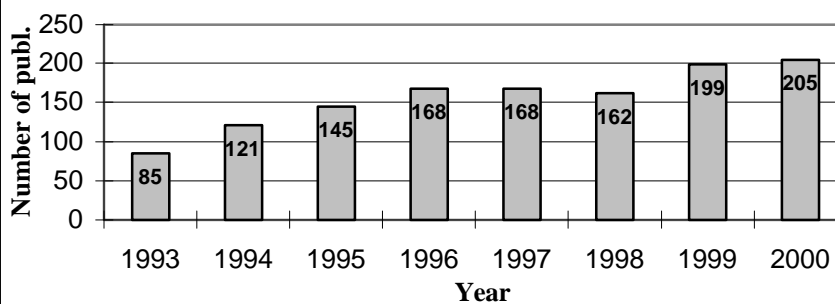
**Fig. 2. Deduction % from grants to the infrastructure**



**Fig.3. Staff**



**Fig. 4. Number of publications**



# CRYSTAL PHYSICS

Head of Division *Dr. P.Kulis*

## Research Area and Main Problems

Research area of the division is concerned with three main projects:

1. Recombination mechanisms of the electronic excitations in new optical binary and ternary compounds - the project is aimed to investigate the exact mechanisms of annihilation, localization and recombination of the electronic excitations and their relationships in new binary and ternary inorganic compounds (nominally pure and doped with some active impurities).
2. Technology of Al-Ga nitride semiconductor heterostructures for light-emitting and laser diodes for violet and ultraviolet spectral regions - the goal of the project is the development of light-emitting diodes and laser diodes for violet and ultraviolet spectral region. The project involves synthesis and design of corresponding new materials on the basis of the third group nitrides, elaboration of the thin film heterostructures and further development of production of multifunctional photonic devices in joint stock company "Alfa".
3. ODMR and multifrequency EPR investigations of the structure of defects - investigation of geometrical and electronic structure of actual defects by optically detected magnetic resonance (ODMR) and multifrequency EPR methods in some important for applications memory screen and scintillator materials.

## Scientific Staff:

1. Mg. J.Jansons
2. Dr. P.Kulis
3. Dr. A.Pujats
4. Dr. hab. U.Rogulis
5. Dr. E.Ruža
6. Dr. hab. M.Spriodis
7. Prof. Dr. hab. I.Tâle
8. Dr. V.Tâle
9. Dr. J.Trokšs
10. Dr. Â.Veispals
11. Dr. hab. V.Ziraps

## Technical Staff:

1. Dz.Bçrziðð
2. R.Erts
3. A.Guiâns
4. A.Muhins
5. Dr. A.Nagornijs
6. V.Ogorodiks
7. P. Zarâns
8. E.Zîle

## Students:

1. Dz.Bçrziðð
2. R.Erts

3. A.Guiāns
4. V.Ogorodniks
5. P.Zarāns
6. E.Zīle

#### **Scientific visits abroad:**

1. Dr.hab. U.Rogulis - University of Paderborn, Germany (6 months).
2. Dr.hab. I.Tale - University of Rostock, Germany (2 weeks)
3. Dr.hab. I.Tale – Johannesburg, South Africa (1 week)
4. Dr.hab. M.Spriodis – Johannesburg, South Africa (1 week)
5. Dr.hab. U.Rogulis – Johannesburg, South Africa (1 week)

#### **Cooperation:**

##### **Latvia:**

Joint stock company “Alfa”

##### **Germany:**

1. University of Paderborn, Germany (Prof. J.-M. Spaeth).
2. University of Rostock, Germany (Prof. H.-J. Fitting, Prof. H. Stolz).
3. University of Osnabruck, Germany (Dr. H. Reyher)
4. Greifswald University, Institute of Chemistry, Greifswald, Germany (Prof. H.Wulff)

#### **Main Results**

#### **THERMAL RELAXATION OF COLOUR CENTRES IN LiBaF<sub>3</sub> CRYSTALS**

*P.Kulis, I.Tale, M.Springis, U.Rogulis, A.Veispals, H.-J.Fitting\**

Processes in LiBaF<sub>3</sub> crystals caused by the thermal decay of F-type centres created by X-irradiation at room temperature have been examined. It is shown that the thermal decay of F-type centres results in the formation of two kinds of electron centres peaking at 630 nm and 740 nm differing in thermal stability. Weak TSL intensity, accompanying the decay of F-centres, also observed as well as the low value of the process activation energy suggest that due to the presence of moving anion vacancies a random walk of the F-centres occur. We propose that in course of the random walk of the F-centres both the aggregate F-centres are created and the annihilation with some complementary radiation defect take place.

*\*Physics Department, University of Rostock, Germany*

#### **SELF-TRAPPED HOLES IN LIBAF<sub>3</sub> CRYSTALS**

*I.Tale, M. Springis, U. Rogulis, V. Ogorodnik, P. Kulis, V. Tale,  
A. Veispals and H.-J. Fitting*

Self-trapped holes ( $V_K$ - centres) in  $x$ -irradiated  $\text{LiBaF}_3$  crystals were investigated by electron paramagnetic resonance (EPR), recombination afterglow and thermostimulated luminescence (TSL). The  $^{19}\text{F}$  hyperfine interaction parameters of  $V_K$ - centres estimated from EPR angular dependencies are:  $A_{\parallel} = 2520$  MHz;  $A_{\perp} = 200$  MHz; the  $g$ -tensor parameters are:  $g_{\parallel} = 2.002$  and  $g_{\perp} = 2.024$ .

\**Physics Department, University of Rostock, Germany*

## **ADVANCED TRAP SPECTROSCOPY USING THE GLOW RATE TECHNIQUE AND THERMOSTIMULATED BLEACHING OF COLOR CENTRES**

**P.Kulis, I.Tale, G.Rudlof\***

The glow rate technique like the fractional glow technique offers a procedure for evaluation of the activation energy of trap emptying of arbitrary thermostimulated relaxation kinetics. The experimental procedure involves at least two subsequent measurements of thermostimulated recombination kinetics at different heating rates. The extension of the glow rate technique to the direct measurements of thermostimulated bleaching of the radiation-induced color centers is presented. The experimental procedure performs measurements of the decay of radiation-induced absorption spectra of color centers in irradiated materials during linear heating. Methods for evaluation of trap depths are considered. Results of the application of glow rate technique for the parameters of thermostimulated decay of color centers are presented for the case of decay of the radiation-induced defects in  $\text{LiBaF}_3$  crystal.

\**Physics Department, University of Rostock, Germany*

## **IONIC, ELECTRONIC AND ION-DIFFUSION CONTROLLED RELAXATION PROCESSES IN $\text{CaF}_2$ , $\text{BaF}_2$ AND $\text{LiBaF}_3$ CRYSTALS**

*V. Ziraps, P. Kulis, I. Tale and A. Veispals*

The ionic, electronic and anion-diffusion controlled thermally stimulated relaxation (TSR) processes at 80–700 K in  $\text{CaF}_2$ ,  $\text{BaF}_2$  and  $\text{LiBaF}_3$  crystals ( X-ray irradiated or non-irradiated) have been investigated by means of the ionic conductivity, ionic thermally stimulated (TS) depolarization current (TSDC), as well as the current (TSC), luminescence (TSL) and bleaching (TSB) techniques. Above 250–290 K broad and overlapping anion TSDC peaks and correlated TSB stages are detected. The TSB kinetics is initiated and controlled by the anion detrapping and interaction with the localized charges, i.e., the anion-diffusion controlled TSR processes take place in fluorides. The TSL and TSC data for  $\text{LiBaF}_3$  evidence that the lifetime and drift of electrons at 80–250 K are very small because of deep retrapping. The main TSL peaks at 132 K, 170 K and 220 K are caused by the  $V_k$  centre detrapping and hole-diffusion controlled tunnel recombination within pairs like  $\{D_n e^- \dots V_k\}$ .

## **ION AND ELECTRON TRAPPING, RELEASE AND RELAXATION PROCESSES IN FLUORIDE CRYSTALS**

The thermally stimulated relaxation (TSR) processes in CaF<sub>2</sub>, BaF<sub>2</sub> and LiBaF<sub>3</sub> crystals have been investigated by means of the ionic conductivity, thermally stimulated (TS) ionic depolarization current (TSDC), TS current (TSC), TS luminescence (TSL) and thermal bleaching techniques. The ionic TSDC measurements evidence that under DC field fluorides accumulate large ionic space-charge as a result of the migrating anion interstitial and/or vacancy capture on defects. In the ionic conductivity region (290–650 K) the thermoelectret state anneals, and several wide and overlapping anionic TSDC peaks are detected. The ionic TSDC stages correlate with the X-ray induced absorption band (F-type and other) thermal bleaching stages. These data evidence that the TSR processes are initiated and controlled by the anion defect thermal detrapping and interaction with the colour centres and other localized charges. The anion diffusion-controlled TSR processes take place in fluorides. The TSL, TSC and TSL efficiency (TSL/TSC) data evidence that holes and, probably, the interstitials are detrapped: in CaF<sub>2</sub> - at 125–190 K, 260–320 K; in LiBaF<sub>3</sub> - at 132 K, 170 K and 220 K. The hole or interstitial diffusion-controlled radiative recombination (TSL) takes place above LNT.

### **MOLLWO-IVEY RELATIONS FOR OPTICAL ABSORPTION BANDS OF THE ATOMIC AND F' CENTRES IN ALKALI HALIDES**

V. Ziraps

Evidences are given that two classes of the transient IR-absorption bands: (a) with max. at 0.27–0.36 eV in NaCl, KCl, KBr, KI and RbCl (due to "shallow electron traps" or "bounded polarons and (b) with max. at 0.15–0.36 eV in NaI, NaBr, NaCl:I, KCl:I, RbCl:I and RbBr:I (due to "on-centre STE localised at iodine dimer" are caused by the same defect – "atomic alkali impurity" centre  $[M^+]_c^0 e^-$  (electron  $e^-$  trapped by a substitutional smaller size alkali cation impurity  $[M^+]_c^0$ ). The *Mollwo-Ivey* plots (for the transient IR-absorption bands) of the zero-phonon line energy  $E_0$  (for NaCl, KCl, KBr, RbCl and NaBr, KCl:I) and/or the low-energy edge values  $E_0$  (for NaI, RbCl:I, RbBr:I) *versus* anion-cation distance (d) evidence that two types of the  $[M^+]_c^0 e^-$  centres are predominant: (a)  $[Na^+]_c^0 e^-$  in KX and RbX host crystals with the relation  $E_0 \approx 6.15/d^{2.74}$ ; (b)  $[Li^+]_c^0 e^-$  in NaX host crystals -  $E_0 \approx 29.4/d^{4.72}$ . The *Mollwo-Ivey* relation  $E_0 \approx 18.36/d^{2.70}$  is fulfilled as well for the F' band in NaCl, KCl, KBr, KI, RbCl, RbI if we use the F' centre optical binding energy values  $E_0$  eV.

### **STRUCTURE AND LUMINESCENCE OF GaN LAYERS**

*T.Barfels\**, *H.-J. Fitting\**, *J.Jansons*, *I.Tale*, *A.von Czarnowski\**, *H.Wulff\*\**

The growth of thin GaN films on Si substrates by means of low pressure MOCVD technique in a horizontal flow quartz reactor is investigated. The polycrystalline hexagonal structure of GaN layers has been checked by means of grazing incidence X-ray diffractometry and IR spectroscopy. Cathodoluminescence spectra and their kinetics are studied. The mean decay time of the 3.44 eV UV bound exciton transition is below 1 ns, whereas the 3,26 violet band shows a slow hyperbolic decay over 1  $\mu$ s. The third yellow band appears at 2.25 eV due to transitions via localized states.

\**Physics Department, University of Rostock, Germany*

\*\**Institute of Chemistry, Greifswald University, Germany*

## **LUMINESCENCE AND ELECTRON TRANSPORT PROPERTIES OF GaN AND AlN LAYERS**

*T. Barfels\*, H.-J. Fitting\*, A. Gulans, J. Jansons, M. Springis,  
H. Stolz\*, I. Tale, A. Veispals*

Third group nitrides being wide gap semiconductors are prospective for application as materials for both the luminescence transformers and the selective photo - detectors in visible and ultraviolet spectral region. Thin GaN and AlN films were grown on sapphire substrates by means of low pressure MOCVD technique in a horizontal flow quartz reactor. In our preparation the growth temperature was 900 – 1000 °C. Trimethylgallium or trimethylaluminium with flow rates of 3 – 8 µmol/min and a N<sub>2</sub> flow of 10 l/min as the carrier gas were used as group-III source; NH<sub>3</sub> with flow rates 0.25 – 0.5 mol/min as group-V source. Luminescence, free electron density and Hall mobility of obtained monocrystalline GaN, GaN(Mg) and AlN films of thickness ranging from 0.1 µm to 0.2 µm was investigated.

\**Physics Department, Rostock University, Germany*

## **OPTICALLY DETECTED MAGNETIC RESONANCE INVESTIGATIONS OF OXYGEN LUMINESCENCE CENTRES IN BaFCl**

**S. Schweizer\*, U. Rogulis, K.S. Song\*\* and J.-M. Spaeth\***

The structure of oxygen-related luminescence centres in oxygen-doped BaFCl was investigated by photoluminescence-detected electron paramagnetic resonance (PL-EPR). It turned out that one of the oxygen-related luminescence centres is due to an excited triplet state. The structure of the centre can be described as an oxygen-vacancy complex where the oxygen substitutes for fluorine with a next nearest chlorine vacancy.

\* *Physics Department, University of Paderborn, Germany*

\*\**Physics Department, University of Ottawa, Canada*

## **RbBr AND CsBr DOPED WITH Eu<sup>2+</sup> AS NEW COMPETITIVE X-RAY STORAGE PHOSPHORS**

*S. Schweizer\*, U. Rogulis, S. Assmann\* and J.-M. Spaeth\**

Photostimulated luminescence and the paramagnetic defect centres generated upon x-irradiation were studied in CsBr and RbBr doped with divalent Eu. The influence of the Eu<sup>2+</sup> aggregation on the energy storage and read-out process is under investigation.

\* *Physics Department, University of Paderborn, Germany*

## THE F-TYPE CENTRES IN YAG CRYSTALS

A. Pujats, M. Springis

The comparative study of optical properties of thermochemically reduced undoped YAG ( $\text{Y}_3\text{Al}_5\text{O}_{12}$ ) crystals is reported. A particular type of the centres often observed in YAG crystals synthesized as well as treated under the reducing atmosphere is related to an anion vacancy with one or more trapped electrons (F-type centres in YAG crystals). The changes of photoluminescence intensity and absorption bands intensity of the observed centres under X - irradiation as well as the speculations support the F- and  $\text{F}^+$ -centre models. It is shown that the F-centre absorption involves at least two bands at 195 nm and 240 nm, where the broad F-centre luminescence band at 460 nm can be excited. It is suggested the existence of the F-centre could be connected with the absorption bands at 360 nm, 480 nm, and 830 nm.

### Scientific Publications

Published in 2000

1. I.Tale, V. Tale, P. Kulis, M. Springis, A.Veispals, H.-J. Fitting. *Mechanism of the recombination luminescence of  $\text{LiBaF}_3$  crystals*, Proceedings of the 5-th International Conference on INORGANIC SCINTILLATORS and THEIR APPLICATION, August 16-20, 1999, Moscow State University, Moscow, Russia, 2000, ed. V. Mikhailin, p. 236-241.
2. M.Springis, P. Kulis, I. Tale, A. Veispals, H.-J. Fitting. *Defect luminescence of  $\text{LiBaF}_3$  perovskites*, Proceedings of the 5-th International Conference on INORGANIC SCINTILLATORS and THEIR APPLICATION, August 16-20, 1999, Moscow State University, Moscow, Russia, 2000, ed. V. Mikhailin, p. 555-559.
3. A.N.Trukhin, H.-J.Fitting, T.Barfels, A.Veispals. *Defect Luminescence Study in Tetragonal  $\text{GeO}_2$  Crystals*. - NATO Sciences Series, 3. High Technology – Vol.77, Kluwer Academic Publishers, 2000., p.379-386.
4. V.Ziraps, P.Kulis, I.Tale and A.Veispals. *Thermally Stimulated Ionic and Electronic Processes and Radiation- Induced Defect Annealing in  $\text{LiBaF}_3$  Crystals*. NATO Sciences Series, 3. High Technology – Vol.77, Kluwer Academic Publishers, 2000., p.387-392.
5. P.Kulis, I.Tale, M.Springis, U.Rogulis, J.Trokss, A.Veispals and H.-J.Fitting. *Radiation Defects in  $\text{LiBaF}_3$  Perovskites*. - NATO Sciences Series, 3. High Technology – Vol.77, Kluwer Academic Publishers, 2000., p.393-398.
6. M.Springis, P.Kulis, I.Tale, A.Veispals, H.-J.Fitting. *Defect Luminescence of  $\text{LiBaF}_3$  Pervoskites*. - NATO Sciences Series, 3. High Technology – Vol.77, Kluwer Academic Publishers, 2000., p.479-484.
7. U.Rogulis, S. Schweizer, S. Assmann and J.-M. Spaeth, *Photostimulated luminescence process in the X-ray storage phosphor  $\text{CsBr:Ga}$* . J. of Applied Physics, 2000, vol. 87, pp. 207-211.
8. S.Schweizer, U. Rogulis, J.-M. Spaeth, L. Trinkler and B. Berzina, *Investigation of oxygen-related luminescence centres in AlN ceramics*. Phys. Status. Sol. (b), 2000, vol. 219, pp. 171-180.
9. S.Schweizer, U. Rogulis, K.S. Song and J.-M. Spaeth, *Optically detected magnetic resonance investigations of oxygen luminescence centres in  $\text{BaFCl}$* , J. Phys.: Condens. Matter, 2000, vol. 12, pp. 6237-6243.



### In Press

1. I.Tale, M.Springis, U.Rogulis, P.Kulis, V.Tale, A.Veispals and H.-J.Fitting, *Self – Trapped Holes in LiBaF<sub>3</sub> Crystals*. - Radiation Effects and Defects in Solids, (in press)
2. P.Kulis, I.Tale, M.Springis, U.Rogulis, V.Tale, A.Veispals and H.-J.Fitting, *Thermal Relaxation of Colour Centres in LiBaF<sub>3</sub> Crystals*. - Radiation Effects and Defects in Solids, (in press)
3. A.Pujats, M.Springis, *The F-type centres in YAG crystals*. - Radiation Effects and Defects in Solids, (in press)
4. V.Ziraps, P.Kulis, I.Tale and A.Veispals, *Ionic, Electronic and Ion-Diffusion Controlled Relaxation Processes in CaF<sub>2</sub>, BaF<sub>2</sub> and LiBaF<sub>3</sub> Crystals*. – Radiation Effects and Defects in Solids, (in press).
5. U.Rogulis, S.Schweizer, J.-M.Spaeth, L.Trinkler and B.Berzina, *Magnetic resonance investigations of oxygen-related luminescence centres in AlN ceramics*, Radiation Effects and Defects in Solids, (in press).
6. T.Klempt, S.Schweizer, O.Kanert, D.Suter, U.Rogulis and J.-M.Spaeth, *Magnetic resonance investigations of F centres in LiF caused by ionising radiation*, Rad. Eff. and Def. in Solids, (in press).
7. T.Barfel, H.-J.Fitting, A.Gulans, J.Jansons, M.Springis, H.Stolz, I.Tale and A.Veispals, *Luminescence and Electron Transport Properties of GaN and AlN Layer*. Radiation Measurements, (in press).
8. P.Kulis, I.Tale and G.Rudlof, *Advanced Trap Spectroscopy by Glow Measurements Rate Technique using Thermostimulated Bleaching of Color Centers*. Radiation Measurements, (in press).
9. P.Kulis, I.Tale, A.Veispals, V.Tale and H.-J.Fitting, *The Mechanism of Thermally Stimulated Decay of F-Type Centers in LiBaF<sub>3</sub> Crystals*. Radiation Measurements, (in press).
10. V.Ziraps, *Mollwo-Ivley Relations for Optical Absorption Bands of the Atomic and F' - Centres in Alkali Halides* Radiation Measurements, (in press).
11. V.Ziraps, P.Kulis, I.Tale and A.Veispals, *Ion Diffusion – Controlled Processes in Fluoride Crystals*. Radiation Measurements, (in press).
12. S. Schweizer, U. Rogulis, S. Assmann and J.-M. Spaeth, *RbBr and CsBr doped with Eu<sup>2+</sup> as new competitive x-ray storage phosphors*, Radiation Measurements, (in press).
13. P.Kulis, I.Tale and G.Rudlof, *Advanced Trap Spectroscopy in LiBaF<sub>3</sub> by Thermostimulated Bleaching of Color Centers*. Latvian J.Phys.Techn.Sci, (in press).
14. V.Ziraps, P.Kulis and I.Tale, *Ion and Electron Trapping, Release and Relaxation Processes in Fluoride Crystals*. – Proceedings of SPIE, (in press).
15. V.Ziraps, *Shallow Electron Traps in Alkali Halide Crystals: Mollwo-Ivey Relations of the Optical Absorption Bands*. – Proceedings of SPIE, (in press).

### Lectures on Conferences

#### 16th Scientific Meeting of the Institute of Solid State Physics, University of Latvia, Riga, 1998.

1. M.Springis, P.Kulis, I.Tale, A.Veispals and H.-J.Fitting. *Polarized luminescence of LiBaF<sub>3</sub> Crystals*, - 16<sup>th</sup> Scientific Conference. Abstracts (Institute of Solid State Physics, University of Latvia, Riga, 2000), pp. 17. (oral presentation).
2. P.Kulis, I.Tale, M.Springis, U.Rogulis, A.Veispals and H.-J.Fitting. *Thermal relaxation of colour centres in LiBaF<sub>3</sub> crystals*, - Ibid, pp. 18. (oral presentation).

3. A.Pujats and M. Springis. *Luminescence of intrinsic defects in YAG crystals*, - Ibid, pp. 19. (oral presentation).
4. V.Ziraps, *Shallow Electron Traps in Alkali Halide Crystals: Optical Absorption Spectra Mollwo-Ivey Relations*. – Ibid, pp. 22-23. (oral presentation).
5. J.Jansons, M.Springis and V.Ziraps, *Change of Cathodoluminescence under X-Irradiation of LiBaF<sub>3</sub>*. - Ibid, pp. 24. (oral presentation).
6. J.Jansons, *Founding of technical committee for lighting standartisation*, - Ibid, pp. 80. (oral presentation).
7. U. Rogulis, V. Ogorodniks, I. Tale un A. Veispals, EPR spectra of LiBaF<sub>3</sub> crystals, - Ibid, pp. 20. (oral presentation).

14<sup>th</sup> International Conference on Defects in Insulating Materials, ICDIM-2000. Eskom Conference Center, Johannesburg-Midrand, South Africa, 2000

1. A.Pujats and M.Springis, *The F-type centres in YAG crystals*, - 14<sup>th</sup> International Conference on Defects in Insulating Materials, ICDIM-2000. Programme and Abstracts (Eskom Conference Center, Johannesburg-Midrand, South Africa, 2000), p. 34. (poster presentation).
2. V.Ziraps, P.Kulis, I.Tale and A.Veispals, *Ionic, Electronic and Ion-Diffusion Controlled Relaxation Processes in CaF<sub>2</sub>, BaF<sub>2</sub> and LiBaF<sub>3</sub> Crystals*, - Ibid, p. 64. (poster presentation).
3. V.Ziraps, *Shallow Electron Traps in Alkali Halide Crystals*, - Ibid, p. 65. (poster presentation).
4. I.Tale, M.Springis, U.Rogulis, P.Kulis, V.Tale, A. Veispals and H.-J.Fitting. *Self-traped holes in LiBaF<sub>3</sub> crystals*, - Ibid, p. 88. (poster presentation).
5. P.Kulis, I.Tale, M.Springis, U.Rogulis, A.Veispals and H.-J.Fitting, *Thermal relaxation of colour centres in LiBaF<sub>3</sub> Crystals*. - Ibid, p. 115. (poster presentation).

4<sup>th</sup> Euroconference "Luminescent Detectors and Transformers of Ionizing Radiation" LUMDETR'2000, Rīga-Jūrmala, Latvia, August 14-17, 2000

1. V.Ziraps, *Mollwo-Ivey Relations for Optical Absorption Bands of the Atomic and F' Centres in Alkali Halides*. – 4<sup>th</sup> Euroconference "Luminescent Detectors and Transformers of Ionizing Radiation" (LUMDETR'2000). Book of Abstracts (Rīga-Jūrmala, Latvia, August 14-17, 2000), p. 96. (poster presentation)
2. S.Schweizer, U.Rogulis, S.Assmann and J.-M. Spaeth, *RbBr and CsBr doped with Eu<sup>2+</sup> as new competitive x-ray storage phosphors*, - Ibid, p. 80. (poster presentation)
3. V.Ziraps, P.Kulis, I.Tale and A.Veispals, *Ion diffusion-controlled processes in fluorite crystals*, – Ibid, p. 97. (poster presentation)
4. P.Kulis, I.Tale and G.Rudlof, *Advanced trap spectroscopy by glow rate technique using thermostimulated luminescence or bleaching of color centers*, – Ibid, p. 129. (poster presentation)
5. I.Tale, M.Springis, U.Rogulis, V.Ogorodnik, P.Kulis, V.Tale, A.Veispals and H.-J.Fitting, *Self-traped holes in LiBaF<sub>3</sub> crystals*, – Ibid, p. 130. (poster presentation)
6. I.Tale, V.Tale, P.Kulis, M.Springis, J.Jansons, A.Veispals and H.-J.Fitting, *Radiative recombination processes in LiBaF<sub>3</sub> crystals*, – Ibid, p. 131. (poster presentation)
7. A.Pujats, *Luminescence of intrinsic defekts in YAG*, – Ibid, p. 132. (poster presentation)
8. T.Barfels, H.-J.Fitting, A.Gulans, J.Jansons M.Springis, H.Stolz, I.Tale and A.Veispals, *Luminescence and electron transport properties of GaN and AlN layers*, – Ibid, p. 133. (poster presentation)

2<sup>nd</sup> International Conference "Advanced Optical Materials and Devices" ADOM-2, Vilnius, Lithuania, August 16-19, 2000

1. U.Gross, A.Ubelis and J.Jansons, *Iodine and mercury resonance lamps and their spectrum in far UV*, – 2<sup>nd</sup> International Conference "Advanced Optical Materials and Devices" (ADOM-2). Abstracts (Vilnius, Lithuania, August 16-19, 2000), p. 24. (poster presentation)
2. V.Ziraps, *Shallow Electron Traps in Alkali Halide Crystals: Mollwo-Ivey Relations of the Optical Absorption Bands*. – Ibid, p. 54. (poster presentation)
3. V.Ziraps, P.Kulis and I.Tale, *Ion and Electron Trapping, Release and Relaxation Processes in Fluoride Crystals*. – Ibid, p. 83. (poster presentation)

5<sup>th</sup> Euroconference on Application of Polar Dielectrics, ECAPD-5 Riga(Jurmala), Latvia, August 27-30, 2000

1. V.Ziraps, *Thermoactivated Electronic and Ionic Relaxation Processes in Irradiated YScO<sub>3</sub> and YScO<sub>3</sub>:Nd Crystals*. – 5<sup>th</sup> Euroconference on Application of Polar Dielectrics (ECAPD-5). Programme and Abstracts (Jurmala, Latvia, August 27-30, 2000), p. 123.

13<sup>th</sup> International Symposium on Exoemission and Related Phenomena, Jurmala, Latvia, August 21-25, 2000

1. V.Ziraps, V.Graveris and I.Krumins, *Electronic and Ionic Processes in Sapphire*. - 13<sup>th</sup> International Symposium on Exoemission and Related Phenomena. Abstracts (Latvia, August 21-25, 2000), pp. 22-23. (poster presentation)
2. J.Jansons, M.Springis and V.Ziraps, *Influence of Charge Relaxation in Surface Layer on Cathodoluminescence under X-Irradiation of LiBaF<sub>3</sub>*. - Ibid, p. 27. (poster presentation)
3. P.Kulis, I.Tale and G.Rudlof, *Advanced trap spectroscopy in LiBaF<sub>3</sub> by thermostimulated bleaching*, - Ibid, p. 27. (poster presentation)

The American Ceramic Society's 102<sup>nd</sup> Annual Meeting and Exposition: "6<sup>th</sup> Symposium on Fabrication and Properties of Ceramics for Fusion Energy and Other High Radiation Environments"

1. V.Ziraps, *Radiation-Induced Ionic and Electronic Charge Accumulation and Release in Alumina*. – The American Ceramic Society's 102<sup>nd</sup> Annual Meeting and Exposition: "6<sup>th</sup> Symposium on Fabrication and Properties of Ceramics for Fusion Energy and Other High Radiation Environments". Abstracts (St. Louis, Missouri, USA, April 30-May 3, 2000), Abstract ID=427. (poster presentation)

# DISORDERED MATERIAL PHYSICS

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

## Research Area and Main Problems

The time-resolved spectroscopy of luminescence and absorption is used for the study of recombination process as well as charge trapping or/and self-trapping in complex oxides. The main objects of the study are pure and doped ( $\text{LiNbO}_3$  and  $\text{KNbO}_3$ ) and tungstates ( $\text{PbWO}_4$ ,  $\text{CdWO}_4$ ,  $\text{ZnWO}_4$ ).

The transient absorption band below 1.3 eV in niobates is identified as absorption due to self-trapped polaron states. The absorption due to luminescence center excited state is observed in  $\text{CdWO}_4$  and  $\text{ZnWO}_4$ . The spacing of electrons and holes are strongly affected by presence of dopands in  $\text{PbWO}_4$ .

### Scientific Staff:

1. Dr. hab.phys. S.Chernov
2. Dr. hab.phys. L.Grigorjeva
3. Dr. hab.phys. D.Millers
4. Dr. hab.phys. I.Plavin
5. Dr.phys I.Hinoverova
6. Dr.phys. A.Tale

### Technical Staff:

1. Ing. A.Sitdikov

### Ph.D. Students:

1. Mg. Phys.V.Pankratov

### Students:

1. I.Lubina
2. K.Shmits

### Scientific Visits Abroad:

1. Dr. hab.phys. L.Grigorjeva, CERN, Geneva, Switzerland (4 days)
2. Dr.hab.phys. L.Grigorjeva, South Africa (7days)
3. Mag.V.Pankratov, Aachen, Germany (5 days)
4. Mag.V.Pankratov, Rostock, Germany (14 days)
5. Dr.hab.phys.D.Millers, University of Osnabruck, Germany (6 days)

## Cooperation

### Latvia

1. University of Latvia, (Prof. J.Tiliks).
2. University of Latvia, Institute of Biology (O.Mutere)
3. SIA "Baltic Scientific Instruments" (Dr.V.Gostillo)
4. SIA "Ritec" (Dr. V.Ivanov)

### USA:

Prof. R.T. Williams, Dr.H. Yochum

### Czech Republic:

Academy of Sciences, Institute of Physics (Dr.M.Nikl)

**Germany:**

University of Osnabruck, Department of Physics (Prof.S.Kapphan)

**Estonia:**

Institute of Physics, Tartu (Dr.V.Nagirnyj)

**Hungary:**

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

**Russia:**

1. University of Kemerovo (Prof.E.Aluker)
2. GOI, St.Peterburg, Dr.L.Maksimov
3. Phys.Tech.Inst. RAS, Dr.V.Trepakov, Dr. A.Badaljan

**Ukraine:**

University of Lvov, Prof. Voloshinovskii

**Switzerland:**

1. CERN, CRYSTAL CLEAR PROJECT, Geneva (Prof.P.Lecoq, Dr.A.Belskii)

## Main Results

### TRANSIENT ABSORPTION AND LUMINESCENCE OF LiNbO<sub>3</sub> AND KNbO<sub>3</sub>

*L. Grigorjeva, V. Pankratov, D. Millers, G. Corradi\*\* , K. Polgar\*\* , R.T.Williams\* ,  
H.M.Yohum\**

The time-resolved optical absorption spectra in congruent and stoichiometric LiNbO<sub>3</sub> as well as KNbO<sub>3</sub> crystals are reported. The fraction of transient absorption at 1.0 eV in LiNbO<sub>3</sub> and KNbO<sub>3</sub> is due to electron polarons. The part of transient absorption above 1.5 eV is due to secondary defects. These defects are formed from primary intrinsic polarons trapped at lattice imperfections. The main relaxation processes in LiNbO<sub>3</sub> and KNbO<sub>3</sub> occur within niobium-oxygen complexes and are only slightly affected by alkali ion.

The excited states responsible for luminescence are created via recombination. In the creation of these excited states participate spaced electrons and holes, possibly geminate pairs.

A strong infrared transient absorption band centered below 1.3 eV is found in stoichiometric LiNbO<sub>3</sub>. The band is much weaker in congruent LiNbO<sub>3</sub> and then is only observed on subnanosecond time scales. This absorption band is attributed to intrinsic electron polarons in undoped stoichiometric LiNbO<sub>3</sub>. Its formation time is <300 fs at room temperature and its decay is ~1 ns at 295 K and a few μs at 77 K.

*In cooperation with:* \* Wake Forest University, USA

\*\* Hungarian Academy of Sciences, Research Inst. for Solid State  
Physics & Optics, Crystal Physics Laboratory

## EXCITED STATE ABSORPTION AND LUMINESCENCE IN $\text{ZnWO}_4$

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

The spectra and decay kinetics of luminescence and transient absorption in  $\text{ZnWO}_4$  were studied. The pulsed electron beam and nitrogen laser were used for luminescence excitation, the transient absorption was measured under electron beam excitation. The slow exponential decay component (15  $\mu\text{s}$  at 300K) was observed under electron beam excitation in both luminescence and absorption decay. This slow decay fraction (~60% of total transient absorption) is due to transitions from luminescence center excited state (ESA). The ESA was observed earlier in  $\text{ZnWO}_4$  and in  $\text{CdWO}_4$ . The activation energy of luminescence center thermal quenching is estimated from luminescence and ESA temperature dependencies. The effects of Fe doping on ESA spectrum and luminescence decay times under laser excitation are discussed. The other fraction of transient absorption is fast, nonexponential and may be due to trapped charge carriers.

*In cooperation with:* Hungarial Academy of Science, Research Inst. for Solid State Physics & Optics.

## TRANSIENT ABSORPTION IN $\text{PbWO}_4:\text{Nb}$

*D.Millers, S.Chernov, V.Pankratov, L.Grigorjeva*

The transient absorption spectra and kinetics of absorption relaxation have been studied in  $\text{PbWO}_4:\text{Nb}$  (PWO:Nb) under pulsed electron beam ( $10^{-8}$  s) irradiation at RT. The spectra and kinetics are quite different for pure PWO and  $\text{Nb}^{+5}$  doped PWO crystals. The kinetics of absorption relaxation in PWO:Nb are different within absorption spectrum. The contribution of absorption slow decay component ( $<10^{-6}$  s) is large than that in pure PWO. These effects are responsible for significant differences in spectra measured under irradiation pulse and at time delay. One absorption band (3.5 eV) of two known bands (3.0 eV and 3.5 eV) of hole centers is observed in pure as well as La doped PWO whereas both absorption bands are observed in PWO:Nb.

### Scientific Publications Published in 2000

1. V.Pankratov, L.Grigorjeva, D.Millers, G.Corradi, K.Polgar. *Luminescence of ferroelectric crystals  $\text{LiNbO}_3$  and  $\text{KNbO}_3$* . Ferroelectrics, v.239, p.241-250, 2000.
2. E.Kotomin, R.I. Eglitis, G. Borstel, L.G.Grigorjeva, D.KMillers and V.Pankratov. *Theoretical and experimental study of radiation defects in  $\text{KNbO}_3$  perovskite crystals*. Nucl. Instrum. and Methods in Phys. Research, B, v.166-167, p.239-304, 2000.
3. L. Grigorjeva, D. Millers S. Chernov, M. Nikl, Y. Usuki, V. Pankratov. *The study of time resolved absorption and luminescence in  $\text{PbWO}_4$  crystals*. Nucl. Instrum. and Methods in Phys. Research, B, v.166-167, p.323-333, 2000.
4. D. Millers, S. Chernov, L. Grigorjeva, V. Pankratov, M. Nikl, Y. Usuki. *Luminescence and transient absorption of doped  $\text{PWO}_4$  scintillator crystals*. Proc. 5<sup>th</sup> International Conference on Inorganic Scintillators and their application. SCINT'99, Moscow, Russia, p. 613-617, 2000.
5. R.T. Williams, H.M. Yochum, K.B.Ucer, D.K. Millers, L.G.Grigorjeva, S.Chernov. *Picosecond and nanosecond time-resolved study of luminescence and absorption of  $\text{CdWO}_4$  and  $\text{PbWO}_4$* . Ibid, p.336-341, 2000.

6. H.M.Yohum, K.B.Ucer, R.T.Williams, L.Grigorjeva, D.Millers, G.Corradi. *Subpicosecond laser spectroscopy of blue-light-induced absorption in  $KNbO_3$  and  $LiNbO_3$* . NATO Science Series, 3 High Technology, v.77, p.125-138, 2000.

### In Press

1. S.Chernov, D.Millers, L.Grigorjeva, V.Pankratov. *Transient absorption spectra and relaxation kinetics in the  $PbWO_4$ -Nb scintillation crystals*. Radiation Measurements, 2001 accepted.
2. L.Grigorjeva, D.Millers, S.Chernov, V.Pankratov, A.Watterich. *Luminescence and transient absorption in  $ZnWO_4$  and  $ZnWO_4$ -Fe crystals*. Ibid., 2001, accepted.
3. L.Grigorjeva, V.Pankratov, D.Millers, G.Corradi, K.Polgar. *Transient absorption and luminescence of  $LiNbO_3$  and  $KNbO_3$* . Ferroelectrics, 2001, accepted.
4. L.Grigorjeva, V.Pankratov, D.Millers, G.Corradi, K.Polgar. *Relaxation of electronic excitations in  $LiNbO_3$  crystals*. Ibid., 2001, accepted.
5. D.Millers, L.Grigorjeva, V.Pankratov, S.Chernov, A.Watterich. *Time-resolved spectroscopy of  $ZnWO_4$* . Radiat.Effects and Defects in Solids, 2001, accepted.
6. R.T.Williams, K.B.Ucer, H.M.Yochum, L.Grigorjeva, D.Millers, G.Corradi. *Self-trapped electron and transient defect absorption in niobate and tungstate crystals*. Ibid., 2001, accepted.
7. A.Tale, I. Plavina, Spatial correlation of latent image centres active in photostimulable luminescence of irradiated doped alkali halides. In: "Advanced Optical Materials and Devices," 16-19 August, 2000, Vilnius, Lithuania, Proc. SPIE, 2000, accepted.
8. I.Plavina, A. Tale, Luminescence responses of KBr:In at room temperature in the case of electron irradiation, Latvian J. of Phys. and Techn. Sci., accepted.
9. Īëÿàëíŭ È.È., Òàëà À.È. Īðñòðãñòààíííâ ðãñðããããëãëã äãòãëòíã â òðòñðèíóëèðóãíŭò ùãëí-ñ-ããëëãíŭò êðèñòãëëò. – Àãðñãððëÿ, 2000 (accepted).

### Lectures at Conferences

#### 16th Scientific Conference of ISSP, February 14-16, 2000

1. I.Piaviða, A.Tãle. *Fotostimlçtãs luminiscences spektri KBr:Tl kristãlã.*
2. V.Pankratovs, L.Grigorjeva, D.Millers, S.Èernovs. *Ierosinãtã stãvokia absorbcija un luminescence  $ZnWO_4$  kristãlã.*
3. D.Millers, S.Èernovs, L.Grigorjeva *Ísi dzívojoðã absorbcija PWO:Nb kristãlã.*
4. V.Pankratovs. *Fotonikas materiãlu spektrãlie pçtñjumi ar laika izðkirðanu.*

#### International workshop on "Microstructure of Oxide Materials" Universitate of Osnabruck, June 13-15, 2000.g

5. D.Millers, L.Grigorjeva, S.Chernov, V.Pankratov. *Relaxation of electronic excitations in tungstates and niobates.*, (oral presentation)

#### International Conference Advanced Optical Materials and Devices, AOMD-2, Vilnius, Lithuania, August 16-19, 2000.

6. A.Tale, I.Plavina. *Spacial distribution of the latent image centers active in photostimulable luminescence*, (poster presentation)

#### The 5-th Euroconference on Application of Polar Dielectrics. ECAPD-5, Jurmala, Latvia, August 27-30, 2000.

7. L.Grigorjeva, V.Pankratov, D.Millers, G.Corradi, K.Polgar *Electronic excitations relaxation in  $LiNbO_3$  crystals*, (poster presentation)

#### 12-th International Sumposium on Integrated Ferroelectrics, ISIF-2000, Aachen, Germany, March 12-15, 2000.

8. L.Grigorjeva, V.Pankratov, D.Millers, G.Corradi, K.Polgar. *Transient absorption and luminescence of LiNbO<sub>3</sub> and KNbO<sub>3</sub>*. (poster presentation)

14-th International Conference on Defects in Insulating Materials, ICDIM-2000, Johannesburg, South Africa, April 3-7, 2000.

9. D.Millers, L.Grigorjeva, V.Pankratov, S.Chernov, A.Watterich. *Time-resolved spectroscopy of ZnWO<sub>4</sub>*. (poster presentation).  
10. R.T.Williams, K.B.Ucer, H.M.Yochum, L.Grigorjeva, D.Millers, G.Corradi *Self-trapped electron and transient detected absorption in niobate and tungstate crystals*. (oral presentation)

The 4-th Euroconference Luminescent Detectors and Transformers of Ionizing Radiation, Jurmala, Latvia, August 15-17, 2000.

15. S.Chernovs, D.Millers, L.Grigorjeva, V.Pankratov. *Transient absorption spectra and relaxation kinetics in the PbWO<sub>4</sub>-Nb scintillator crystals*, (oral presentation).  
16. L.Grigorjeva, D.Millers, S.Chernov, V.Pankratov, A.Watterich. *Luminescence and transient absorption in ZnWO<sub>4</sub> and ZnWO<sub>4</sub>-Fe crystals*, (poster presentation).  
17. I.Plavina, A.Tale. *Optically stimuable luminescence of irradiated alkali halides and possibility of operative dosimetry*. (poster presentation).

#### **Lectures at universities, institutes, companies**

1. L.Grigorjeva, D.Millers. Luminescence in TlBr crystals.
2. D.Millers. X-ray tomography.

#### **Thesis**

I.Lubina. Cr(VI) sorption by intact and dehydrated *C.utilis* in the presence of Me<sup>2+</sup>. Bachelor thesis, University of Latvia, Faculty of Biology, Riga, 2000.



# SEMICONDUCTOR MATERIALS AND SOLID STATE IONICS

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

## Research Area and Main Problems

### Research areas:

- Electrophysics and electrochemistry of specific semiconductor materials, mixed conductors, ion conductors, high temperature superconductors (transition metal oxides, bronzes, metal hydrates, solid electrolytes, etc.);
- Material preparation methods: thin and thick film technologies, sol-gel process;
- Material characterisation by spectroscopic methods (Raman scattering, optical and X-ray absorption, electrical and electrochemical impedance, magnetic susceptibility, ESR, etc);
- Solid state ionics and optics:
  - electro-, photo-, thermo-, chemo- or gaso-chromic phenomena,
  - structural changes due to ion intercalation,
  - lattice dynamics and structural and electronic phase transitions,
  - solid state reactions at interfaces electrode – solid electrolyte,
  - solid state reactions in bulk of electrode and solid electrolyte materials,
  - two and three phases electrode reactions,
  - gases and ions sensing phenomena and detection technologies;
- Functional coatings and multi layer electrochemical systems;
- New measurement technologies and instruments with artificial intelligence;
- Miniaturisation of solid state ionic devices:
  - physical and chemical sensors (ChemFET) and actuators compatible with Si-technology for MST, ASIC or MCM (smart devices),
  - variable optical coatings for micro optics and smart optical sensors and windows;
- Application specific semiconductor materials and solid-state ionic devices in micro systems for electronic nose.

### Research problems and tasks:

1. Stability of materials for electrochromic devices.
2. Improvements in x-ray absorption spectroscopy methodology and local structural anomalies in the mixed transition metal oxide compounds.
3. Inter-grain activity of solid electrolyte layers based on  $ZrO_2:Y_2O_3$  ceramics.
4. Ion ( $H^+$ ,  $OH^-$ ,  $Li^+$ ) insertion (extraction) in solid electrolytes and electrodes.
5. Metal hydride electrode for Ni / MH battery.
6. Microwave absorption and Josephson junctions based on high temperature superconductors.
7. Research and development of an electronic nose
  - 7.1. Software Environment for Electronic Nose and Electronic Nose Module;
  - 7.2. Preparation of sensor elements and testing their sensitivity and selectivity;
  - 7.3. Application methodology of electronic nose for food quality and water pollution control.
8. Environmental pollution monitoring methods and instrumentation.

9. Testing and certification of materials and accreditation of testing laboratories.

**Scientific staff:**

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

**Technical staff:**

1. A.Kursitis
2. J.Pinnis
3. M.Purane

**Postgraduate students:**

1. Ī.Vçveris
2. J.Zubkâns

**Students:**

1. L.Grînberga
2. U.Klavins
3. L.Jçkabsone
4. K.Paegle

**Visitors from abroad:**

1. Prof. E.Cazzanelli – University of Calabria, Italy (5 days)..
2. Ing. A.Pede – senior scientist, Rome International University, Rome, Italy (8days).

**Scientific visits abroad:**

- Dr. P.Cikmacs: University of Roma (Tor Vergata), Italy (2 months.)
- Dr. J.Gabrusenoks: Conference IME-4, Uppsala, Sweden.
- Dr. J.Kleperis: 1) 7<sup>th</sup> Int. Symp. “Olfaction & Electronic Nose” Brighton, England;  
2) 51<sup>st</sup> ISE Meeting, Warsaw, Poland;
- Dr. A.Kuzmins: 1) Joint Institute for Nuclear Research, Dubna, Russia (14 days);  
2) CNR CeFSA, Trento, Italy (4 months).
- Dr. A.Lusis: 1) Conference IME-4, Uppsala, Sweden.  
2) EC project consortium meeting (EGLE Technology), London, UK.  
3) Conference BEC’2000, Tallinn, Estonia
- Dr.. J.Purans: 1) Laboratory of Synchrotron Radiation, Orsay, France (3 months);  
2) Conference IME-4, Uppsala, Sweden.
7. Dr. M.Shirokov: 1) Laboratory of Inorganic Materials Structural Chemistry ( prof. E. Antipov), Moscow State University.  
2) Laboratory of Spin Tracer Biophysics ( Prof. A.Tikhonov), Moscow State Un  
3) Magnetic Resonance Laboratory ( Dr. A.Timoshin), Cardiology Centre, Mosc
- Dr. G.Vaivars: 1) Poznan Central battery laboratory, Poland (4 week);  
2) Conference IME-4, Uppsala, Sweden;  
3) 51<sup>st</sup> ISE Meeting, Warsaw, Poland
- Dr. A.Vitins: Int. conf. “Solid State Chemistry 2000”, Prague, Czech Republic

- L.Grînberga: 1<sup>th</sup> School “*Fundamentals on sensors and sensor systems for electronic nose application*”, Alpbach , Austrija.
- K.PaeGLE: 1<sup>th</sup> School “*Fundamentals on sensors and sensor systems for electronic nose application*”, Alpbach, Austrija.

## Cooperation

### Latvia

1. Riga Technical University (RTU) – Faculty of Radioengineering and telecommunications (Doc. I.Slaidins, Doc. P.Misans)
2. Riga Technical University - Institute of Inorganic Chemistry (Dr. J. Grabis, Dr. I.Zalite, Dr. A. Dindune).
3. Information technology division of UL (Doc. H.Bondars).
8. Certification centre of Latvian Academy of Sciences (Prof. J.Matiss).
9. Institute of Physical Energetics of Latvian Academy of Science (Dr. N.Zeltið).
10. Laboratory for Mathematical Modelling of Environmental and Technological Processes, University of Latvia (Dr.A.Jakovics)

### Denmark

Technical university of Denmark (Dr. K.West )

### France

1. LURE, Lab. of Synchrotron Radiation (Orsay, France) – Prof. S. Benazeth, Dr. Ph. Parent.
2. University of Marseille II: Lab. of Condensed Material Physics (Prof. Y.Mathey).
3. Institut de Physique Nucléaire, Orsay, France (Dr. F. David).

### Italy

1. University of Roma (Tor Vergata) – Department of Physics (Prof. M.Iannuzi).
2. University of Trento – Department of Physics (Prof. G.Mariotto, Prof. G.Dalba).
3. University of Cosenza – Department of Physics (Prof. E.Cazzanelli).

### Poland

Poznan Central Battery Laboratory (Dr. M.Kopczyk, Dr. G.Wojcik)

### Russia

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

### Sweden

1. Uppsala University (Prof. C.-G. Granqvist, Dr. A.Azens)
2. Stockholm University, Arrhenius laboratory (Dr. J.Greens)
3. Linköping University – Laboratory of Applied Physics (Prof. I.Lundstrom)

### Switzerland

Universite de Lausanne – Prof. A.E. Merbach

**NEXUS** – Network of excellence in multifunctional microsystems (EC program ESPRIT). Office (Berlin) in Fraunhofer-ISiT (Dr. H.-C.Petzold). NEXUSPAN - Specific program for CEE countries (Dr. A.Lusis - NEXUS Board member and coordinator in Latvia).

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

**COST** programme: Project D18 "Lanthanide Chemistry for Diagnosis and Therapy" (Dr.J.Purâns – member of project management committee).

## Main results

### **ION ELECTRON PHENOMENA IN SYSTEM: INTERCALATION ELECTRODE – SOLID ELECTROLYTE**

*A.Lusis, J.Kleperis, E.Pentjuss, G.Vaivars, J.Garbusenoks,  
Z.Kanepe\*, A.Dindune\**

1. **Materials for electrochromic devices.** Phase transitions in crystals, nano-crystals and amorphous materials will be investigated by Raman scattering and IR reflection methods. Analyses of experimental results on bases of numerical calculation of lattice dynamic and determination of the vibrations symmetry. The materials for investigations are oxides of transition metals ( $\text{WO}_3$ ,  $\text{MoO}_3$ ,  $\text{CrO}_3$ ,  $\text{Nb}_2\text{O}_5$ ,  $\text{CdWO}_4$ ), oxychlorides and solid solutions  $\text{A}_x\text{B}_y\text{O}_z$ . The materials for wider atomic structure will be synthesized by several methods (growing of crystals, sputtering in vacuum).

The poly-chromic phenomena (i.e. electro-, photo-, chemo- gaso-, cathodo-, thermo-chromic) of amorphous tungsten trioxide (a- $\text{WO}_3$ ) films are described by processes on inner surfaces. The a- $\text{WO}_3$  films were prepared by thermal evaporation of tungsten trioxide powder in the presence or with out of  $\text{H}_2\text{O}$  vapour. The constitution of such films is heterogeneous and built up of nano size particles, pores and adsorbed substances. From the TGA, IR spectra and quartz resonator micro-balance data we find that the density of  $\text{WO}_3$  films from amorphous to crystalline state is in the range 5,6÷7,3  $\text{g cm}^{-3}$ , weight losses 7% (i.e. losses of water 45÷55%). The value of molar fraction of water content in a- $\text{WO}_3$  films calculated from these data is  $\approx 0,5$  or  $\approx 13\%$  of the film molar volume, which means that a- $\text{WO}_3$  films have developed internal surface ( $>5 \times 10^6 \text{ cm}^2/\text{g}$ ). Part of this surface is closed for direct interaction with gas atmosphere or liquid electrolyte leading to inner and outer interfaces. From the analysis of data on composition, constitution and structure we found that a variety of a- $\text{WO}_3$  film properties in many cases can be explained if one assumes that films are composites based on nano size particles or phases. The physical and chemical properties as composition, constitution and structure of the a- $\text{WO}_3$  films depend on interaction with environment and the type of external influences or excitations of chemical species on the particles of different tungsten trioxide phases. The investigation covers main types of multi - phase interfaces on tungsten trioxide particles in the a- $\text{WO}_3$  film as electrochemical electrodes. *The adsorbed gases and water in pores on the surface of oxide form different interfaces. The hydration level of  $\text{WO}_3$  films is more or less constant for substrate temperature up to 200 °C during deposition of films. In that region the values of electron and proton conduction are the same values. Above 200 °C the electronic conduction dominates. Adsorbed water serves as a source of hydrogen ions (protons,  $\text{H}_3^+\text{O}$ ) and electrolyte for ion transfer inside film. Any adsorbed chemical compound interacts with electronic and ionic defects on nano-size crystal particles and changes conductivity of the oxide phase. Boundary between adsorbed water (liquid phase) oxide (solid phase) interacts with the gas phase. For investigation of poly-chromic phenomena in*

*WO<sub>3</sub> films such assumption is very important. The boundary WO<sub>3</sub>-film with electrode is a more complicated case: in the electrode processes three (electrode - metal layer, oxide and water or gas) and four (electrode - metal layer, oxide, water and gas) phases can be involved. The colour centres, for example, can be induced thermally (increase of non-stoichiometry) or electrically (injected ions). The poly-chromism of a-WO<sub>3</sub> films can be directly related to ion insertion / extraction processes. These processes or solid state redox reactions in a-WO<sub>3</sub> films are sensitive to external forces which induce reversible optical effects.*

## **2. Synthesis and testing of the new proton conducting polymer composites electrolytes.**

The ECD need proton conducting polymer electrolytes with good optical transparency in visible region and stable up to 120 - 140°C. Proton conducting polymer complexes with inorganic acids (H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>) show excellent electrical and optical properties. Their high chemical activity is, however, a serious drawback for practical applications. The electrolytes were tested in electrochromic devices with thin film electrodes based on WO<sub>3</sub> (cathode) and NiO<sub>x</sub> and CrO<sub>x</sub> (anode). The porous nickel oxide films shows different from traditional electrochromic behaviour. According with the new developed model, fresh-prepared porous nickel oxide films could adsorb the water from electrolyte and act as an proton donor.

4. *Structure and conductivity in AgM(III)P<sub>2</sub>O<sub>7</sub> (M = Sc, Fe).* The difference in structure types of AgScP<sub>2</sub>O<sub>7</sub> and AgFeP<sub>2</sub>O<sub>7</sub> is introduced by different ion radii,  $r(\text{Sc}^{3+}) = 0.81$  and  $r(\text{Fe}^{3+}) = 0.68$  Å. The Arrhenius plot of Ag<sup>+</sup> ion conductivity is not linear. Such a behavior should be related to changes in correlation of Ag<sup>+</sup> ions and to changes in the interaction of Ag<sup>+</sup> ions with the cage lattice. At 450-713 °C NaScP<sub>2</sub>O<sub>7</sub> shows activation energy of conductivity  $E = 0.36$  eV, whereas at low temperatures it increases to 0.99 eV. AgFeP<sub>2</sub>O<sub>7</sub> shows  $E = 0.88$  eV at 167-345 °C and  $E = 0.46$  eV at 450-700 °C. At 300 °C conductivity for AgScP<sub>2</sub>O<sub>7</sub> is  $1.1 \times 10^{-4}$  S/cm at 300 °C, which is for two orders higher than for NaScP<sub>2</sub>O<sub>7</sub>, having the same structure type as AgScP<sub>2</sub>O<sub>7</sub>. The increased conductivity in AgScP<sub>2</sub>O<sub>7</sub> is due to the large polarizability of Ag<sup>+</sup> ions, which facilitates delocalization of Ag<sup>+</sup>. However the structures of AgFeP<sub>2</sub>O<sub>7</sub> hinder the ion transport and conductivity is of  $3 \times 10^{-6}$  S/cm at 300 °C.

\*) In cooperation with: Institute of Inorganic Chemistry of Riga Technical University

## **X-RAY ABSORPTION SPECTROSCOPY OF TRANSITION METAL AND RARE-EARTH OXIDE COMPOUNDS**

J. Purans, A. Kuzmin, R. Kalendarev

X-ray absorption spectroscopy is relatively novel and rapidly developing experimental technique, those use provides with unique information on the structure and dynamics of solids, liquids and gases. The availability of synchrotron radiation sources, characterized by very intense x-ray radiation flux (up to  $10^{20}$  photons/sec) and high energy resolution (about 0.2-5 eV) in wide available energy range (100-100000 eV), allows for a precise determination of structural parameters (e.g. of interatomic distances with picometric accuracy) in multicomponent materials, having small concentration of the probed element, independently from the presence or absence of the structural order in a system. In spite of the method has been widely used for about 10-15 years both in fundamental and applied research, there are still many open questions to be solved in experimental and data analysis/interpretation fields.

Our laboratory is the only one in three Baltic republics, which is directly involved in the research and development of x-ray absorption spectroscopy instrumentation and methodology. Our main achievements and research topics are related to (1) the in-lab EXAFS-spectroscopy; (2) development of original methods for

EXAFS data analysis and interpretation; (3) investigation of a role of different processes, occurring upon the photoabsorption process, in a formation of the EXAFS signal and (4) use of x-ray absorption spectroscopy in Materials Science for the study of disordered, nanocrystalline and diluted systems.

The main studies were carried out in the following directions: (a) preparation and characterisation of novel thin-film materials based on the transition metal oxides; (b) local atomic and electronic structure investigations by x-ray absorption spectroscopy (EXAFS and XANES) and complementary techniques (XRD, Raman spectroscopy, optical spectroscopies, atomic force microscopy (AFM)) of pure and doped polycrystalline compounds, nanocrystalline mixed oxide thin films, chalcogenide solid solutions, rare-earth ions doped glasses, transition metal and rare-earth ions in solutions; (c) further developments of the EXAFS interpretation methodology.

The experimental EXAFS measurements were performed using synchrotron radiation in LURE (Orsay, Paris) and ESRF (Grenoble) international laboratories.

The local structure anomalies were studied in nanocrystalline mixed transition metal oxide thin films  $\text{WO}_3\text{-IrO}_2$ ,  $\text{NiO-WO}_3$ ,  $\text{WO}_3\text{-ReO}_3$ ,  $\text{IrO}_2\text{-TiO}_2$  in comparison with pure oxides, all prepared by reactive dc magnetron sputtering of metal targets in  $\text{Ar/O}_2$  atmosphere. The obtained results allowed us to conclude on the nano-phase formation depending on the chemical composition and the local environment relaxation as a function of nanocrystalline grains size. The influence of the size effect on the chemical metal-oxygen bonding was observed and studied in details in  $\text{WO}_3$ ,  $\text{NiO}$  and  $\text{NiO-WO}_3$  systems. An application of the EXAFS spectroscopy to the studies of structural phase transitions caused by temperature change was demonstrated on an example of polycrystalline molybdenum trioxide-hydrates  $\text{MoO}_3 \cdot n\text{H}_2\text{O}$ . We found that the phase transition is accompanied by strong distortions of the metal-oxygen polyhedra, caused by large modifications of the crystal lattice topology.

The above mentioned results were obtained with the help of the EXAFS data analysis software package "EDA", originally developed and significantly improved during the past four years in our laboratory. In particular, the original method for model-independent reconstruction of the radial distribution function from EXAFS data was suggested and successfully implemented. At the moment, several promising data analysis techniques are at the development stage. The "EDA" program is recognized at the international level and is now used in more than 40 laboratories, located in 15 countries all around the world.

Finally, the obtained experimental results and the developments in the EXAFS data analysis methodology were used as a basis for the review on "EXAFS spectroscopy using synchrotron radiation", written in collaboration with our colleagues V.L.Aksenov and S.I.Tiutiunnikov from Joint Institute of Nuclear Research (Dubna, Russia, 2000).

## **PREPARATION AND INVESTIGATION OF SOLID OXIDE ELECTROLYTE CERAMICS**

*A.Vitins and A.Lusis*

Materials and technology for developing solid oxide fuel cells, particularly based on  $\text{ZrO}_2\text{-Y}_2\text{O}_3$ , and electrochemical cells based on them are connected with conduction mechanism and constitution of solid electrolyte.

*Electrical properties of  $\text{ZrO}_2\text{-7.5 mol\% Y}_2\text{O}_3$  ceramics.* Impedance spectra were measured using two-probe technique for a  $\text{ZrO}_2\text{-7.5 mol\% Y}_2\text{O}_3$  ceramic specimen with silver electrodes in the frequency range 20 Hz - 1 MHz by means of a HP 4284A precision LCR meter. The experimental data of plots ((Im(Z))-(Re(Z))) represent the frequency response function of complex dielectric permeability of ceramic sample. The intragrain polarization and conduction in the ceramics determine the spectra measured.

The impedance spectra were interpreted according to the approach [1]. The method to determine a value of the intragrain dc electrical conductivity ( $\sigma_0$ ) from an impedance spectrum was developed. Two kinds of systematic deviations from a depressed circular arc were observed: a deviation in a high frequency part is in agreement with [1], a deviation in a low frequency part is presumably due to polarization in the grain boundaries of the ceramics. The frequency range investigated may be subdivided into two domains, below and above the transition frequency ( $\tau$ ), where a power-law dependence is observed for the imaginary part of the dielectric response, but with different exponents  $n$ : 0.83-0.84 and 0.57-0.59, respectively. The ( $\tau_r$ ) is a frequency, where the absolute value of the reactance reaches its maximum. The ratio ( $\tau/\tau_r$ ) was in a range 3.0-4.1. The plots of  $\log_{10}(\sigma_0(T))$ ,  $\log_{10}(\tau)$  and  $\log_{10}(\tau_r)$  vs.  $1/T$  gave the activation energies 1.113(0.004), 1.07(0.04) and 1.11(0.06) eV respectively in the temperature  $T$  range 457-523 K.

Study of the a.c. electrical properties of  $ZrO_2$ -7.5 mol%  $Y_2O_3$  ceramics at 457-595K. *The intragrain part of the impedance spectra for the frequency range 20 Hz - 1 MHz of a  $ZrO_2$ -7.5 mol%  $Y_2O_3$  ceramic specimen was analyzed on the basis of the approach proposed in the literature [1] for impedance of  $ZrO_2$ -12 mol%  $Y_2O_3$  single crystals. The method to determine a value of the intragrain d.c. electrical conductivity from an impedance spectrum has been developed. Frequency dependence of the intragrain complex dielectric response was interpreted according to the common model used in the literature. Frequency domains, where a power-law dependence having different exponents  $n_1=0.825-0.844$  and  $n_2=0.571-0.592$  is observed, were found. Inner consistency of the model used is verified. Values of the transition frequency and the relaxation frequency were determined for the grain interiors and compared with each other. They are comparable with the inverse of mean residence time of an oxygen vacancy obtained from the Nernst-Einstein relationship assuming jumps of oxygen vacancies to be random and independent of each other. The values of the activation energies of the d.c. conductivity, the transition frequency and the relaxation frequency are found to be the same within experimental uncertainty and equal to 1.1 eV in the temperature range 457-523 K.*

## **SUPERCONDUCTOR, AS INTELLIGENT MATERIAL: MICROWAVE LOSSES TEMPORAL SELFORGANIZATION**

*M. Shirokov*

1) Microwave modulated magnetoabsorption ( ESR-detected signal) establishment processes are investigated in high- $T_c$  superconductors repeated remagnetization cycles. The signal hysteresis loop drift, observed both in  $Y-Ba_2-Cu_3-O(7-\delta)$ ,  $Tm-Ba_2-Cu_3-O(7-\delta)$  ( $T_c=90$  K) single crystals and ceramics cycling, saturates in uncommon, inmonotonous way. The saturation loop broadens significantly and has opposite by-pass direction, but the following cycles expose oscillations around equilibrium position. Wide diapazone of the saturation types is found, from two-cyclic up to unobservable one during experiment, depending on the sample preparation and the cycling parameters. Based on microwave absorption surface barrier model with shielding currents contours broad distribution at superconductor surface, pair Neel type contours interactions are taken into account. Then the drift is the result of the currents system equilibrium violation as the modulation induced current reaches critical value in some contours and there appears intrinsic contribution to the magnetic field, which is trapped in each cycle by pinning centres. The drift saturation follows from the current and magnetic field redistribution along the precritical contours. The saturation type diversity depends on the pair number in interaction. Its striking and inmonotonous character indicates the precritical contours transition to the critical ones in order to compensate equilibrium violation and the

critical ones – to zero current state for weak sites breaking. Such self-organization mechanism corresponds to universal critical state establishment phenomena in superconductors and can be controlled by the sample surface treatment, shape and defects (weak sites and pinning centres) concentration and distribution.

2) In mercury saturating high-T<sub>c</sub> superconductors, Hg-Ba<sub>2</sub>-Cu-O(4+δ), Hg-Ba<sub>2</sub>-Ca-Cu<sub>2</sub>-O(6+δ), with critical temperatures T<sub>c</sub>=97 K and T<sub>c</sub>=125 K, respectively, two pronounced features are observed. In regime nonlinear on modulation amplitude, when modulation induced critical shielding currents are present, the remagnetization cycles drift shows regular oscillations, from cycle to cycle, with amplitude of the same order that shift of the signal itself caused by the drift, both relaxing slowly. Another effect is that the reverse branch of the hysteresis signal intersects the direct branch, and the magnetic field interval, in which this intersection takes place, grows with modulation amplitude. It is well known, that, though of the highest T<sub>c</sub>, critical currents and higher critical magnetic fields in these compounds, Hg-1-2-0-1, 1-2-1-2, yield appreciably to ones in classical Y-1-2-3. So, far from thermodynamical equilibrium nonlinear effects of the critical state are more available at the same temperature, and besides far from T<sub>c</sub>. The oscillations are due to equilibrium between processes of currents (and corresponding magnetic fluxes) redistribution, from critical to precritical contours, and weak sites effect, when microwave absorption concentrates at the sample perimeter – in most long and so most precritical contours, which are of maximal weak sites content. This instability occurs each time after absorption optimization period, i.e. after each two cycles. The intersection effect can be explained by the fact, that different contours change the currents sign at magnetic field sweeping reverse points in different time interval, proportional to the currents value. Then the last series of the contours with the maximal currents, giving the maximal contribution to absorption, which is proportional to the current value in quadrat, experience additional magnetic field from already reversed ones, which gives rise to local signal line shift in magnetic field, i.e. in x-axis of the line. Actually, the effect is seen only at steep region of the line, where such line transition along x-axis is the most sensible. This mechanism, moreover, resembles Neel's result for ferromagnet statical magnetization hysteresis loop drift in repeated remagnetization cycles, due to distributed magnetic domains interactions.

3) Hg-1-2-0-1 clean sample, doped with Fe, showed resonant (ESR) signals, belonging to Cu<sup>2+</sup> and Fe<sup>3+</sup> paramagnetic centres. It is interesting that these centres concentrations ratio is approximately 1.5. This gives rise to idea that Cu<sup>2+</sup> signal give only those Cu ions, in which neighbourhood Fe<sup>3+</sup> ion is present. This can elucidate mechanism of well known fact, that there is no Cu<sup>2+</sup> paramagnetic centre signal in clean high-T<sub>c</sub> superconductor phase.

#### Resume:

Novel independent information on isolating then micro-impurities (weak sites) and pinning centres (artificial point defects), so important for improving of critical current and higher critical magnetic field parameters in Hg-based superconductors with maximal known T<sub>c</sub>, is expected in further experiments.

## **HYDROGEN ENERGETICS - MATERIALS AND DEVICES**

*J.Kleperis, G.Vaivars, G.Vitins, G.Mlynarek\*, G.Wojcik\*, M.Kopczyk\**

Metal hydride electrode impedance measurements are continued. New AB<sub>2</sub> electrode materials were synthesized in the Central Laboratory of Batteries and Cells in Poznan, their electrochemical characteristics (charge transfer resistance, exchange current, equilibrium potential) and impedance were measured in Riga and Poznan by G. Vaivars.



It was found that the behavior of the sintered electrode was much stable in comparison with the pressed one. Changes of the double layer capacitance  $Q$  for the pressed electrode during charging/discharging were drastic, which was the reason for the electrode disintegration. The charge transfer resistance  $R_{ct}$ , which is the most important parameter for an application in batteries, was much higher for the Fe containing electrode. However, during pretreatment it was possible seriously decrease the charge transfer resistance for the Fe containing electrode. The addition of the Fe was for commercial reasons. It allows dramatically reduce the price of the electrode material.

Solar-hydrogen energy system is assumed to be most efficient power source for Latvia in future. Actual task now is to develop the concept of solar-hydrogen energy powered house and to built-up experimental model to show the advantages of hydrogen energy. Hydrogen-related investigations in the Institute of Solid State Physics (metal hydride, hydrogen conducting solid electrolyte) were reported in different conferences by J. Kleperis and G. Vaivars.

Improving of the impedance analysis model for metal hydride batteries as a part of cooperation with Poznan Battery Centre. Previously used adsorption model was developed by Prof. Breiter 30 years ago for hydrogen adsorption on palladium and was noncritically applied to metal hydride electrodes. It was found that the behavior of the sintered electrode was much stable in comparison with the pressed one. Changes of the double layer capacitance  $Q$  for the pressed electrode during charging/discharging were drastic, which was the reason for the electrode disintegration. The charge transfer resistance  $R_{ct}$ , which is the most important parameter for an application in batteries, was much higher for the Fe containing electrode. However, during pretreatment it was possible seriously decrease the charge transfer resistance for the Fe containing electrode. The addition of the Fe was for commercial reasons. It allows dramatically reduce the price of the electrode material.

*\*)In cooperation with: Central Laboratory of Batteries and Cells (CLA), Poznan (Poland)*

## INVESTIGATION OF THE Nb OXIDATION AT THE DIFFERENT INTERFACES FOR TO USE IN THE JOSEPHSON TUNNEL JUNCTIONS

*P.Cikmacs, F.d'Acapito<sup>\*</sup>, I.Davoli<sup>\*\*</sup>, J.Klavins, V.Merlo<sup>\*\*</sup>, S.Mobilio<sup>\*\*\*</sup>*

The oxidation of Nb/Al interface is particularly interesting in the field of the Josephson tunnel junction. Two Nb film sandwiching a thin insulator gap realize a weak superconductor where a small dc supercurrent can flow giving origin to number of interesting effects, all going under the common name of Josephson effect. We report on the modification of the local order of Nb at the Nb/Al interface upon different oxidation processes, using reFLXAFS spectroscopy under grazing incidence conditions. In this geometry the EXAFS gains a surface sensitivity. The data show that a thin (60Å) Al cap do not completely prevent the oxidation of the Nb even if the film is simple exposed to air at room temperature. The thin layer of niobium oxide, observed at the interface has a more ordered phase than the bulk one. A light annealing (200°C) in air leads to an O release from the Nb substrate, while a stronger thermal treatment (600°C) leads to the formation of a NbAl alloy phase in agreement with literature. The presence of Nb oxide at the interface is expected to slower the transformation rate to Nb aluminide structures.

In cooperation with: <sup>\*</sup>) INFM, Grenoble, France

<sup>\*\*</sup>) Roma II University "Tor Vergata", Italy

<sup>\*\*\*</sup>) University "Roma Tre", Italy

## RESEARCH AND DEVELOPMENT OF ELECTRONIC NOSE

*J. Kleperis, J. Zubkans, M. Veidemanis, K. Paegle, V. Eglitis,  
A. Lusis, P. Misans\*, A. Jozapovics\*, I. OSMANIS\**

During this year an electronic nose from Nordic Sensors AB was used to supplement the "odour map" collection. Different examples from food (sausages, breads, coffees, teas), beverages (juices, waters, beers), vegetables (apples, bananas) and spirits were tested. Principal Coordinate Analyses was recognized as more convenient and more obvious in discussions and presentations were product producers participated. Some representatives of basic odours were used to make absolute (human panel) orientation of odour maps. As test example the results collected during exhibition "Riga Beer'98" were used and best beer sort determinate. The concept of mobile nose was further elaborated (P. Misans et al) on base of micro-controller TI 3705x and (or) signal-processor TI 3205x. By using only one signal-processor the functions of potential device will be shortened.

*\*<sup>1)</sup> In cooperation with: Department of Electronics and Telecommunications, Riga Technical University*

### DEVELOPMENT OF SIGNAL PROCESSING AND IDENTIFICATION HW/SW FOR E-NOSE MINI MODULES

*V. Eglitis, J. Kleperis, A. Lusis, P. Misans\*, J. Zubkans*

The goal of this research project is to develop micro system prototypes for the mobile intelligent or artificial human sensing instruments. The HW/SW co-design is one of the tools for creation of such micro systems. There will be presented one of first steps in HW/SW co-design of prototype modules. The module of mobile e-nose (MEN) is a prototype for this research project.

The **hardware** (HW) for one of the basic version included the control module (CM) that provided: delivering of gas, control of sensor array and data acquisition. The brain of CM was a micro controller (MC) (Texas Instrument 3705x). On the one hand we were able to use this control module as autonomous portable device for simple tasks of identification or recognition. On the other hand we had a possibility to connect the CM through RS232 interface to IBM PC compatible computer for more complicated recognition tasks. In this case we have very flexible and complex system that can be used for research goal, for creation and extension of databases of smells or for development of next versions of electronic nose (EN).

The change of MEN brain to DSP is motivated at least by three important signal processing tasks: 1) digital filtering of sensor signals, 2) sensor signal pre-processing by fast linear transforms and 3) speech synthesis for indication the recognised smells or classes of smells.

The **software** (SW) plays the general role for development and use of electronic nose. Our system and its parts constantly are under continuous changes and development. In such a situation is very important a choice of flexible environment for programming and driving of system

MATLAB was chosen as basic software for development of EN from its first version. Our experience during last four years confirms that such choice is absolutely true. In previous stages of work we used MATLAB only for the programming and driving of general control program (GCP) on the PC. In the recent versions of EN for GCP we use mostly SIMULINK environment

For programming we used (and we still use) four different programming environments and languages: MATLAB, C language, assembler for TMS 3705x and assembler for TMS3205x. We use the C language and assemblers for writing of programs for MEN. For early versions of MEN we used mostly hand-written C and assembler's codes. MATLAB was used only to prove the algorithms. Presently pure C-coding and inline assembler have been used for optimisation of several pieces of codes.

There are three main features of EN: 1) a data acquisition system, 2) a signal processing and pattern recognition system and 3) a communication system. The first two points were background for previous versions of EN. When we incorporated modem in the architecture of EN, we obtained new system with new features. Presently we can consider our EN as remote for: 1) data acquisition system and 2) signal processing and pattern recognition system. In such a way we can install the minimum of necessary functions on the MEN. This allows significant reduction of costs of MEN. Last months we concentrate main efforts on the development of EN as communication tool for remote sensing and recognition of smelts.

We use MATLAB and SIMULINK environment to develop the software for separate parts of electronic nose and for the system as whole. The developed software for electronic nose is a large and open collection of MATLAB functions, scripts, MEX-files, "nose" library of SIMULINK blocks, model files, C codes, data files and hand-written inline assembler codes. We do not prepare here all of details. The developed set of tools we use: 1) to simulate behaviour of EN for different configuration (research tool, mobile electronic nose, remote mobile electronic nose) as whole, 2) to simulate behaviour of different parts of EN (control program for MEN, switch terminal, GCP), 3) for calibration (temperature, sensor type, etc.) and 4) as parts of control programs for different parts of electronic nose (MEN, switch terminal, GCP). The collection includes several general parts of programs and SIMULINK blocks: 1) for sensor array support, 2) for data acquisition service, 3) for communication service, 4) for database management, 5) for digital signal processing, 6) for preliminary displaying of results and 7) for pattern recognition.

The sensor array support includes: 1) the setting of currents for MOSFET gas sensor array, 2) the temperature setting and control and gas delivery control.

We reduced the number of current sources in the recent versions of EN. Such approach led to the simplification of hardware and software for the control of currents. It also led to the change of shape of corresponding window for temperature control. The recent version of EN also allows a remote control of sensor.

\*) *Department of Electronics and Telecommunication of Riga Technical University*

## **REMOTE HEAT LOSS DIAGNOSTICS USING THERMOGRAPHIC MEASUREMENTS**

*U.Kanders, J.Klavins, I.Viksna\*, N.Zeltins\**

Nowadays thermographic measurements have been applied to provide data about a heat loss through building envelopes and thermal conditions of different heat distributing elements of houses as pipes and vessels, elevators and radiators, pumps and valves, etc. Thermographic method particularly plays a significant role in situations where the visible parts of building envelope or technological and electrical equipment being under high voltage or other dangerous location cannot be reached by other measuring technique for an examination. Besides the inaccessibility of points which are to be measured other most important advantage of thermography is that the object under observation is totally unaffected by the measurement process. Thus thermography provides data about object within their normal operating environment. The information obtained by single point temperature measurement technique is generally comparable with that got by thermographic measurements. However, in order to measure the

corresponding trajectory on the wall of building from outside or respective object under dangerous conditions it might take several hours while thermography provides a quick and complete overview of the entire object's temperature.

Practical thermographic in situ measurements of the building envelope (of ISSP) have been carried out in order to examine the heat loss through different elements of outside wall like lightweight concrete panels, wood boards with mineral fiber insulation, 2-panes windows, 2-panes windows with mineral fiber insulation. Temperature profiles corresponding the 12m-long trajectories along outside walls have been calculated from thermographic pictures. Thermobridges and other thermal defects of perimeter walls have been detected.

\*) In cooperation with LAS FEI Energy Efficiency Centre

### Scientific Publications

Published in 1999

1. A.Lusis. Role of Internal Multi Phase Surfaces on the Poly-Chromic Phenomena in the Amorphous Tungsten Trioxide Thin Films. In: Abstr. Int. Meet. on Electrochromism. August 21-23, 2000, Uppsala, Sweden.
2. A.Lusis. Role of Internal Multi Phase Surfaces on the Poly-Chromic Phenomena in the Amorphous Tungsten Trioxide Thin Films. Iesniegts: *Electrochimica Acta*, 2000.
3. G.Vītiðð, Z.Kaðepe, A.Vītiðð, J.Ronis, A.Dindûne, A.Lûsis. Structure and conductivity studies in  $\text{LiFeP}_2\text{O}_7$ ,  $\text{LiScP}_2\text{O}_7$ , and  $\text{NaScP}_2\text{O}_7$ .// *J. Solid State Electrochem*, 2000, **4**, p.146.
4. K.West, G.Vitins, R.Koksbang. Synthesis and host properties of tetragonal  $\text{Li}_2\text{Mn}_2\text{O}_4$  and  $\text{Li}_2\text{Co}_{0.4}\text{Mn}_{1.6}\text{O}_4$ .// *Electrochimica Acta*, 2000, **45**, p.3149.
5. Ī. Vītiðð, G. Íizâne, A. Lûsis, J. Tīliks. Electrical conductivity studies in the system  $\text{Li}_2\text{TiO}_3\text{-Li}_{1.33}\text{Ti}_{1.67}\text{O}_4$ .// Iesniegts: *J. Solid State Electrochemistry*, 2000.
6. G.Vaivars, A.Azens and C.G.Granqvist. Proton conducting polymer composites for electrochromic devices. In: Abstr. Int. Meet. on Electrochromism. August 21-23, 2000, Uppsala, Sweden.
7. G.Vaivars, A.Azens and C.G.Granqvist. Proton conducting polymer composites for electrochromic devices. Iesniegts: *Electrochimica Acta*, 2000.
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9. G.Vaivars, M.Furlani, B.E.Mellander un C.G.Granqvist. DSC analysis of the proton conducting PVA/Glycerine gel composite with zirconium phosphate. In: Abstr. 10<sup>th</sup> Int. Conf. Solid State Protonic Conductors, Montpellier, September 24-28, 2000. P. 84.
10. P.Misans, J.Kleperis, J.Zubkans, V.Eglitis, A.Lusis "The MATLAB and SIMULINK-based Software Environment for Development of Mobile Electronic Nose", BEC '2000, Tallin, October 8-11, 2000, pp. 295-298.
11. J. J. Kleperis, L. Grinberga, K. Paegle and A. Lusis, Two Possible Applicators of Electronic Nose: Bear Producer and Customs Inspector, Proceedings of 7<sup>th</sup> International Symposium Olfaction & Electronic Nose 2000, July 20-24, 2000, Brighton (England), p.97-101.
12. Instruments with Artificial Intellect in Fight against the Fraud, Jānis Kleperis and Andrejs Lûsis, Materials of 6<sup>th</sup> Nordic-Baltic Conference in Regional Science, Riga, Latvia, October 4-7, 2000. p.34-39.
13. G. Vaivars, J. Kleperis, G. Mlynarek, A. Sierczyńska, G. Wójcik and M. Kopczyk. The ac impedance behaviour of the  $\text{AB}_{2+x}$  (A-Zr, Ti, B-V, Ni, Cr, Fe) type metal

- hydride electrodes. Accepted for publishing in *Proceedings of Hungarian Academy of Science* (2000).
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  20. A.Kuzmin, J. Purans. Extended x-ray absorption fine structure spectroscopy of perovskite-type compounds. In "Defects and Surface-Induced Effects in Advanced Perovskites", edited by G. Borstel, A. Krumins, and D. Millers, NATO ASHT, Ser. 3, Vol. 77, 139-144, Kluwer, Dordrecht, 2000.
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  23. A.P.Menushenkov, K.V.Klementev, S.Benazeth, J.Purans, P.V.Konarev. A.A.Meshenkov. The double-well oscillating potential of oxygen atoms in perovskite system Ba(K)BiO<sub>3</sub>: EXAFS analysis results. *Nucl. Instrum. Methods A* 448 (2000) 340-344.
  24. M. I Shirokov. HTSC and related compounds microwave absorption evolution in remagnetization cycles. Proc. Int. Conf. "Magnetic and superconducting materials (MSM-99)". M. Akhavan et al (eds), World Sc. Publ. Co., Inc. 2000, p. 287-294.
  25. M. I. Shirokov. Surface induced drift and self-organization features of microwave losses in high-Tc superconductor perovskites. Proc. Int. Workshop, NATO ASI "Defects and surface-induced effects in advanced perovskites". G. Borstel et al.(eds), Kluwer Acad. Publ., 2000, p. 167-172.
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1. A.Lasis. Role of Internal Multi Phase Surfaces on the Poly-Chromic Phenomena in the Amorphous Tungsten Trioxide Thin Films, *Electrochimica Acta* (2001) .
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- Fe) type metal hydride electrodes. Accepted for publishing in *Proceedings of Hungarian Academy of Science* (2000.).
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  4. E. V. Antipov, V. A. Aljoshin, M. I. Shirokov, A. A. Timoshin. Microwave magnetoabsorption reptation effect and defects in Hg-2101 and Hg-2112 superconducting phases. *Physica C: Superconductivity*. 2001 (in press).
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  6. N. Mironova, V. Skvortsova, A. Kuzmin, I. Sildos, N. Zazubovich. One- and two-magnon contributions in optical spectra of KNiF<sub>3</sub> single-crystal. *Ferroelectrics* (2000) [iesn.].
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  12. J.H. Agondanou, J. Purans, A. Coutsolelos, S. Bénazeth, G.Spyroulias, C. Souleau. XAFS study of gadolinium and samarium bis and monoporphyrinate complexes. *Inorg. Chem.* (2000) [iesn.].

### Lectures on Conferences

#### Int. Meet. on Electrochromism. August 21-23, 2000, Uppsala, Sweden:

- 1) A.Lusis. *Role of Internal Multi Phase Surfaces on the Poly-Chromic Phenomena in the Amorphous Tungsten Trioxide Thin Films.*
- 2) G.Vaivars, A.Azens and C.G.Granqvist: *Proton conducting polymer composites for electrochromic devices.*
- 3) A.Azens, G.Vaivars, M.Veszelei, L.Kullman and C.G.Granqvist: *Electrochromic design with chemical compatibility: devices with W oxide / Ni oxide tandem layers*
- 4) A.Kuzmin, J.Purans, R.Kalendarjov: *Local structure and vibrational dynamics in NiWO<sub>4</sub>.*

#### Int. conf. "Solid State Chemistry 2000", Sept.3-8, 2000Prague, the Czech Republic.:

A. Vitins. *Study of the a.c. electrical properties of ZrO<sub>2</sub>-7.5 mol% Y<sub>2</sub>O<sub>3</sub> ceramics at room temperature and at 457-594 K.*

#### 10<sup>th</sup> Int. Conf. Solid State Protonic Conductors, Montpellier, September 24-28, 2000, France:

G.Vaivars, M.Furlani, B.E.Mellander un C.G.Granqvist. *DSC analysis of the proton conducting PVA/Glycerine gel composite with zirconium phosphate.*

51<sup>st</sup> ISE (International Electrochemical Society) Meeting, September 3-8, Warsaw, Poland:

- 1) G.Vaivars, J.Kleperis, G. M<sup>3</sup>ynarek, G. Wójcik and M. Kopczyk. *The ac Impedance Behavior of the AB type Metal-Hydride Electrodes.*
- 2) J. Kleperis, G. Vaivars, A. Lūsis, G. Wojcik. *Photoelectrochemical hydrogen battery.*

7th International Symposium Olfaction & Electronic Nose ISOEN 2000, July,20-24, 2000, Brighton, England:

J.Kleperis, L.Grinberga, K.Paegle,A.Lūsis. *Two possible applicators of Electronic Nose: Bear Producer and Customs inspector.*

BEC '2000, Tallin, October 8-11, 2000, Estonia:

P.Misans, J.Kleperis, J.Zubkans, V.Eglitis, A.Lūsis *The MATLAB and SIMULINK-based Software Environment for Development of Mobile Electronic Nose.*

International Workshop: Microstructure of Oxide Materials, June 13-15, 2000, Osnabrūke, Germany: J. Purans (Invited Speaker)

BioXAFS 2000, EuroWorkshop, July 3-4, 2000, Orsay, France:

J. Purans (Invited Speaker)

European Conference on Application of Polar Dielectrics (ECAPD-5), Aug.27-30, 2000, Jūrmala, Latvia:

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

Euroconference on Luminescent Detectors & Transformers of Ionizing Radiation (LUMDETR-4), Aug.14-17, 2000, Jūrmala, Latvia:.

A. Kuzmin, J.Purans,

Scientific Practical Meeting "Thermotechnics of the boundary constructions of buildings", Riga, March 16-17, 2000:

J.Klavins, J.Pinnis, M.Springis, *Testing of the water permeability and absorption of the building materials.*

16<sup>th</sup> Scientific Conference of ISSP UL, Rīga, February 21-23, 2000:

- 1) Ī. Vītiðð, Z.Kaðepe\*, A.Lūsis, A.Dindūne. *AgM(III)P<sub>2</sub>O<sub>7</sub> (M = Sc, Fe) struktūra un jonu vadītspēja.*
- 2) A.Kuzmins. *Nature luminescence centers in porous silicon.*
- 3) P.Cikmacs, F.d' Acapito, I.Davoli, J.Klavins, V.Merlo, S.Mobilio, *Investigation of the Nb oxidation at the different interfaces for to use in the Josephson tunnel junctions.*
- 4) U.Kanders, J.Klavins, I.Viksna, N.Zeltins, *Remote heat loss diagnostics using thermographic measurements.*

#### **Participation in Exhibitions**

1. E-NOSE: Hanovera, Germany, April 22-26, 2000.
2. E-NOSE: 2nd International Trade Fair For Beer And Brewing Technology RIGA BEER 2000, 2-4 March, 2000, Riga, Kipsala.
3. E-NOSE: Baltic Dynamics 2000, Riga, Skonto Halle.

# **DIDACTIC SYSTEMS**

*Head of Division Assoc. Prof., Dr. J.Kuzmin*

## **Research Area and Main Problems**

The main problem studied in the laboratory is programming of education material for Latvian schools.

### **Scientific Staff:**

Assoc.Prof.,Dr.J. Kuzmin

### **Technical Staff:**

Ing.,R.Tilgase

### **Scientific Visits Abroad:**

J.Kuzmin, COMPUTAS AS, Oslo, Norway (5 days)

## **Cooperation**

### **Latvia**

1. Faculty of Education and Psychology (A.Geske, L.Kuzmina)
2. Riga Pedagogic and Education Management Higher School (J.Valbis)
3. Institute of Solid State Physics, University of Latvia (A.Kuzmin)

### **Norway**

COMPUTAS AS, Oslo (M.Sorgard, T.Christianden)

## **Main results**

## **DIDACTIC SYSTEMS FOR SCHOOLS IN LATVIA**

### **J.Kuzmin**

In year 2000 our studies of methods of educational material programming were continued with a special focus on frontal educational process computerization. Second activity were concerned with testing of our results under existing conditions in Latvian Schools. As a result of an existing CAL and CAI systems examination were found that existing client-server technology implementation in these systems is extremely hard for a programming of educational materials. It is necessary to elaborate special educational materials programming language for a CAL and CAI systems on the base of client-server technology.

For purpose of testing of research results 4 CD-ROM s were presented to Informatics Chare of University of Latvia and 2 Latvian Schools.

First CD-ROM contains information for teachers about methods and details of preparing and programming CAL and CAI materials in T-language. Editor for preparing educational materials in Latvian, English, German and Russian, as well as T-language interpreter also is included. This CD-ROM contains ready examples



of courses, tests and drills for a novices. CD-ROM can be used in a distance education systems for a corresponding materials preparing.

Second CD-ROM contains special shell for a graphical educational materials elaboration. It is developed special programming technology, which can be used when is necessary combine large amount of graphical and sound information in one educational material. Main efforts are made to easing job of such material elaboration.

Third and fourth CD-ROM s are designated for a teachers and instructors

## **Scientific Publications**

### **Published in 2000**

1. L.Kuzmina and J.Kuzmins, PASCAL valoda skolEniem un skolotâjiem. "Lielvârs", 2000, p.105.
2. J.Kuzmins, L.Kuzmina. Izglîtība 2010. gadâ. Prognoze un iespçjas. – LU 58. konference. Izglîtības vadîbas sekcijas materiâli. 2000.g.31.janvâris.

# NONLINEAR PROCESSES IN SOLIDS

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

## Research Area and Main Problems

Our main research activities deal with the study of non-linear processes in condensed matter with emphasis on point defects and surfaces. This research consists of two directions: the kinetics of processes with emphasis on self-organization and catalytic surface reactions, and the electronic structure calculations of defective solids. We combine many different techniques, including analytical formalisms and large scale computer simulations (both quantum chemical methods and Monte Carlo/cellular automata modelling). These studies are performed in a close collaboration with 15 International groups listed below, and with several laboratories inside the Institute of Solid State Physics, Riga. We have good computer facilities including 3 Silicon Graphics Workstations, several Pentiums with extended memory.

### Scientific staff:

1. Dr.hab. J.R.Kalnin
2. Dr.hab. E.Kotomin
3. Dr.hab. V.Kuzovkov
4. Dr. A.Popov
5. Dr. R.Eglitis
6. Dr. Yu.Zhukovskii

### Postgraduate Students:

G.Zvejnieks

### Students:

V.Kashcheyevs

### Scientific visits abroad:

1. Dr. R.Eglitis, Osnabrueck University (6 months)
2. V.Kashcheyevs, Niels Bohr Institute, Denmark (1 week)
3. Dr.hab. E.Kotomin, Osnabruck University, Germany (5 month), Max Planck Institute in Stuttgart, Germany (3 months)
4. Dr.hab. V.Kuzovkov, Eindhoven University of Technology, The Netherlands (2 months), Braunschweig University, Germany (3 months)
5. 5. Dr. A.Popov, RIKEN Institute, Japan (8 months)
6. Dr. Yu.Zhukovskii, University College London (2 months), Uppsala University (3 months)
7. G.Zvejnieks, Osnabrueck University, Germany (5 months)

## Cooperation

Belgium	University of Antwerpen (Belgium, Prof. J.T.Devreese)
Denmark	University of Aarhus (Denmark, Prof. N.E.Christensen)
Great Britain	Royal Institution of Great Britain, London (Great Britain, Prof. C.R.A.Catlow)
	University College London (Great Britain, Prof. A.M.Stoneham)
Finland	Helsinki University of Technology (Finland, Prof. R.Nieminen)
France	CIRIL, Lab. CEA/CNRS, GANIL, Caen, (France, Prof. E.Balanzat)
Germany	University of Freiburg (Germany, Prof. A.Blumen)
	University of Osnabrück (Germany, Prof. G.Borstel)
	Gesellschaft für Schwerionenforschung (GSI) (Germany, Prof. R.Neumann)
	Max Planck Institut für Festkörperforschung (Germany, Prof.

	J.Maier)
	Braunschweig University of Technology (Germany, Prof. W.von Niessen)
The Netherlands	University of Groningen (the Netherlands, Prof. H.W den Hartog)
	University of Eindhoven (the Netherlands, Prof. A.P.J.Jansen)
Spain	University of Carlos III de Madrid (Spain, Prof. R.Gonzalez)
Sweden	University of Uppsala, (Sweden, Prof. K.Hermansson)

## Main Results

### THEORY OF SURFACE AND BULK PROCESSES IN WIDE GAP SOLIDS

In year 2000 our studies of defects and processes in advanced oxide materials were continued with a special focus on highly defective solids, perovskite surfaces and solid solutions.

#### First Principles Modelling of Metal Oxidation and Corrosion

Despite considerable experimental and theoretical efforts, understanding of technologically very important processes of the oxidation of metals and corrosion on an atomic scale are still not very well developed and their probable mechanisms have not been identified so far. The same is true for the structure and various properties of interfaces between metal and metal oxide. The main aims of this work are to perform detailed first principles theoretical studies of the initial stages of the oxidation of aluminium and magnesium as well as the formation of metal coatings on the surfaces of alumina and magnesium oxide.

We perform comprehensive quantum chemical calculations using mainly *ab initio* CRYSTAL98 simulation for different stages of the initial oxidation of light metals (in the framework of collaboration with Prof. P.W.M. Jacobs, University of Western Ontario, London, Canada and Prof. B.I. Lundqvist, Chalmers University of Technology, Göteborg, Sweden). To construct periodic models for the corresponding theoretical simulations we consider perfect and defective densely-packed monocrystalline surfaces. The sequence of performing simulation is the following: substrate interaction with molecular oxygen, its further dissociative chemisorption, surface diffusion of adatoms and their absorption inwards substrate, as well as formation of the first oxide units in the O/Me interface. To study possibilities of initial oxidation deeper we consider such defects of the substrate as steps on the metal surface and vacancies of metal atoms. When modelling all the stages of initial oxidation we simulate both relaxation and reconstruction of the metal surface. The analogous methodology is applying for theoretical study of different densely-packed Me/MeO interfaces: Ag/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub>, Ag/MgO, Al/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub>, and Cu/MgO when varying coverage of oxide substrates and considering different kinds of defects (see paper [1]). When combining the corresponding calculations with thermodynamic approach we describe mechanism of metal film growth on oxide substrate (see paper [2]). Metal/oxide interfaces are studied in collaboration with Prof. A.M. Stoneham (University College, London, UK), Prof. K. Hermansson (Uppsala University, Sweden) and Prof. V.Kemper (Clausthal University, Germany).

As a result of these comprehensive computer simulations and theoretical analyses, we describe mechanisms of initial low-temperature oxidation of Al as well as formation of metallic coatings on various surfaces of alumina and magnesium oxide. We clarify what is an influence of different surface defects on the rate of interfacial

processes, when they can be accelerated and intensified but when they can be considered as protectors. Very important part of the study proposed is a comparison with various experimental and theoretical data to make the corresponding correlations for both models and computational schemes.

#### Defects and Surfaces of Advances Perovskites

Perovskites is a wide class of materials with numerous technological applications in electro- optics, waveguides, laser frequency doubling, high capacity memory cells, substrates for high Tc superconductors etc. However, efficiency of relevant devices is affected by structural defects and impurities, whereas further nano-scale miniaturisation of devices is limited by quantum surface effects. The main aim of this work package is to perform detailed theoretical studies of these effects in technologically important ABO<sub>3</sub> type perovskites.

We plan large scale first principles and quantum chemical calculations for a number of materials, including SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, KNbO<sub>3</sub>, KTaO<sub>3</sub> and their solid solutions, widely used in technological applications. Methods to be used are:

Hartree-Fock with the electron correlation corrections, full potential LMTO, semi empirical Intermediate Neglect of the Differential Overlap (INDO), and lastly, the shell model. Combination of a wide range of methods and techniques will permit to get reliable information on the atomic, electronic structure and optical properties of basic impurities in these materials, including O vacancies (F type centers), hole polarons, common metal impurities (e.g., Fe) and hydrogen. This is of a key importance for defect identification. One of particular purposes of our study is identification of defects responsible for the blue-light-induced-infrared-adsorption (BLIIRA) effect which strongly affects efficiency of laser frequency doubling in KNbO<sub>3</sub>-based devices. We have a rich experience in such large scale computer modelling of advanced materials and have very good collaboration with five partner laboratories: prof. J.Maier (Max Planck Institut, Stuttgart, Germany), prof. N.E.Christensen (Inst. of Physics, Aarhus University, Denmark), prof. G. Borstel (Dept of Physics, University of Osnabrueck, Germany), prof. R.Nieminen (Lab. of Physics, Helsinki University of Technology, Finland), prof. C.R.A.Catlow (Royal Institution of Great Britain, London, UK). Another activity will focus on the quantum effects in surface limited nanoscopic-size perovskite crystals. For this purpose, we will model different types of surfaces (100, 110, 111) with emphasis on near-surface atomic reconstruction, surface defects, surface-induced polarization and ferroelectric properties. Quality of these surfaces are extremely important for applications, e.g. for a growth of qualitative high Tc superconductors.

As a result of these large scale computer simulations, we expect to get a sound understanding of properties and thus to make the spectroscopic identification of basic defects in advanced ABO<sub>3</sub>-type perovskites, first of all, O vacancies (F centers) and hole polarons. This will be used for understanding the nature of point defects responsible for the BLIIRA effect. We expect also to shed light on the atomic and electronic structure of the basic surfaces and surface defects, which could be checked by means of the low-energy-electron-diffraction (LEED) experiments. As a result, we could conclude at which monocrystalline sizes quantum surface effects become predominant, which is extremely important for the further opto- and microelectronic applications of perovskites.

In collaboration with Prof. R. Gonzalez (Madrid University, Spain) and Prof. K. Kimura (RIKEN, Japan) optical absorption and luminescence experiments were used to study the photoconversion of neutral oxygen vacancies which trapped two electrons (F centers) in MgO single crystals thermochemically reduced (TCR) at elevated temperatures. It is shown that in crystals with an undetectable concentration of hydride ions and a moderate concentration of F centers ( $10^{17}$  cm<sup>-3</sup>), excitation with UV-light

produces positively charged anion vacancies (F<sup>+</sup> centers) and electrons which are subsequently trapped at impurities. Under continuous excitation, the F<sup>+</sup> centers release holes which are trapped at cation vacancies, charge compensated by impurities. In crystals with high concentrations of both hydride ions and F centers ( $10^{18}$  cm<sup>-3</sup>), the electrons from the F to F<sup>+</sup> photoconversion are trapped mainly at the hydride ions to form H<sup>2-</sup> ions, which are metastable at room temperature.

We performed simultaneous in situ luminescence and optical absorption studies in scintillator CsI and CsI-Tl crystals, exposed to very dense electronic excitations induced by <sup>86</sup>Kr ions (8.63 MeV/amu). This study is performed in collaboration with Dr E. Balanzat (CIRIL, France) and Prof. K. Kimura (RIKEN, Japan). Irradiation at 15 K leads to the formation of the prominent F absorption band. In addition, several other features of the broad absorption between exciton and F bands were ascribed to an anion vacancy, a-centre (240 nm), self-trapped hole, Vk centre (410 nm) and interstitials, H centres (560 nm). We have found that low doping of thallium ( $10^{17}$  cm<sup>-3</sup>) causes the F centre formation to proceed more rapidly than in pure crystal. On the other hand, we were not able to create any amount of F centres in heavily doped CsI-Tl. The production efficiency (electron volts/center) of F band absorption in CsI was found to be  $2.5 \cdot 10^7$  eV/center. Such a quite high value defines the appropriate radiation hardness of CsI scintillators.

## **SELF-ORGANIZATION PHENOMENA AND KINETICS OF NON-LINEAR PROCESSES IN CONDENSED MATTER**

The second aim of our activities is the study of many-particle (cooperative) effects in bimolecular reaction kinetics in condensed matter.

Catalytic surface reactions are of enormous importance in industrial (synthesis of NH<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>, cracking and reforming processes) and environmental chemistry (catalytic control of emission CO, SO<sub>2</sub>). For each particular reaction a specially adapted catalyst is demanded. Therefore a computer aided design of catalyst would be a great progress in optimizing the selectivity, yield and performance of the reaction. Although surface reactions have been intensively investigated in the last 20 years, surprisingly little is known about the elementary reaction steps, which take place on the atomic length scale of these reactions. The CO+O<sub>2</sub> and the CO+NO reaction systems are by far the best-explored ones, both on low index single crystal and polycrystalline surfaces, but experimental investigations using new spectroscopic methods are very demanding to carry out and frequently cannot resolve the individual reaction steps. On the other hand, standard theoretical approaches do not master the complexity of most of the important reaction steps including correlations, fluctuations, formation of spatio temporal patterns and energetic interactions, both in the adsorbate layer and between the adsorbates and the surface. In this case computer simulation may be a good tool to study details of these reactions. Certain aspects of the reaction can be simulated to examine the system behavior as function of these control parameters.

The occurrence of kinetic oscillations in catalytic surface reactions such as the oxidation of CO on Pt(100) and Pt(110) is a well known phenomenon and has been investigated extensively in the recent past. Experimental results show that the temporal- and spatial kinetic oscillations are closely connected with the propagation of chemical waves, i.e. with the propagation of the borders between CO- and O- covered regions on the catalyst surface. In the case of the Pt(100) surface adsorbed CO is able to reverse the 1x1 -> hex surface reconstruction. As O adsorbs essentially only on the 1x1 phase, which initiate the reaction, continuous structural transformations are propagated along with chemical waves. Therefore the system of the CO + O<sub>2</sub> reaction is in principle able to show the kinetic oscillations as soon as one takes these structural transformations into

account. The questions that arise, which basic processes among the vast number of proposed reaction steps have to be included to describe the kinetic oscillations and how should these elementary reaction steps be modeled on an atomic length scale. We have a rich experience in large scale computer modelling of surface reactions combining Monte Carlo and cellular animation simulations, analytical methods: mean-field, pair mean-field, cluster approximations and correlation analysis. Cooperation with prof. W. von Niessen (TU Braunschweig, Braunschweig, Germany), prof. A. Blumen (Freiburg University, Germany), prof. A.P.J. Jansen (Eindhoven University, the Netherlands).

In collaboration with Prof. W. von Niessen (TU Braunschweig, Germany), the problem of oscillation synchronisation in oxidation catalytic reaction on metal surface has been also investigated. The key process appears to be the transition from a local oscillation regime to the macroscopic one that affects the whole system.

As a result of these large-scale computer simulations, we expect to get a sound understanding of essential processes for the surface reconstruction and catalytic surface reactions of single crystal surfaces. Our theory explains the most important experimental phenomena. Thus, for the first time this mechanism can be brought to light, which has remained obscure because experiments by their very nature mix a lot of individual processes.

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#### *Intern. Conf. on Excitonic Processes in Condensed Matter. Osaka, Japan, 2000*

3. K. Kimura, S. Sharma, and A.I. Popov. Novel 100 ps-lived luminescence in insulator crystals excited at extremely high density with heavy ions. -Abstracts, p.58.
4. A.I. Popov and E. Balanzat. *In situ* luminescence and optical absorption studies of CsI scintillators under 8.63 MeV/amu 86Kr ion irradiation at 15-300 K. –Abstracts, p. 101

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5. K. Kimura, S. Sharma, and A.I. Popov. Novel ultra-fast luminescence from incipient ion tracks in insulator crystals. –Abstracts, p.25.

6. A.I. Popov and E. Balanzat. *In situ* studies of point defect creation in CsI scintillaions. - Abstracts, p. 115.

*International Conference on Defects in Insulating Materials (ICDIM). Johannesburg, South Africa, 2000*

- 7 V.N. Kuzovkov, A.I. Popov, E.A. Kotomin, M. Monge, R. Gonzalez and Y. Chen. The kinetics of F center aggregation in Thermochemically Reduced MgO single crystals. - Abstracts, P.
8. E.A. Kotomin, V.N. Kuzovkov, and A.I. Popov. The kinetics of defect aggregation and metal colloid formation in ionic solids under irradiation. - Abstracts, P.
9. V. Kashcheyevs, E.A. Kotomin, and V.N. Kuzovkov. Computer modeling of metal colloid formation in tracks of swift ions in ionic solids. – Abstracts, P.

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10. V.N. Kuzovkov, O. Kortlüke, and W. von Niessen. Nucleation and island growth kinetics on reconstructing surface.- Abstracts, P. 172: P1-241.
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12. J.R. Kalnin, E.A. Kotomin, and V.N. Kuzovkov. The effective diffusion coefficient in inhomogeneous solids.- Abstracts, P. 182: P2-17.



# OPTICAL RECORDING

Head of Division *Dr. J.Teteris*

## Research Area and Main Problems

Synthesis and research of amorphous chalcogenide semiconductor (As-S, As-Se and As-S-Se) and fullerene C<sub>60</sub> thin films for optical recording and electron beam lithography have been performed. Photoinduced changes of optical properties, holographic recording and hologram self-enhancement effects, and relaxation processes in amorphous films were studied. The main task was R&D of high sensitive photoresists in the visible region for holography and electron-beam resists for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed.

### Scientific Staff

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

### Technical Staff

1. J.Gurovs
2. D.Popele

### PhD Students

1. K.Jefimovs

### Students

1. J.Berzins
2. I.Kuzmina
3. M.Stagitis
4. I.Kaufmanis

### Visitors from Abroad:

1. Prof. K.Schwartz, GSI Darmstadt, Department Material Sciences, Germany (3 days).

### Scientific Visits Abroad:

1. Mg. K.Jefimovs, University of Joensuu, Finland (12 months).
2. Dr. P.Stradins, Thin Film Silicon Solar Cells Super laboratory, Electrotechnical Laboratory, Japan (12 months).

### Cooperation

#### Latvia

1. Riga Technical University (prof. A.Ozols).
2. Daugavpils Pedagogical University (Dr. V.Pačkšvics 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)

#### Japan

5. Electrotechnical Laboratory, Thin Film Silicon Solar Cells Super Lab. (Dr. P. Stradins).

**Austria**

**6. Holography Center Austria (Dr. I. Wöber).**

**Main Results**

**ANISOTROPIC DIFFRACTION BY VECTOR HOLOGRAMS IN  
AMORPHOUS As – S – Se FILMS**

*A.Ozols and M.Reinfelde*

Vector holographic grating recording in amorphous As-S-Se films and anisotropic light diffraction by these elementary holograms is experimentally studied in details and compared with scalar recording. It is holographically established that a linearly polarized 632.8nm light produces photoinduced anisotropy and the chalcogen related  $D^+$ ,  $D^-$  center reorientation and generation mechanism is proposed. It is used to explain the observed peculiarities of vector recording in comparison with scalar recording based on photoinduced structural changes: much lower diffraction efficiency ( $4 \times 10^{-3}$  % versus 4 %), much larger specific recording energy (6.4 kJ/(cm<sup>2</sup>%) versus 20 J/(cm<sup>2</sup>%)), difference in spatial frequency response, instability (vector hologram lifetime of about two days versus practically permanent scalar holograms), the absence of hologram self-enhancement (present in scalar recording), near perfect reversibility. It is also experimentally found that vector holograms in a-As-S-Se films indeed reconstruct the signal wave polarization but only in the minus first diffraction order. It is also shown that photoinduced anisotropy also contributes to the scalar hologram recording in amorphous chalcogenides stimulating it by means of subbandgap readout light and enabling a subbandgap recording.

**ELECTRON BEAM INDUCED PROCESSES IN AMORPHOUS  
CHALCOGENIDE FILMS**

**K.Jefimovs and J.Teteris**

The As<sub>2</sub>S<sub>3</sub> and As-S-Se systems were studied as a resist material for Electron Beam Lithography (EBL). These systems belong to the class of so-called Chalcogenide Vitreous Semiconductors (ChVS). Obtaining the profile after electron beam irradiation is an important property of the resist, because it makes possible to copy the recorded elements by using replication techniques.

The films used were prepared by thermal evaporation method. As-evaporated as well as thermally annealed in air films were studied. The films of different thickness (0.5-3.0 μm) were tested and different electron energies (10-40 keV) and doses (25-2000 μC/cm<sup>2</sup>) were used for film exposures. An organic alkaline developer was used for film etching after exposure. The test gratings of period 30 μm were recorded at different recording parameters. It was found that as-evaporated As-S-Se films behave as a negative resist for the developer used, whereas films annealed at 180°C behave as a positive resist. It was found that the profile-depth dependencies on dose are almost linear which makes it easy to design three-dimensional elements of given profile shape on this resist base. The profile depth obtained for 2 μm thick films was 1.25 μm, which means,

that elements with high diffraction efficiency for He-Ne laser wavelength (633 nm) can be fabricated. Some slanted gratings were recorded.

## **HOLOGRAPHIC PROPERTIES OF DIELECTRIC CRYSTALS AND AMORPHOUS SEMICONDUCTOR FILMS**

*A.Ozols and M.Reinfelde*

Holographic recording properties and mechanisms are analysed and compared in dielectric electrooptic crystals (EOC, e.g., doped and undoped LiNbO<sub>3</sub>, LiTaO<sub>3</sub>, SBN, KTN), dielectric colored alkali halide crystals (AHC, e.g., additively and electrochemically colored KBr, KCl, NaCl) and amorphous semiconductor films (ASF, e.g., As-S, As-Se, As-S-Se, Ge-Te) basing on author's investigations as well as on the literature data. Holographic photosensitivity parameters are introduced enabling the characterization of the recording mechanism efficiency independently of the particular optical and geometrical sample parameters, and allowing also for recording optimization. Ultimate specific recording energies for EOC, AHC and ASF are theoretically estimated to be  $5.0 \cdot 10^{-7}$ ,  $1.5 \cdot 10^{-5}$  and  $1.4 \cdot 10^{-6}$  J/(cm<sup>2</sup>%), respectively. Therefore, it is concluded that the ultimate recording energy for both crystalline and amorphous materials is of order of about  $10^{-6}$ (cm<sup>2</sup> %). Now the best holographic parameters for the scalar hologram recording are achieved in EOC. Then come ASF and AHC. Yet AHC so far are superior at vector hologram recording. Finally, the conclusion is made that ASF can become serious rivals of EOC in holography and optical information processing if other material properties are taken into account such as hologram lifetime, sample size and cost, hologram self-enhancement possibilities.

### **holographic RECORDING in amorphous AS-S-SE films**

*J.Teteris and I.Kuzmina*

The relaxation self-enhancement (RSE) phenomenon of the holographic gratings in amorphous As-S-Se films was studied. The changes of the diffraction efficiency were measured as a function of the aging time and the recording light intensity. The role of the internal mechanical stress of the films in the self-enhancement phenomenon has been discussed. It was shown that the RSE has a vectorial character owing to the uniaxial periodically distributed stress relaxation. A model based on the photo-induced stress relaxation and viscous flow of amorphous film is proposed to explain the experiments qualitatively.

The dependence of the holographic recording self-enhancement on the illumination intensity of the holographic gratings has been experimentally studied in amorphous as-evaporated As-S-Se films. The relaxation time of the self-enhancement was found to decrease exponentially as a function of the exciting laser beam intensity. Results were explained by assuming that light induces the decrease of the viscosity of amorphous films.

### *AMORPHOUS CHALCOGENIDE SEMICONDUCTOR RESISTS FOR HOLOGRAPHY AND ELECTRON-BEAM LITHOGRAPHY*

**J.Teteris, D.Popele and M.Reinfelde**

The photo- or e-beam stimulated changes in the rate of wet etching of amorphous chalcogenide semiconductor (AChS) thin films obtained by vacuum deposition method is the basis for development of a new class of inorganic resists. AChS resists are characterized by very high resolution ( $> 10000$  lines/mm), wide spectral range of photosensitivity (UV and visible up to 700 nm) and they have a number of peculiarities that make them very attractive for application in many photo- and e-beam lithographic processes. The possibility of light- and thermo-induced amplification of holographic recording in amorphous semiconductor films is especially important for the further improvement of the light sensitivity of these photoresists. The amorphous chalcogenide photoresists for production of embossed rainbow holograms have been used. The negative photoresist elaborated at Institute of Solid State Physics (University of Latvia) possesses light sensitivity of  $\sim 100$  mJ/cm<sup>2</sup> and spectral sensitivity range at  $\lambda \leq 700$  nm. Thus it is possible to record holograms by means of semiconductor diode or solid state lasers.

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1. A.Ozols and M.Reinfeldē. *Vector holograms in amorphous As-S-Se films*. Abstracts, p.27.
2. J.Teteris, M.Reinfeldē, D.Popele and J. Berzins. *Application of amorphous chalcogenide semiconductor thin films in holography*. Abstracts, p.83.
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4. V.Paskevics, J.Maniks, J.Teteris and R.Pokulis. *Relaxation of mechanical stresses in fullerene C<sub>60</sub> and amorphous As<sub>2</sub>S<sub>3</sub> films*.

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5<sup>th</sup> Conference of the Latvian Physical Society, Daugavpils, Latvia, June 8-11, 2000.

6. **A.Ozols and M.Reinfeldē. *Anisotropic diffraction of laser beams by vector holograms in amorphous As-S-Se films*. Abstracts, p.17.**

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7. B.Ōāđāđēñ. Āīēīāđāōē÷āñkāy çāīēñū ā àīīđôīúō vēāīēāō ðāēüēīāāīēāīūō īēōīđīāīāīēēēā.
8. Ē. Īāīēēā, B. Īāīēēñ, B.Ōāđāđēñ, B.Ēāēīā÷ñ, Đ.Īīēóēēñ. Ōīđōđāīñōīđīā-ōēy è ðāđīē÷āñēīā īēēñēāīēā iēēđīēđēñðāēēē÷āñēēō vēāīēē ðóēēāđēðō. Ñ

Int Conf. Holography 2000, St.Polten, Austria, 10-14 July

9. **J.Teteris. *Holography in Latvia*.**
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13. J.Teteris. *Amorphous chalcogenide semiconductor resists for holography and electron-beam lithography*. Abstracts, p.36.

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15. A.Ozols and M.Reinfeldē, *Holographic properties of dielectric crystals and amorphous semiconductor films*. Abstracts, p.7.

# DEFECT PHYSICS IN IONIC MATERIALS

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

## Research Area and Main Problems

The research field is connected with properties of radiation defects and their accumulation in ionic materials such as *alkali halides, alkali earth halides* and *aluminum nitride ceramics*. Optical research methods based on luminescence are applied.

### Scientific Staff:

1. Dr. hab., assoc. Prof. B. Berzina
2. Dr. L. Trinkler

### Ph. D. Students:

1. J. Sils

### Scientific Visits Abroad:

1. J. Sils, Freie Universitaet Berlin, Germany (3 month).
2. J. Sils Ludvigs Maximillian University Munich, Germany (3 month).

## Cooperation

### Latvia

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

### Denmark

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

### Germany

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

Paderborn Universitaet (Dr. S. Schweizer)

Freie Universitaet Berlin (Prof. E. Matthias)

## Main results

### LUMINESCENT AND DOSIMETRIC PROPERTIES OF AlN CERAMICS

*L. Trinkler and B. Berzina*

Luminescence mechanisms of the oxygen-related defects and UV light induced energy accumulation in aluminum nitride crystalline lattice were investigated. AlN-Y<sub>2</sub>O<sub>3</sub> ceramics sintered at Institute of Inorganic Chemistry, RTU as well as partly transparent AlN ceramics without Y<sub>2</sub>O<sub>3</sub> additive prepared in Japan were used as samples for study. Investigations of ultraviolet-blue luminescence behavior caused by oxygen-related defects together with the research using sensitive magnetic-resonance technique (at Paderborn University, Germany) allow interpretation of the luminescence center structure and the luminescence mechanism (see publications [3,5] and lectures [2,4]). Studies of the dosimetric characteristics of AlN-Y<sub>2</sub>O<sub>3</sub> ceramics after UV irradiation (in cooperation with colleagues from RISO National Laboratory, Denmark) allow consideration of the AlN ceramics as a perspective material for use in UV dosimetry

(see publications [2,4] and lectures [1,5]). The studies of dosimetric characteristics of AlN are in progress.

## LASER DAMAGE INVESTIGATIONS IN ALKALI EARTH FLUORIDES

*J.Sils*

Investigation of laser damage on several alkaline earth fluoride single crystals including CaF<sub>2</sub> has been continued. The damage mechanism has been studied using 14 ns laser pulses at 248 nm. The origin of different damage mechanisms has been discussed in the publication [6] and presented in the international conference [6].

## CONVERSION OF EXCITON-CREATED DEFECTS IN PURE AND DOPED ALKALI HALIDES

*B.Berzina and J.Sils*

The role of the exciton-created defects in energy accumulation and energy transfer from the host lattice excitations to the impurities was examined in some alkali iodide crystals (KI-Tl, RbI-Tl). The results obtained affirm the hypothesis worked out in our laboratory revealing the role of the exciton-created F<sub>H</sub> center pairs in impurity excitation. The proposed mechanism of energy transfer was discussed in the publication [1] and the international conference [3].

### Scientific Publications

#### published in 2000

1. B.Berzina and J.Sils, *Exciton-created defects and their participation in energy transfer from excitons to Tl ions in KI-Tl crystal*. Nuclear Instruments and Methods in Physics Research B, **166-167** (2000) 586-591.
2. L.Trinkler, L.Botter-Jensen, P.Christensen, B.Berzina, *Studies of aluminum ceramics for application in UV dosimetry*. Radiation protection dosimetry, **92** (2000) 299-306 .
3. S.Schweizer, U.Rogulis, J.M.Spaeth, L.Trinkler and B.Berzina, *Investigation of oxygen-related luminescence centers in AlN ceramics*. Phys. Stat. Sol. (b), **219** (2000), 171-180.

#### in press

4. L.Trinkler, L.Botter-Jensen, P.Christensen, B.Berzina, *Stimulated luminescence of AlN ceramics by ultraviolet radiation*. Radiation measurements (2000) submitted.
5. *B.Berzina, L.Trinkler, J.Sils and E.Palcevskis*, Oxygen-related defects and energy accumulation in aluminum nitride ceramics. *Radiation Effects and Defects in Solids* (2000) submitted.
6. *J.Sils, H.Johansen, E.Matthias, M.Reichling*, Approaching the perfect CaF<sub>2</sub> surface for 248 nm optics applications. *Appl.Surface Sci.* (2000) submitted.

## Lectures on Conferences

### 16<sup>th</sup> Scientific Conference of the Institute of Solid State Physics (Riga, Febr. 2000)

1. L.Trinkler, B.Berzina, *Application of AlN ceramics for UV dosimetry*, (oral presentation).

### International Conference on Defects in Insulating Materials ICDIM'2000

(Iohannesburg, South Africa, April 2000)

2. B.Berzina, L.Trinkler, J.Sils and E.Palcevskis, *Oxygen-related defects and energy accumulation in aluminum nitride ceramics*, (oral presentation).
3. B.Berzina and J.Sils. *Conversion of exciton-crated defects in pure and doped alkali halides*, (poster presentation).

### 4<sup>th</sup> Euroconference on Luminescent Detectors and Transformers of Ionizing Radiation

LUMDETR'2000 (Riga, Aug. 2000)

4. B.Berzina, L.Trinkler, J.Sils, E.Palcevskis and A.Bluma, *Luminescence of oxygen-related defects and energy accumulation in aluminum nitride ceramics*, (oral presentation).
5. L.Trinkler, L.Botter-Jensen, P.Christensen and B.Berzina, *Application of AlN ceramics for UV dosimetry*, (oral presentation).

### International Conference ICPS' 2000 (Zadara, Hrovatia 2000)

6. J. Sils, *Approaching the perfect CaF<sub>2</sub> surface for 248 nm optics application*, (oral presentation).



# OPTICAL MATERIALS

*Head of Division Dr. hab. phys. Prof. I.Lacis*

## *Research Area and Main Problems*

Lot of new materials are investigated for application or already are in use in a variety of noncontact and contact vision correction devices (goggles, telescopes, contact lenses, intraocular lenses, light protection goggles). Still there are lot of unsolved problems for advanced vision correction simple aids and devices. They exhibit high dispersion, thus resulting in a variety of aberrations in a lens and the eye. The most important aberration effecting the qualitative vision correction is the transversal chromatic aberration of the oblique beam propagation. The influence of spectacle lens aberrations on vision quality depending on task, environment and visual training are studied. The impact of different external parameters on visual fatigue will be analyzed.

The electrooptically tunable light scattering in PLZT ceramics for simulation of eye segments optical properties are applied in new instrument constructions on in new visual ability tests. The sensitivity of the binocular visual system to luminance and contrast distribution of two monocular half-images are studied.

The main aim of this laboratory is experimental studies of the newest optical materials and lenses usable for vision correction devices and model studies of the optical system eye - corrective element for evaluation of the human adaptation ability, especially binocular, to different geometry construction of the vision correction devices.

### **Scientific Staff:**

1. Dr.habil.phys. I. Lacis
2. Dr.habil.phys. M.Ozolinsh

### **Graduate Students:**

1. B.Sc. O.Cirpone;
2. B.Sc. A.Svede;
3. B.Sc. L. Viesture

### **Postgraduate Students:**

1. M.Sc. A.Balgalve
2. M.Sc. G.Papelba
3. M.Sc. J. Fridrihsons

### **Visitors from Abroad:**

1. Prof. O.Franzen, Mid Sweden University, Sundwall, Sweden (1 month);
2. Prof. S.Villani, Florence University , Italy (12 days).
3. Prof. Kenneth J. Ciuffreda. State College of Optometry, USA (9 days).

### **Cooperation**

#### **Italy**

1. Istituto Internazionale Delle Scienze Ottiche e Visive "Vasco Ronchi"  
(Prof. S. Villani)
2. II. Universita` di Roma "Tor Vergata", (Prof. I. Davoli)

## Norway

3. Buskerud Høgskolan, Institut for optometri, (Prof. K. I. Daae)

## Sweden

4. Mid Sweden University, Sundswall, (Prof. O. Franzen)
5. Lund University, (Prof. S.Svanberg).
6. Department of Clinical Science of Karolinska Institute, (Dr. H. Richter)

## Main Results

### COORDIMETER'S STRUCTURE, MECHANISM AND INTERPRETATION OF RESULTS

#### *A. Svede*

In the case of incomitant strabismus there is important not only to find an affected muscle, but also to follow up possible changes in ocular motility. Coordimetry (Lancaster, Hess and Lee screens) provides a readily repeatable graphic recording to monitor the ocular motility defect, finding the affected muscle, seeing signs of recovery or deterioration, muscle sequelae development, type and proximal size of deviation. As there are none working mentioned tests in Latvia for now, new experimental methods are developed.

### BINOCULAR CONTRAST SENSITIVITY SUMMATION AND INHIBITION

#### *A. Balgalve, J. Fridrihsons and I. Lacis*

It is generally accepted that binocular spatial contrast sensitivity in normal observers is higher than monocular sensitivity by some 42% across all spatial frequencies, as a result of neural summation of the two monocular responses. Recent experimental data have shown, that reduction in monocular sensitivity caused by reduced luminance can, in some subjects, lower binocular sensitivity to a level below that of the other eye. It seems to be an analogue of Fechner's brightness paradox. There are also another subjects where the expected summation occurs and binocular sensitivity always remains at or above the monocular level.

**The influence of eye dominance degree on binocular inhibition have been studied.**

### STEREOVISION UNDER EXTERNAL INFLUENCE

#### *G. Papelba, I. Lacis, M. Ozolinsh, and K.I. Daae<sup>a</sup>*

<sup>b</sup> *Institute for optometry, Norway*

*Introduction:* Stereopsis is that unique quality of binocular vision that enables to perceive depth in visual space. It arises from horizontal retinal image disparity between the two *foveas* or other corresponding retinal points: differing amounts of such disparity give

rise to differing sensations of depth. Just as visual acuity is graded in terms of minimum angular resolution of two distinct points, stereopsis can be graded (stereoacuity) in terms of the smallest horizontal retinal disparity of images that gives rise to a sensation of depth. The main goal of this investigation was studies of the stereovision threshold under static and dynamic conditions. These stimuli were optical overcorrection or blurring of the stimulus for one eye.

*Subject:* In this experiment were 125 subject, who had good visual acuity (1,0 or 0,9) with or without correction. Age of subjects was from 14 to 74 years. Presbyops had the near correction in 40cm distance. In this experiment was different ametropias.

*Method:* Three different test techniques were developed. First, studies of stereovision quality in near using monocular overcorrection with a standard TNO test (random elements combined with anaglip method). The monocular alternative overcorrection was made with lenses from  $-2.50$  D to  $+2.50$  D with step 0.5 D. Replacing of the colour filters changed the disparity type (crossed or uncrossed). Subject must determine the ring's segment place.

Second, determination the influence of monocular overcorrection on the maximum stereoangle in far using an original projection line test technique with polaroids or colour (red and green) filters for stimuli separation. There was the same diapason of the lenses. Subject must determine depth localisation of lines in regard to the fixation point (before or behind a screen).

Third, studies in static and dynamic conditions of correlation between the decrease of the monocular acuity and the stereothreshold using a light scattering obstacle placed between one eye and a random dot stereopair. The obstacle made of electrooptic PLZT ceramics provided a continuo quasistatic and dynamic change of blurring of a retinal image, thus decreasing the contrast of the stimuli. Subject must determine the figure with the highest stereoangle seen when the light scattering is dynamically switched on.

*Results and Conclusions:* For tests both in near and in far a decrease of the stereovision quality with overcorrection is close to linear. A ratio between the stereothreshold (in lines for TNO test) and overcorrection would be taken as a measure for a stereoresistance. The stereoresistance differs for positive and negative overcorrection and for near vision has an averaged for 125 patients value of 0.58 and 1,6 (D/lines), having the tendency for negative value being smaller. Using the third method, light scattering induced by applying the voltage to the PLZT ceramics obstacle decreased the monocular acuity in far down to 0.5, causing the loss of the stereosense for the value of disparity of  $2^{\circ}$  within 0.5 s after switching on scattering.

*Conclusions:* Three different test methods are used to evaluate the external influence to the stereovision quality. A new term - stereoresistance is proposed to characterise diminishing of the stereosense with overcorrection. More detailed studies comparing stereovision changes caused by overcorrection and by blurring due light scattering would give an additional information of the impact of anisometropia on the stereothreshold.

## TOLERANCE TO SPECTACLE TRANSVERSE ABERRATION

*J. Fridrihsons*

Several authors who studied the influence of spectacle lens transverse chromatic aberration on visual acuity found out that the subject tolerance to the TCA was remarkably different although the criteria of the subject selection were similar. Up to now no attempt was made to explain this phenomena. It is proposed that visual contrast sensitivity has its role in difference of subject tolerance to the TCA. Theoretical concepts and proposal to the experimental test of the hypotesis have been studied.

## **PROBLEMS IN BINOCULAR VISION RESEARCH**

*O. Cirpone*

Physiology of binocular vision continuously attracts interest of researchers. No unified opinion is reached because of contradictions in different studies. Separation of visual fields is necessary to explore such phenomena as suppression or abnormal retinal correspondence. On the other hand separation of visual fields affects properties of binocular fusion. This necessary evil means that results must be analysed taking account the applied method of investigation in every research.

## **POLARIZATION-OPTICAL VISUALISATION OF EYE INHOMOGENEITIES**

*M. Ozolinsh and G. Papelba*

Investigation of transparent eye segments usually are done by various techniques (split lamp, handheld ophthalmoscope, digital microscopy etc.). Light scattering and birefringent inhomogeneities in eye caused by cataract, scarring after accidents or corneal surgery can be studied using polarization-optical methods. Similar techniques are reported previously<sup>1</sup> for studies of polarization sensitive backscattering in human tissues in order to assess skin lesions. Subtracting of two images captured by a digital video camera using backscattered light, correspondingly, with two orthogonal polarization planes allows visualisation of the superficial skin avoiding the nonpolarized light scattering from the deeper dermis. Authors<sup>1</sup> are using mechanically adjustable polarization filters, thus the method is critical to small displacements of a test object during the procedure, and increasing of the signal/noise ratio by summation of a number of images is not effective.

We have modified the reported technique introducing of an electrooptically controllable polarization plane switching unit consisting of a transparent PLZT (lead-lanthanum zirconate titanate) ceramics phase plate and of a sheet polarization filter. The data acquisition rate - 10 frames per second (5 frames for each of two polarization plane directions) allows to minimise the influence of the test object movement for investigation of skin and as we believe - for polarization-optical imaging of eye tissues.

### **Method of stereosense time response studies by use of dynamic suppressing of retinal images**

*M. Ozolinsh, I. Lacis and K.I. Daae\**

The novel technique for determination the stereopsis dynamic response, using as stimulus a random dot stereopair was developed. Stereopsis can be evoked or depressed by continuous or flash illumination of the stimulus with simultaneous control of a special light scattering obstacle built in the visual path of one eye. The obstacle - a thin plate of electrooptical PLZT ceramics - exposes (by applying of the voltage to semitransparent gold electrodes deposited on both surfaces of the plate) light scattering so blurring the retinal image, similar as for an eye with a cataract, depressing stereopsis. The random dot stereopair contains contours of images with a different stereodisparity. The PLZT plates active (covered with electrodes and light scattering) part influences a

part of the image of one eye so ensuring the continuous fusion of both eye stimuli and supplying a reference stereoisimage in the clear region of the stimulus. The degree of blurring one can vary continuously by changing the voltage applied to the PLZT ceramics plate. The dynamically controlled light scattering induced in the obstacle has much greater switching speed (in sub-millisecond range) as compared with the human ocular and oculomotoric responses.

*\*In cooperation with Institutt for optometri Høgskolen i Buskerud, NORWAY*

## **Scientific Publications**

### **Published in 2000**

1. M.Ozolinsh, K.I.Daae, D.Bruenech and I.Lacis, Studies of time response of the vision binocularity by use of dynamic suppressing of retinal images. In: 1999 International Conference on Biomedical Optics (BMO), Qingming LUO et.al., Editors, Proceedings of SPIE Vol. 3863, 1999, p. 214-218.
2. M. Ozolinsh, I. Lacis, M. Livinsh, S. Svanberg, S. Anderson-Engels, and J. Swartling. Spectral Scattering Dependencies of Controllable PLZT Occluder for Vision Science Applications. In: 5<sup>th</sup> Euroconference on application of polar dielectrics, August 27-30, 2000, Jurmala, Latvia, p. 68.
3. G. Papelba, I. Lacis, M. Ozolinsh, Stereoresistance-a new characterization of stereothreshold under external influence. – In: Sixth International meeting of American Academy of Optometry, Madrid, 2000, p.13.
4. M. Ozolinsh and G. Papelba “Polarization-optical visualisation of eye inhomogeneities”, Proc.SPIE, Vol.4160 (in print).
5. M. Ozolinsh, I. Lacis, K. I. Daae, Method of stereosence time response studies by use of dynamic suppressing of retinal images. – In: 16<sup>th</sup> Scientific Conference of the University of Latvia, February 14-16, 2000, Riga, p. 32.
6. G. Papelba, I. Lâcis, Overcorrection effect to stereovision. - In: 16<sup>th</sup> Scientific Conference of the University of Latvia, February 14-16, 2000, Riga, p. 33.
7. A. Balgalve, J. Fridrihsons, I. Lâcis, Binocular contrast sensitivity summation and inhibition. - In: 16<sup>th</sup> Scientific Conference of the University of Latvia, February 14-16, 2000, Riga, p. 35.

### *Lectures on Conferences*

Int. Meeting of American Academy of Optometrists (AAO) - Madrid, April 2000.

G. Papelba, I.Lacis, M.Ozolinsh, and K.I.Daae “Stereoresistance - a new characterization of stereothreshold under external influence.”

EOS/SPIE European Biomedical Optics Week EBiOS2000 - Amsterdam, July 2000.

M. Ozolinsh and G.Papelba “Polarization-optical visualisation of eye inhomogeneities.”

OSA Annual Meeting 2000, Providence RI, November 2000.

I. Lacis, M. Ozolinsh, and G. Papelba “Influence of dynamic monocular image blurring on stereo threshold.”

5th European Conference on Application of Polar Dielectrics ECAPD5 - Riga, August 2000.

M. Ozolinsh, I. Lacis, M. Livinsh, S. Svanberg, S. Andersson-Engels, and J. Swartling “Spectral Scattering Dependencies of Controllable PLZT Occluder for Vision Science Applications.”

16<sup>th</sup> Scientific Conference of the University of Latvia, February 14-16, 2000, Riga.

1. A.Balgalve, J.Fridrihsons and I.Lacis, Binocular contrast sensitivity summation and inhibition.
2. G.Papelba and I.Lacis, Overcorrection effect to stereovision.
3. A.Svede, Coordimeter’s structure, mechanism and interpretation of results.
4. J. Fridrihsons, Tolerance to spectacle transverse aberration.
5. M. Ozolinsh, I. Lacis and K.I. Daae, Method of stereosense time response studies by use of dynamic suppressing of retinal images.
6. M.Ozolinsh, G.Papelba and A.Hermerschmidt, Elipsometrical visualisation of inhomogeneities in eye.

30<sup>th</sup> Congress of the European Contact Lens Society of Ophthalmology. September, 27-30, 2000, Antalya, Turkey.

A. Balgalve. Using of CCRLU grading Scales in Practice.

5th European Conference on Application of Polar Dielectrics ECAPD5 - Riga, August 2000.

M. Ozolinsh, I. Lacis, M. Livinsh, S. Svanberg, S. Andersson-Engels, and J. Swartling “Spectral Scattering Dependencies of Controllable PLZT Occluder for Vision Science Applications.”

### **Thesis**

1. J. Fridrihsons, “Tolerance to spectacle transverse aberration,” Master Thesis, University of Latvia, Riga, 2000, p.52.
2. N. Stotika, “Adaption by prisms induced heterophoria”, Master Thesis, University of Latvia, Riga, 2000, p. 87.

# **SURFACE PHYSICS**

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

## *Research Area and Main Problems*

- micromechanical properties of near-surface layers of solids and thin films,
- photo- and atmosphere-induced effects in micromechanical properties of optical and other materials,
- the strength properties of phase boundaries and interfaces in heterogeneous systems,
  - the adhesion of coatings and solids.

### *Main Problems:*

- microhardness and dislocation mobility, photo- and thermo-induced structural changes and environmental effects in fullerite  $C_{60}$  crystals and thin films ;
- the adhesion and micromechanical properties of tribological nitride multilayer and other coatings;
- the adhesion of atomically-clean and real surfaces of solids, mechanical properties of phase boundaries.

### **Scientific Staff:**

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

### **Students:**

4. A.Kozelis
5. Z. Jonelis

### **Scientific Visits Abroad:**

1. Dr.F.Muktepavela, Joint Nordic Powder Technology Conference, Stockholm, Sweden (7 days)
2. Dr. I.Manika , A.Joffe Physico-Technical Institute, Sankt-Petersburg, Russia (7 days).
3. Dr.I.Manika, ADOM-2 conference, Vilnius, Lithuania (7 days)
4. Dr. habil. J.Maniks, ADOM-2 conference, Vilnius, Lithuania (7 days)
5. Dr.I.Manika, CSEM Instr., Neuchatel, Switzerland (7 days).

### **Cooperation**

#### **Latvia**

1. Institute of Physical Energetics, Latvian Academy of Sciences (Dr.J.Kalnacs).

- 2 Riga Technical University (Prof.V.Mironovs).
- 3.Daugavpils Pedagogical University (R.Pokulis).
- 4.Institute of Solid State Physics, University of Latvia (Dr.J.Teteris).

#### **Ukraine**

**Institute of Metal Physics, Ukrainian Academy of Sciences, Kiev (Dr. M.Vasiljev)**

Czech Republic

**Institute of Scientific Instruments, Brno (Dr.J.Sobota).**

#### **Main Results**

### **EFFECT OF LIGHT EXPOSURE ON DISLOCATION MOBILITY IN FULLERITE C<sub>60</sub> CRYSTALS: THE WAVELENGTH DEPENDENCE**

*I.Manika, J.Maniks, J.Kalnacs<sup>\*</sup>, R.Pokulis<sup>\*\*</sup>*

The illumination-time evolution and the wavelength dependence of the photoinduced structural transformation in near-surface layer of C<sub>60</sub> single crystals in air have been investigated by use of the dislocation mobility method. Investigations were performed on the (111) face of crystals at power densities 0.2-2 mW/cm<sup>2</sup> in the wavelength range of 150-900 nm. The results show that the light exposure in air leads to the decrease of the dislocation mobility. The magnitude of the effect as a function of the illumination time was investigated and a two-stage relationship was obtained. The ultraviolet light was found to be more effective than the visible light in the photo-induced reduction of dislocation mobility. In the wavelength range of 350-700 nm, the reduction of dislocation mobility under light irradiation linearly increased with increasing the photon energy. The obtained results are discussed in terms of the photo-induced polymerisation, which proceeds through different stages including the formation of dimers, polymer chains and cross-linked polymerised structures.

The results at short-wave ultraviolet light illumination (147 nm) indicate to participation of the gaseous medium in the photochemical transformation of fullerite. The immobilization of dislocations was observed not only on the illuminated part of the crystal but over its entire surface. Obviously, at the photon energies greater than the O<sub>2</sub> dissociation energy, the oxidation reaction of fullerite at room temperature becomes possible.

*In cooperation with Institute of Physical Energetics<sup>\*</sup>, Latvian Academy of Sciences and Daugavpils Pedagogical University<sup>\*\*</sup>.*

### **INDENTATION CREEP AND STRESS RELAXATION IN FULLERITE C<sub>60</sub> CRYSTALS AND AMORPHOUS As-S-Se FILMS**

*J.Maniks, I.Manika, J.Teteris, R.Pokulis<sup>\*</sup>*

The photo-induced polymerization of fullerite as well as amorphous chalcogenide is accompanied by the generation of significant mechanical stresses, which can cause ageing effects, stress-promoted reactions and mechanical damage. The stress relaxation has been investigated by the indentation creep method. The results show pronounced



relaxation of mechanical stresses at room temperature. The relationship  $\dot{\epsilon} = B \dot{\sigma}^m$  between the deformation rate and the applied stress was observed. For As-S-Se films the values of the deformation rate sensitivity exponent  $m=0.04-0.09$  were obtained depending on deposition conditions, applied indentation load, structural state of the material and light irradiation during the creep test. In the case of fullerite single crystals and polycrystalline films, the values of  $m=0.02-0.03$  were observed. The data obtained show comparatively low rate sensitivity of the flow stress for investigated materials. The coefficient of viscosity was found to be dependent on the applied stress and deformation rate.

<sup>8</sup>In cooperation with Daugavpils Pedagogical University.

## C-N/MeN<sub>x</sub> NANOCOMPOSITE COATINGS USED AS HARD SOLID LUBRICANTS

I.Manika, F.Muktepavela\*

Nanocomposite coatings enable, by using an optimal ratio of individual components, combination of properties conventionally considered as excluding one another, such as high hardness and high toughness. We investigated nanostructured multilayer coatings of the C-N/MeN<sub>x</sub> type, where Me could be Ti, Nb or Zr. Various substrates, such as tungsten carbide, steel, and silicon, were used. The microhardness, friction coefficient, wear and the film transfer in a reciprocating ball on the disk tribometer were measured. The potential application of C-N/MeN<sub>x</sub> nanostructured multilayers as a hard solid lubricant is discussed. Indentation criteria for polycrystalline, amorphous and nanostructured multilayer coatings are compared. For hard multilayer coatings on a soft substrate at  $H_f / H_s = 10$  the values of film thickness to critical indentation depth ratio  $t/h_c = 10$  were obtained, and in this case the Bückle's one-tenth rule is valid. For hard single layer coatings on a soft substrate this rule is broken, and values of  $t/h_c$  as high as 13-17 at  $H_f / H_s > 10$  are experimentally observed. It means that the plastic deformation in multilayer coatings is highly localised and such coatings in the indentation test behave like amorphous ones.

<sup>8</sup>In cooperation with Institute of Scientific Instruments, Brno

## Scientific Publications

### Published in 2000

1. H.Jensen, G.Sorensen, I.Manika, F.Muktepavela, J.Sobota. *Reactive sputtering of nanostructured multilayer coatings and their tribological properties*. Surface and Coatings Technology, 1999, v.119, p. 1016-1021.
2. I.Manika, F.Muktepavela, G.Sorensen. *Mechanical behaviour and limits to the microhardness testing of hard multilayer coatings on soft substrates*. 3-rd Int. Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering, A.I.Melker, Editor, Proc. SPIE, 2000, vol.4064, p.351-354.
3. J.Maniks, A.Simanovskis. *The joining of LiNbO<sub>3</sub>, quartz, TlBr-TlI and other optical materials by the use of thin metal films as bonding agents*. In: "Defects and Surface-Induced Effects in Advanced Perovskites (G.Borstel, A.Krumins, D.Millers, eds.)",

NATO Science Series 3.High Technology, Kluwer Academic Publishers, 2000,vol.3, p. 267-272.

4. I.Manika, J.Maniks, J.Kalnacs. *Photo-, thermo- and stress-promoted transformations in fullerite C<sub>60</sub>*. Latvian Journal of Physics and Technical Sciences, 2000, 4, p.48-59.

5. M.A.Vasiljev, V.E.Panarin, A.A.Deina, B.B.Straumal, F.O.Muktepavela. *Increase of the corrosion-resistance after low energy ion treatment*. Czechoslovak Journal of Physics, 2000, vol.50, Suppl.53, p.1-4.

### **In Press**

6. F.Muktepavela, M.Vasiljev. *Hydrogen formation on phase boundaries of Sn/Al*. NATO Science Series.

7.J.Maniks, I.Manika, J.Teteris, R.Pokulis. *Indentation creep and stress relaxation in amorphous As-S-Se and As-S films*. Proceedings SPIE .

8. I.Manika, J.Maniks, R.Pokulis, J.Kalnacs. *Effect of light exposure on dislocation mobility in fullerite C<sub>60</sub> crystals*. **Proceedings SPIE .**

9. F.Muktepavela, I.Manika, J.Kalnacs. *Investigation of mechanically alloyed metal/oxide coatings by SIMS method*. Latvian Journal of Physics and Technical Sciences.

### **Lectures on Conferences**

16<sup>th</sup> Scientific Conference of Institute of Solid State Physics, University of Latvia, Riga, February 14-16, 2000:

1.J.Maniks, I.Manika, J.Kalnacs. *Photo-, thermo- and stress-promoted transformations in fullerite C<sub>60</sub>*. Abstracts, p. 48.

2.J.Maniks, I.Manika, J.Pokulis, J.Kalnacs. *Relaxation of mechanical stresses in fullerite C<sub>60</sub>*, Abstracts, p. 47.

Conference on Applied Physics, Kaunas, Lithuania, 13-14 April 2000:

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4.V.Mironov, F.Muktepavela. *Al-B composite powders and their compaction*. Proceedings, p.51.

5.V.Mironov, F.Muktepavela. *Iron-copper composites received by magnetic-pulse pressing and Cu-impregnating*. Proceedings, p.27

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6.M.A.Vasiljev, V.E.Panarin, A.A.Deina, B.B.Straumal, F.O.Muktepavela. *Increase of the corrosion-resistance after low energy plasma treatment*.

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7. R.Pokulis, I.Manika, J.Maniks, J.Kalnaès. *Fotoinducēto mikrocietības un dislokāciju kustīguma izmaiņu spektrālā atkarība fullerīta c<sub>60</sub> kristālos*.

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8. I.Manika, J. Maniks, J.Teteris, J.Kalnacs, R.Pokulis. *Phototransformation and thermal oxidation of microcrystalline C<sub>60</sub> films*. Abstracts, p.54.
9. M.Abdulagabov, G.Shahshaev, G.Safaralijev, A.Gamzatov, A.Kosarev, I.Manika. *Thermal properties of a-C:H films*. Abstracts, p.63.

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10. J.Maniks, I.Manika, J.Teteris, R.Pokulis. *Indentation creep and stress relaxation in amorphous As-S-Se and As-S films*, Abstracts, p.34.
11. I.Manika, J.Maniks, R.Pokulis, J.Kalnacs. *Effect of light exposure on dislocation mobility in fullerite C<sub>60</sub> crystals*, Abstracts, p.104.

13<sup>th</sup> International Symposium on Exoemission and Related Relaxation Phenomena, Jurmala, Latvia, 21-26 August 2000:

- 12.F.Muktepavela, I.Manika, J.Kalnacs. *Investigation of mechanically alloyed metal / oxide coatings by SIMS method*, Abstracts, p.23-24.

11<sup>th</sup> European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, Nitrides and Silicon Carbide, Porto, Portugal, 3-8 September 2000:

13. J.Sobota, J.Bousek, G.Sorensen, H.Jensen, I.Manika, F.Muktepavela. *C-N/MeN<sub>x</sub> nanocomposite coatings used as hard solid lubricants*.

Powder Metallurgy World Congress, Kyoto, Japan, 12-16 November, 2000:

14. V.Mironovs, F.Muktepavela. *Copper infiltration of iron powder items using magnetic-impulse compaction*. Abstract 15P-T2-102.

# RADIATION PHYSICS

*Head of Division Dr. hab. J.Berzins*

## Research Area and Main Problems

Laboratory of Radiation Physics was incorporated into Institute of Solid State Physics since 1.01.1999. in connection with the reorganization of Nuclear Research Center of Latvian Academy of Sciences. The laboratory consists of four groups – the nuclear spectroscopy and theory, applied nuclear physics, oxide physics and high temperature superconductivity. The following main problems are developed in the laboratory:

- experimental and theoretical investigation of nuclear structure at normal and exotic states;
- **selective neutron activation methods for the analysis of the technical materials and environment samples of the forest ecosystem;**
- detection of radionuclides (artificial and radioactive decay products) in the nuclear reactor and technological scraps from nuclear facilities and in environmental samples with the nuclear spectrometric methods;
- the analysis of HANES and EXAFS optical absorption and luminescence and neutron diffraction study of MeO - MgO solid solutions. The dependence of the Me-Mg , Me-O and Me-Me distance from the composition and its links with optical and magnetical properties;
- radiation effects in the dielectric crystals ( MgO,  $YAlO_3$  ,  $LiNbO_3$ );
- the use of the physical methods ( MORPHOQUANT, EPR and optical absorption and luminescence) in the medical physics ( retrospective medical dosimetry);
- **flux pinning in neutron irradiated 123 high temperature superconductors and its relationship to magnetic anisotropy.**

### Scientific Staff:

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

## Technical Staff :

1. A.Afanasjeva
2. L.Neiburgs
3. A.Sotaks
5. V.Kurlovics

## Students:

A. Andrejevs

## Visitors from abroad

Dr. K. Starosta New-York University Stony Brook, USA (4 days).

## Scientific visits abroad

Dr. hab. A.Afanasjev Department of theoretical Physics, Technical University Munich, Germany (5 months).

Dr. hab. A.Afanasjev Notre Dame University, Notre Dame, USA (2 month).

Dr. hab. J. Berzins New-York University Stony Brook, Stony Brook, USA (24 days).

Dr. hab. J. Berzins Institute of Transuranium Elements, Karlsruhe, Germany (4 days).

Dr. hab. V. Bondarenko Technical University Munich, Germany (21 + 21 days).

**Dr. hab. N.Mironova - Ulmane Institute of Physics, Tartu, Estonia ( 7 days + 7 days).**

## Cooperation

### Latvia

1. **P. Stradina Medical University ( Dr. hab., prof. M.Eglite, Dr. E.Churbakova).**
2. State Institute of Wood Chemistry ( Dr. hab. G.Dobele, Dr. J.Hrols).
3. Ltd. "Reaktors".
4. Lielriga Regional Board environment(A.Skujina)
5. Riga Technical University, Institute of Inorganic Chemistry( Dr. I.Vitina, Dr. E.Palcevskis).

### 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).

### Canada

Department of Physics and Astronomy, McMaster Univ., Hamilton (Prof. D. G. Burke).

### Czech Republik

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

### Estonia

Institute of Physics , Tartu ( prof. Ch.Luschik, prof. A.Luschik , Dr. A.Sildos Dr.T.Karner).

## **Ukraine**

1. State University “ Lvivska Politechnika” , Lvov ( prof. A.Matkovskii).
- 2.R&D Institute of Materials RPA “ Carat” Lviv ( Dr. D.Sugak, Dr. S.Ubizskii).
- 3.Institute of Physics of the Ukrainian Academy of Science, Kiev (prof. S. Nepijko).

## **Poland**

Institute of Physics, PAS, Warsaw ( Dr. A.Suchocki).

## **Russia**

Metal Physics Institute, Academy of Science , Ural Division ( prof. A.Menshikov).

## **Austria**

**Atomic Institute of Austrian Universities, Vienna (Prof. H.Weber).**

## **Croatia**

**Ruder Boškovic Institute, Zagreb (Prof. S.Music).**

## **Main Results**

### **NUCLEAR STRUCTURE of $^{181}\text{Hf}$ STUDIED in (n, $\gamma$ ) and (d,p) REACTIONS**

*J.Berzins, V.Bondarenko, P. Prokofjevs, L.Simonova, T. v. Egidy, H.-F. Wirth, A.Metz, Y.Eisermann, G.Graw, R.Hertenberg, L. Rubacek, J.Honzatko, and I.Tomandl*

The experimental information about  $^{181}\text{Hf}$  at present is rather unsatisfactory in comparison to neighbour W and Hf nuclei and there are many uncertainties concerning the location of Nilsson states even at energies below 1 MeV excitation energy. In order to obtain a new information of excited states of  $^{181}\text{Hf}$  we performed the measurements with better resolution of the  $^{180}\text{Hf}$  (d,p) reaction with polarised deuterons at the Munich Tandem Van de Graaf accelerator with  $E_d=24$  MeV. Single gamma spectra and gamma-gamma coincidences in (n, $\gamma$ ) reaction were measured at the Nuclear Physics Institute at Řež. As a result 66 energy levels up to 2000 keV were observed most of them for the first time. Part of the levels were grouped into 8 rotational bands. New rotational bands with tentative characteristics were proposed:  $5/2^-$ [512] 1156.0 keV,  $3/2^-$ [501] 1321.8 keV,  $7/2^+$ [633] 1635.9 keV and  $3/2^+$ [642] 1629.4 keV. Some levels above 1 MeV were only obtained in the (n, $\gamma$ ) reaction. Its structure could be connected with the surface vibrations of nucleus. The evaluation of experimental data and theoretical calculations are in progress.

*In cooperation with Technical University of Munich, Nuclear Research Institute, Řež*

### **NUCLEAR STRUCTURE of $^{166}\text{Ho}$ STUDIED in (n, $\gamma$ ), (d,p) and (d, $^3\text{He}$ ) REACTIONS**

*P.Prokofjevs, L.I.Simonova, M.Balodis, J.Čerziðð, V.Bondarenko, H.F.Wirth, T.von Egidy, C.Doll, J.Ott, W.Schauer, R.W.Hoff, R.F.Casten, R.L.Gill, J.Honzatko, I.Tomandl, S.Boneva, V.A.Khitrov, A.M.Sukhovojev, D.G.Burke, J.Kvasil, and A.Mackova*

The odd-odd nucleus  $^{166}\text{Ho}$  was studied with thermal and average resonance neutron capture and with (d,p) and (d, $^3\text{He}$ ) reactions. The  $\gamma\gamma$ -coincidence spectra were measured in the energy interval 50-6243 keV. The  $^{166}\text{Ho}$  level scheme has been developed containing 23 rotational bands below 1 MeV. Six bands of these are new. Several others have been modified and expanded based upon our experimental data. 32 new levels have been identified. Of particular note has been the identification of two rotational bands whose underlying structure consists of  $\gamma$ -vibrational states built upon the two lowest energy quasiparticle states in  $^{166}\text{Ho}$ . The obtained level scheme is in good agreement with semi-empirical and quasi-particle phonon models where residual interactions have been taken into account. Suggestions are given for further experimentation on  $^{166}\text{Ho}$  level structure using existing technology.

*In cooperation with Technical University of Munich, Lawrence Livermore National Laboratory, Brookhaven National Laboratory, Nuclear Research Institute, Rez, Joint Institute of Nuclear Research, Dubna, Department of Physics and Astronomy, McMaster Univ., Hamilton*

## ROTATIONAL BANDS IN $^{124}\text{Ba}$

***J. Berzins, C.J. Chiara, D.B. Fossan, K. Starosta***

The high spin structure of nuclei in  $A=120\div 130$  mass region is very interesting due to the variety of shape coexisting effects. The structure of  $^{124}\text{Ba}$  was investigated in the reaction  $^{64}\text{Zn}(^{64}\text{Zn},4p)^{124}\text{Ba}$ . The double and triple gamma coincidence data processing were performed with the computer code escl8r and eight rotation bands with the high spin levels till 34 were identified. The evaluation of experimental data is in progress.

## THEORETICAL INVESTIGATIONS OF ROTATING NUCLEI AT EXTREME CONDITIONS

*A.V.Afanasjev*

Theoretical investigations of the properties of rotating nuclei at extreme conditions of superdeformation and very fast rotation have been continued in the frameworks of the cranked Nilsson-Strutinsky approach and cranked relativistic mean field theory. The manuscripts devoted to the investigation of band termination features in  $^{86}\text{Zr}$ ,  $^{72,73}\text{Br}$ ,  $^{118}\text{Xe}$ ,  $^{107}\text{Sb}$ ,  $^{119}\text{Ba}$  nuclei, stable triaxiality at the highest spins in  $^{138,139}\text{Nd}$ , highly-deformed structures in  $^{136}\text{Pm}$  and superdeformed structures in  $^{59}\text{Cu}$ , discrete line gamma spectroscopy in the  $50\text{-}60 \leftarrow$  spin domain of  $^{161,162}\text{Er}$  have been published in the international refereed journals. The collaboration with experimental groups from USA, Sweden, Italy, United Kingdom with the aim to understand high-spin properties of rotating nuclei is continued. The investigation of the properties of superdeformed structures in  $^{58,59}\text{Cu}$  nuclei, possible role of proton-neutron pairing at high spin ( $^{72,74,76}\text{Kr}$ ), termination of magnetic and anti-magnetic rotational bands in  $^{105}\text{In}$ ,  $^{110,112}\text{Te}$  and a number of other issues in different nuclei ( $^{113}\text{Sb}$ ,  $^{112}\text{Sn}$  etc.) are in progress and the results of these investigations will be presented in the forthcoming publications.

As an important part of our investigations we have continued the further development of the cranked relativistic mean field theory. The cranked relativistic Hartree-Bogoliubov theory, in which the particle-particle channel is treated in a non-relativistic manner employing the Gogny force and particle number projection is performed by means of the Lipkin-Nogami method, has been developed. Employing this theory very good

description of experimental moments of inertia, quadrupole moments and other physical observables is obtained for the superdeformed rotational bands in the  $A \sim 190$ ,  $A \sim 240$  and  $A \sim 60$  mass regions of superdeformation with no adjustable parameters. The formalism of this theory and the results of the investigations in the above mentioned regions are published in refereed journals. In addition, the investigation of the properties of superdeformed bands in the recently discovered region of superdeformation around  $^{36}\text{Ar}$  is in progress. We are working on the development of the formalism and computer code of the tilted cranked relativistic mean field theory. This theory will allow microscopic investigation of the magnetic and antimagnetic rotation, the properties of shears bands and the role of currents in above mentioned types of rotational bands.

*In cooperation with Technical University of Munich*

## **EXTENSION OF THE STRICTLY RESTRICTED DYNAMICS MODEL APPLICATION REGION**

*J. Tambergs, T. Krasta, J. Ruža, A. Andrejevs*

The systematic calculations [1] of properties of  $\alpha$ -cluster type nuclei, employing microscopic Strictly Restricted Dynamics Model (SRDM), have been extended to  $Z=N$  line nuclei with  $A > 40$ , the study of which presently is very popular. In these calculations our new approximate expressions [2] for  $SU(3)$ -invariant density matrices for  $\epsilon_0 > 2$  were used. The SRDM model parameter set, found via the fit of experimental and theoretical values of nuclear binding and excited level energies, classified according to the ground state  $SU(3)$ -configurations, included nuclear radii parameter  $r_0$ , entering in the expression  $R = r_0 A^{1/3}$  [fm], as well as parameters of the effective central multipole-Gauss-exponent type NN-interaction potential. The fit was made separately for each  $\alpha$ -cluster type nucleus in the region  $4 \leq A \leq 80$ , except for pairs  $^4\text{He}$  and  $^8\text{Be}$ ,  $^{12}\text{C}$  and  $^{16}\text{O}$ ,  $^{36}\text{Ar}$  and  $^{40}\text{Ca}$ , which were calculated together because they have too few states in their respective ground  $SU(3)$ -configurations, and also a group of nuclei  $^{68}\text{Se}$ ,  $^{72}\text{Kr}$ ,  $^{76}\text{Sr}$ ,  $^{80}\text{Zr}$ , which were calculated together due to insufficient experimental data for these isotopes.

The results of our SRDM model calculations allowed to obtain additional information about nuclei along  $Z=N$  line, including binding energies, radii and spectra of low-lying levels. Since calculated binding energy values are very sensitive to the nuclear radii parameter  $r_0$ , directly linked with the nuclear root mean square radius  $\langle r^2 \rangle^{1/2}$ , then it means that  $r_0$  values, obtained via the fit of binding and excited level energies, would provide a valuable information about sizes of nuclei along  $Z=N$  line. Comparing our results with known experimental  $\langle r^2 \rangle^{1/2}$  values when  $A \leq 40$ , the good agreement has been observed for all  $\alpha$ -cluster type nuclei, except for  $^{24}\text{Mg}$ . Unfortunately, we have had no access to experimental radii data for nuclei with  $A > 40$ , though, in this region, one can compare our results with results of calculations using, e.g., Dynamical Microscopic Model (DMM) [3]. These calculations are made, employing deformed single-particle Nilsson potential with pairing forces, i.e., the DMM is based on a completely different understanding of nuclear structure than SRDM. Nevertheless, the results of SRDM and DMM calculations revealed the same trend for  $\langle r^2 \rangle^{1/2}$  values, although SRDM values are somewhat higher.

In order to extend our SRDM model calculations further, we have performed collective density matrix calculations for  $\alpha$ -cluster type nuclei up to  $A \leq 92$ . Also we have started to study the  $SU(3)$ -classification of nuclear states in the unitary scheme chain employing group theory plethysm technique. The results of these investigations would provide us



both with the general classification scheme of SU(3)-states at each A value, covering practically all periodic system, as well as with the classification of SU(3)-states for specific nuclei with given Z and N values, and so would enable us to perform in future systematic SRDM calculations for other type nuclei, not just  $\alpha$ -cluster type ones.

#### DETERMINATION of Sr-90 and Cs-137 IN THE SAMPLES OF RIGA GULF

**A.Skujiòà, S.Puriòà, D.Riekstiòà, V.Bute**

The results demonstrated that the concentration of Cs-137 and Sr-90 in seawater of Riga gulf hasn't changed significantly. The total amount of Cs-137 in the sediments is ever increasing; its concentration in the definite layer is 100 times upwards than that of Sr-90. The concentration of Sr-90 in the seaweed has decreased during last three years but the concentration of Cs-137 hasn't changed essentially. Analysing the fish samples, it was determined that the concentration of Sr-90 in fish is approximately 300 times less than that of Cs-137.

#### DISTRIBUTION OF Sr 90 IN THE FOREST ECOSYSTEMS

*A.Skujina, D. Riekstina, J. Hrols*

The investigation of the environmental pollution has shown that forest is a good pollution accumulator. The aim of this research was to choose the optimal objects for the environmental monitoring of Sr 90 in the regions of possible radioactive contamination. Especially important for the analysis are tree needles; they make it possible to study the dynamics of the pollution within the time interval of 2 5 years.

#### INVESTIGATION DISTRIBUTION OF ELEMENTS IN THE PINS SHOOT WITH DIFFERENT ANALYTICAL METHODS

*D. Riekstiòà, I. Taure, O. Vçveris, A.Vìksna, J. Katkçviès*

The methods of the instrumental neutron activation analysis (INAA), total reflection X-ray spectrometry (TXRF) and electrothermal atomic absorption spectrometry (ETAAS) have been elaborated and applied for determination of the chemical element concentration in the pine needles. The results, obtained with different methods were compared. Variations in the concentration of certain elements in needles depending from their position on the main shoot have been established.

#### STUDY OF CHERNOBYL CLEAN-UP WORKERS TEETH ELEMENTAL CONTENT CHANGES USING INSTRUMENTAL NEUTRON ACTIVATION ANALYSIS

*D.Riekstina. N.Mironova-Ulmane, E.Curbakova*

The instrumental neutron activation analysis (INAA) was used for the investigation the life importance macro- and microelements in the human teeth of clean-up workers Chernobyl s.

The mineralised tissue: tooth enamel and dentine was analyzed. Ten elements: Ca, Sr, Ba, Zn, Fe, Co, Sb, Sc, Br, La of teeth were determined, including such vitally important elements for organism as Ca and its analogue Sr that are mutually replaceable.

The changes of the concentration of Zn and Ca/Sr in the teeth of Chernobyl nuclear power plant accident clean-up workers are connected with the pathology of bones and give the additional information for the diagnosis of diseases.

### **ONE - AND TWO - MAGNON CONTRIBUTIONS IN OPTICAL SPECTRA OF SINGLE - CRYSTAL $\text{KNiF}_3$**

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

The one - magnon and two-magnon contributions were studied in optical absorption spectra of single - crystal  $\text{KNiF}_3$ , measured in the temperature range from 5 K to 300 K. The three absorption bands were considered in details. The first band is due to the magnetic - dipole transition, centred at  $7700 \text{ cm}^{-1}$ , and contains the Brillouin zone - centre one - magnon contribution with the energy  $25 \text{ cm}^{-1}$ . The other two bands are due to the electric - dipole transitions centred at  $16000 \text{ cm}^{-1}$  and  $31200 \text{ cm}^{-1}$  respectively. Both bands contain the Brillouin zone - boundary contribution with the energy  $813 \text{ cm}^{-1}$ .

### **DISPLACEMENT DEFECT FORMATION IN COMPLEX OXIDE CRYSTALS UNDER IRRADIATION**

*S.B.Ubizskii, A.O.Matkovskii, N.A.Mironova - Ulmane V.Skvortsova, A.Sochocki, Y.A.Zhydachovskii, P.Potera*

The work is devoted to an analysis of formation processes of the radiation displacement defects and colour centres in complex oxide crystals under irradiation. The calculation results of the knock-on atoms concentration in some crystals with garnet, perovskite structure are present as well as an analysis of the radiation displacement defects and colour centers accumulation kinetics. New experimental results on additional absorption spectra induced by neutron irradiation of  $\text{LiNbO}_3$  crystals doped with Fe and Cr and  $\text{YAlO}_3$  crystals doped with Nd and Er as well are presented. The obtained results confirm that colour centres causing the irradiation - induced absorption in  $\text{LiNbO}_3$  and  $\text{YAlO}_3$  crystals are formed in secondary processes which are affected by impurities.

### **RADIATION INDUCED DEFECTS IN YTTRIUM ALUMINIUM PEROVSKITE**

*V.Skvortsova, N.Mironova - Ulmane, A.Matkovski, S.Ubizskii*

Optical absorption spectra of  $\text{YAlO}_3$  single crystals with impurities of Nd and Er were measured at room temperature after irradiation with 3,5 MeV electrons, reactor neutrons and gamma-rays. The additional absorption bands at 45000, 42000, 35000, 33000, 26000, 23000 and  $20000 \text{ cm}^{-1}$  were observed. These bands are different thermal stability and irradiation dose dependence. It may be concluded that the electron centres, hole centres and impurity ions take part in the creation and destruction of additional absorption bands in irradiated  $\text{YAlO}_3$  : Nd and  $\text{YAlO}_3$  : Er crystals.

## NEUTRON DIFFRACTION DETERMINATION OF THE STRUCTURE AND MAGNETIC STATES IN THE ANTIFERROMAGNETIC NiO DOPED WITH Li

*A.Menshikov, J.Dorofeev, A.Teplih, B.Gizevski, N.Mironova*

The elastic neutron scattering in ceramic  $\text{Ni}_{1-x}\text{Li}_x\text{O}$  with  $x < 0,1$  solid solutions were studied with neutron diffraction method. At first it is shown, that the incorporation of Li atoms in NiO lattice give the vacancies in the anion sublattice. The concentration of anion vacancies increase with amount of lithium content. The magnetic moment and Neel temperature of NiO - Li decrease with increase of lithium concentration.

## FLUX PINNING IN NEUTRON IRRADIATED 123 HIGH TEMPERATURE SUPERCONDUCTORS AND ITS RELATIONSHIP TO MAGNETIC ANISOTROPY

*A. Petrov*

- 1.The overall contribution of thermal neutron induced Gd--point defects to flux pinning in Gd123- superconductors is small.
- 2.Critical temperature  $T_c$  after pure thermal neutron irradiation remains unchanged within experimental uncertainty in all investigated samples.
- 3.The evaluation of the displacement energy of Gd ions in Gd123- superconductors was done.
- 4.The possible reason of depression of superconductivity after fast neutron irradiation by means of appearance of strongly paramagnetic ions of Gd +3 in "prohibited" sites of the structure is affirming.

### Scientific Publications

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2. P.Prokofjevs, L.I.Simonova, M.Balodis, J.Čerziðð, V.Bondarenko, H.F.Wirth, T.von Egidy, C.Doll, J.Ott, W.Schauer, R.W.Hoff, R.F.Casten, R.L.Gill, J.Honzatko, I.Tomandl, S.Boneva, V.A.Khitrov, A.M.Sukhovej, D.G.Burke, J.Kvasil, A.Mackova, *Nuclear structure of  $^{166}\text{Ho}$  studied in neutron-capture, (d,p), and (d, $^3\text{He}$ ) reactions.* – Phys.Rev. C, vol. 61 (2000) 044305, p.43.
3. J.Döring, Y.A.Akovali, C.Baktash, F.E.Durham, C.J.Gross, P.F.Hua, G.D.Johns, M.Korolija, D.R.LaFosse, I.Y.Lee, A.O.Macchiavelli, W.Rathbun, D.G.Sarantites, D.W.Stracener, G.Z.Solomon, S.L.Tabor, A.Vander Molen, A.V.Afanasjev and I.Ragnarsson, *Band terminations in the valence space of  $^{86}\text{Zr}$ .* – Phys.Rev. C61, 2000, 034310: 1-6.
4. C.M.Petrache, G.Lo Bianco, D.Ward, A.Galindo-Uribarri, P.Spolaore, D.Bazzacco, T.Kröell, S.Lunardi, R.Menegazzo, C.Rossi Alvarez, A.O.Macchiavelli, M.Cromaz, P.Fallon, G.J.Lane, W.Gast, R.M.Lieder, G.Falconi, A.V.Affanasjev and I.Ragnarsson, *Stable triaxiality at the highest spins in  $^{138}\text{Nd}$  and  $^{139}\text{Nd}$ .* – Phys.Rev. C61, 2000, 011305: 1-5 (Rapid Communications).

5. J.F.Smith, C.J.Chicara, D.B.Fossan, G.J.Lane, J.M.Sears, I.Thorslund, H.Amro, C.N.Davids, R.V.F.Janssens, D.Seweryniak, I.M.Hibbert, R.Wadsworth, I.Y.Lee, A.O.Macchiavelli, A.V.Afanasjev and I.Ragnarsson, *Identification of excited states in  $^{119}\text{Ba}$* . – Phys.Rev. C61, 2000, 044329.
6. D.R.LaFosse, C.J.Chicara, D.B.Fossan, G.J.Lane, J.M.Sears, J.F.Smith, K.Starosta, A.J.Boston, E.S.Paul, A.T.Semple, M.Devlin, D.G.Sarantites, I.Y.Lee, A.O.Macchiavelli, A.V.Afanasjev and I.Ragnarsson, *Collective structure and band termination in  $^{107}\text{Sb}$* . – Phys.Rev. C62, 2000, 014305: 1-10.
7. C.Plettner, H.Schnare, R.Schwengner, L.Käubler, F.Döna, I.Ragnarsson, A.V.Afanasjev, A.Algora, G.de Angelis, A.Gadea, D.R.Napoli, J.Eberth, T.Steinhardt, O.Thelen, M.Hausmann, A.Müller, A.Jungclaus, K.P.Lieb, D.G.Jenkins, R.Wadsworth, A.N.Wilson and S.Frauendorf, *Very high rotational frequencies and band termination in  $^{73}\text{Br}$* . – Phys.Rev. C62, 2000, 014313: 1-6.
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  26. N.Mironova, V.Skvortsova, A.Kuzmin, I.Sildos, N.Zazubovich, *Low temperature Optical Absorption by Magnons in KNiF<sub>3</sub> and NiO*. Defects and Surface - Induced Effects in Advanced Perovskites. Ed. G.Borstel et al. 2000, p. 155 - 160.
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  29. S.B.Ubizskii, A.O.Matkovskii, N.A.Mironova, V.Skvortsova, A.Sochocki, Y.A.Zhydachovskii, P.Potera, *Displacements Defects Formation in Complex Oxide Crystals under Irradiation*. Phys. stat. sol. ( a ), **177**, 349 - 366. ( 2000 )
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  32. V.Skvortsova, N.Mironova-Ulmane, U.Ulmanis, A.Matkovskii, *Radiation Effects in Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub> Oxide Crystals*. *ibid* p. 284 - 288.
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35. N.Mironova-Ulmane, V.Skvortsova, A.Kuzmin, I.Sildos, *One - and Two-Magnon Contributions in Optical Spectra of Single-Crystal KNiF<sub>3</sub>*, Ferroelectrics ( in press)
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#### Lectures on Conferences

##### 16<sup>th</sup> Scientific Meeting of institute of Solid state Physics, University of Latvia, Riga, February 14-16, 2000.

- 1 M.Balodis, J.Bçrziòð, N.Krâmere, *<sup>194</sup>Ir spektroskopisks pçtîjums: kâ iegût labâku modelisku izpratni?* – lpp. 57.
2. P.Prokofjevs, L.Simonova, V.Bondarenko, J.Bçrziòð, T.v.Egidy, H.-F.Wirth, A.Metz, V.Eisermann, Graw, R.Hertenberg, I.Rubacek, J.Honzatko, I.Tomandl, *<sup>181</sup>Hf kodolu struktûras pçtîjumi (n,g) un (d,p) reakcijâs*. - lpp. 58.
3. P.Prokofjevs, L.I.Simonova, M.Balodis, J.Bçrziòð, V.Bondarenko, H.F.Wirth, T.von Egidy, C.Doll, J.Ott, W.Schauer, R.W.Hoff, R.F.Casten, R.L.Gill, J.Honzatko, I.Tomandl, S.Boneva, V.A.Khitrov, A.M.Sukhovej, D.G.Burke, J.Kvasil, A.Mackova, *<sup>166</sup>Ho kodolustruktûras pçtîjumi neitronu satverðanas (d,p) un (d,<sup>3</sup>He) reakcijâs*. - lpp. 59.
4. D. Riekstiòda, I. Taure, O. Vçveris, *INAA iespçjas un pielietojums augððu analîzçç*, lpp.84.
5. V.Skvorcova, N.Mironova-Ulmane, A.Matkovskis, S.Ubizskis, *The Radiation Defects in Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> Crystals.*, p. 63.
6. A.Petrovs, I.Kudreòickis, *Magnçtiskâs plûsmas "pinninga" pçtîjumi ar neitroniem apstarotos anizotropiskos augsttemperatûras, 123 struktûras, supravadîtâjos*. – lpp.61.

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7. P.Prokofjevs, L.Simonova, M.Balodis, J.Berzins, V.Bondarenko, H.F.Wirth, T.von Egidy, C.Doll, J.Ott, W.Schauer, R.W.Hoff, R.F.Casten, R.L.Gill, J.Honzatko, I.Tomandl, S.Boneva, V.A.Khitrov, A.M.Sukhovej, D.G.Burke, J.Kvasil, A.Mackova, *Nuclear structure of <sup>166</sup>Ho studied in neutron-capture, (d,p) and (d,<sup>3</sup>He) reactions*. –p.161.
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9. J.Tambergs – report "The analysis of the Unification of Elementary Particle Fundamental Interaction Coupling Constants in Flipped SU(5) String Model"
10. J.Tambergs – report "Binding energies and radii of  $\alpha$ -cluster type nuclei from the strictly restricted dynamics model calculations" at the International nuclear physics conference "Clustering phenomena in nuclear physics".

11. D. Riekstina, N. Mironova-Ulmane, O. Veveris, E. Curbakova, *Study of Chernobyl clean-up workers teeth elemental content changes using instrumental neutron activation analysis*, p. 386.

International Conference Eco – Balt '2000, Riga, 2000

12. D. Riekstiņa, I. Taure, O. Vēveris, *Cs-137 radioaktīvā piesārņojuma sadalījums Latvijas priekšu mežu zemsegā* lpp. 103-104.  
13. A. Skujiņa, S. Puriņa, D. Riekstiņa, V. Bute, *Sr – 90 un Cs-137 noteikšana Rīgas jūras līča paraugos*, lpp. 105-106.  
14. D. Riekstiņa, I. Taure, O. Vēveris, A. Vīksna, J. Katkevičs, *Pētījumi par elementu sadalījumu priekšu dzinuma garumā lietojot daļiņas analīzes metodes* lpp. 107.

Atomic Physics and Spectroscopy Institute at the Faculty of Physics and Mathematics of Latvian University, Rīga, 27 January, 2000

15. J. Ruža -- report “Concept of time in quantum theory”.

Lithuanian Academy of Sciences in memory of prof.V.Vanagas (1930-1990), Vilnius, 28 April, 2000

16. J. Tambergs – report “The Restricted Dynamics Investigations in Last Decade (1990-2000)”.

5th conference of Latvian Physical Society, Daugavpils, 8 June, 2000

17. J. Tambergs – report “Nobel prize in physics in 1999”.

Atomic Physics and Spectroscopy Institute at the Faculty of Physics and Mathematics of Latvian University, Rīga, 19 October, 2000

18. J. Ruža – report “The problem of time symmetry in quantum mechanical measurement process”.

Int. Conf. Mass and Charge Transport in Inorganic Materials. Fundamental to Devices. May 28 - June 2, 2000, Venice, Italy. Abstracts p. 37.

19. V. Skvortsova, N. Mironova – Ulmane, *Single Crystals MeO - MgO Growth and Phase Transformations*.

European Workshop on Individual Monitoring of External Radiation. 4 - 6 September 2000, Helsinki

20. N. Mironova - Ulmane, A. Pavlenko, T. Zvagule, T. Kaerner, *Problems of Absorbed Dose Estimations for Chernobyl Accident Clean-Up Workers*. Abstracts p. 62.

14<sup>th</sup> Intern. Conf. on Defects in Insulating Materials. 3 - 7 April 2000. Johannesburg - Midrand, South. Africa.

21. T. Kaerner, S. Dolgov, A. Luschik, N. Mironova, S. Nakonechnyi, E. Vasilchenko, *High- Temperature Thermoluminescence Manifestations of Anion Interstitials in Neutron Irradiated Pure and Doped Single Crystals of MgO*. Abstracts p. 57.

4<sup>th</sup> Euroconference Luminescent Detectors and Transformers of Ionizing Radiation LUMDETR` 2000 August 14 - 17, 2000, Rīga (Jūrmala), Latvia.

22. T. Kaerner, S. Dolgov, N. Mironova - Ulmane, S. Nakonechnyi, E. Vasilchenko, *Anion Interstitials in Neutron - Irradiated MgO Single Crystals*. Abstracts p. 105.

5-th Euroconference on Application of Polar Dielectrics. August 27 - 30, 2000, Jurmala,

Latvia.

23. N.Mironova - Ulmane, V.Skvortsova, A.Kuzmin, I.Sildos, *One - and Two- Magnon Contributions in Optical Spectra of Single-Crystal KNiF<sub>3</sub>*. Abstracts p. 121.

Spin Waves International Symposium, May 16-19, 2000, St.Peterburg, Russia

24. M.Frischherz, I.Kudrenitskis, A.Petrov, H.Weber, *Thermal Neutron Induced Point Defects in Gd123 Ceramics*. p.14.

International Conference ‘Advances in Modern Natural Sciences’, June 6-9, 2000, Kaluga, Russia

25. A.Petrov, *Magnetism and Magnetic Order in Solids*. p.52

26. A.Petrov, *Magnetism and Magnetic Order in Solids*. (in print).



# **ELECTRONIC ENGINEERING**

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

## **Main Problems**

1. Implement developing and manufacturing of unique measuring and monitoring apparatus and systems, which:
  - provide authorised access on the base of Touch Memory<sup>TM</sup> elements and Proximity Cards to different objects, including
    - ⇒ entrance check-points (entrance gates, access control systems, systems for multilevel parking buildings etc.);
    - ⇒ computers and programmes;
    - ⇒ car and other technical devices (anti-treft systems);
  - execute electronic documentation functions (Touch Memory<sup>TM</sup> -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. I.Gvardina
3. J.Melderis
4. J.Tibergs
5. J.Veinbergs
6. S.Zelenkovs
7. I.Zujevs

### **Cooperation:**

**Latvia:**

1. Joint-stock company *Latvenergo*
2. *Latvijas Krājbanka*
3. *Kokarde Ltd*
4. Latvia Technology Park
5. Riga Technical University
6. Latvian Environment Data Centre
7. Trafik Ltd
8. Sano Ltd
9. GROG Ltd
10. RD Pentano Ltd
11. Apollo AS Ltd

**Denmark:**

DanBalt Electronics

**Estonia:**

OÜ Terg A&K

**Russia:**

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

Lectures on Conferences

16<sup>th</sup> Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2000:

1. A.Kristiðð, G.Matovihs. *Adjustment of temperature in rooms applying heat counters - payment allokators*, Abstracts, p.87.
2. I.Gvardina, A.Kristiðð, J.Melderis, J.Tībergs, J.Veinbergs, I.Zujevs. *Car parking and access control systems*, Abstracts, p.88.

# TESTING LABORATORY

Head of Laboratory *Dr.phys. J.Kiaviðð*

ISSP commenced the evaluation of product conformity assurance since 1996, when the Department of Science of the Ministry of Education and Science rendered support from Market demanded research financing resources for the ISSP in Product testing and quality control pursuant to the requirements of the EU. Some of the staff members of the ISSP participated in the number of projects related to the testing and compliance assurance. Among projects was the establishment of the Testing laboratory (TL). The scope of this project includes a lot of activities. (1) TL preliminary measuring equipment has been supplemented by purchasing several new devices - equipment for determination of the waterproofness of building materials, computerised laboratory and analytical balances etc. (2) The already existing equipment has been repaired. (3) The premises of the laboratory have been repaired and equipped accordingly. (4) In the meantime 7 staff members of the ISSP have completed the training course Preparing the Testing Laboratory Pursuant the Latvian and European Standards , organised by Certification Centre of Latvian Academy of Sciences, some of staff members courses in Germany and England. (5) The quality system has been implemented in the laboratory. (6) TL is operating and currently performs testing according to 6 standard methods. New methods are being acquired.

On January 12, 2001 Latvian National Accreditation Office (LATAK) completed the accreditation of the Testing Laboratory at the Institute of Solid State Physics. It means that the quality system of one of the Institute units is recognized as comformit to international standard LVS EN 45001.

All the ISSP TL spheres applied for accreditation were accredited. They are: (1) concrete watertightness; (2) adhesion and cohesion of adhesives of ceramic linings; (3) release of lead and cadmium from enamelled metallic ware, (4) from ceramic ware, glass – ceramic ware, glass dinner ware, (5) glass hollow ware and (6) ceramic cookware subjected to heating and as in 3, 4, 5, 6 in contact with food.

The activity spheres of the Testing Laboratory will be extended. We've started the testing of water content, water absorbtion, water and vapour permeability and density of building materials. In cooperation with joint stock company *Valmieras stikla ðüedra* we develop the testing of glass fibre and its products' breaking force and chemical resistance.

Test methods and corresponding standards in the scope of accreditation are:

1. Testing hardened concrete. Depth of penetration of water under pressure. PrEN 12364:1996
2. Testing of adhesives for ceramic linings; testing of the deformation of bondings; dispersion adhesives. DIN 53265:1988
3. Ceramic ware, glass-ceramic ware and glass dinnerware in contact with food. Release of lead and cadmium. Part 1: Test method. ISO 6486-1: 1999
4. Vitreous and porcelain enamels. Release of lead and cadmium from enamelled ware in contact with food. Part 1: Method of test. ISO 4531-1: 1998
5. Glass hollowware in contact with food. Release of lead and cadmium. Part 1: Test method. ISO 7086-1: 2000
6. Ceramic cookware in contact with food. Release of lead and cadmium.

Part 1: Method of test. ISO 8391/1 - 1986

Currently not accredited test methods:

1. Floorings. Testing of watertightness. SIS 923511:1974
2. Ceramic tiles - Part 3: Determination of water absorption, apparent porosity, apparent relative density and bulk density. ISO 10545-3: 1995
3. Testing hardened concrete - Part 7: Density of hardened concrete. PrEN 12390-7:1999
4. Testing concrete. Testing of hardened concrete. DIN 1048: 1991
5. Hydrothermal performance of building materials and products – Determination of moisture content by drying at elevated temperature. ISO 12570:2000
6. Thermal insulation products for building applications - Determination of the mechanical properties of glass fibre meshes. PrEN 13496: 1999

Staff:

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

Support Staff:

1. Dr. V.Eglītis
2. Dr.hab. M.Spriððis

Cooperation

1. Latvian National Accreditation Bureau LATAK
2. Latvian Association of Testing Laboratories
3. Certification Center of Latvian Academy of Sciences
4. Testing Laboratory of fresh and hardened concrete of “Kalnozols Building”, Ltd

Publications Published in 2000

1.J.Kiaviðð, M.Spriððis, J.Pinnis, *Testing of Water Transmission and Absorption in Building Materials* – Publications of the Research-Practical Workshop “Thermal performance of the Building`s Envelope”, Riga, March 16-17, 2000, p.17-1 – 17-8.

Lectures on Conferences and Seminars

16th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, February 14-16, 2000.

1.U.Kanders, J.Kiaviðð, I.Viksna, N.Zeltiðð, *Remote Heat Loss Diagnostics Using Thermographic Measurements*. Abstracts, p.91, (oral presentation).

Research-Practical Workshop “Thermal performance of the Building`s Envelope”, Riga, March 16-17, 2000, p.17-1 – 17-8.

2.J.Kiaviðð, M.Spriððis, J.Pinnis, *Testing of Water Transmission and Absorption in Building Materials*, (oral presentation).

Workshop “Energy Audits of Buildings”, Ministry of Environmental Protection and Regional Development of LR, Dep.Building, Riga, April, 19, 2000.

3.J.Kiaviõð, *Practical experience in accounting of energy, in analysing of results and in increasing of energy efficiency of buildings*, (oral presentation).

#### Tests Performed

42 tests were performed in 2000.

## **ORGANIZED CONFERENCES**

### **16th Conference of Institute of Solid State Physics, University of Latvia**

**Riga, February 14-16, 2000**

The Conference of the ISSP, an annual event, takes place at the Institute of Solid State Physics in February.

The 16th Conference worked in 6 sections:

- structure and phase transitions (15 reports),
- non-linear optical properties and problems in optometry (13 reports),
- optical spectroscopy and luminescence (14 reports),
- materials and applications (12 reports),
- nuclear reactions and radiation physics (11 reports),
- solid state electronics and ionics (10 reports).

Alltogether 66 reports each lasting 15 minutes were read. Besides the ISSP and the Department of Optometry, the Faculty of Physics and Mathematics, the representatives of Riga Technical University and Institute of Inorganic Chemistry participated in the Conference.

The aim of the Conference was to inform the physicists in Latvia about the most important results during the last year.

The abstracts of the scientific part of the Conference were published in the Latvian and English languages and offered to the participants before the meeting.

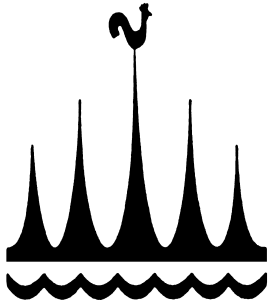
Conference chairman  
Prof. A.Krumins

THE 5<sup>th</sup> EUROCONFERENCE  
ON APPLICATION OF POLAR DIELECTRICS

*ECAPD – 5*

**August 27-30, 2000,**

**Jurmala, Latvia**



Supported by

**the European Commission**

Research D 6, Human Potential Programme

Contract No HPCF – CT – 1999 – 00085

Gordon and Breach Science Publishers

Latvian Council of Science

The 5<sup>th</sup> Euroconference on Application of Polar Dielectrics was organized by the Institute of Solid State Physics, University of Latvia. The Conference continued the series of ECAPD, previously held in Switzerland (Zurich 1988), UK (London 1992), Slovenia (Bled 1996), again Switzerland (Moutreux 1998) and finally Latvia (Jurmala 2000).

ECAPD –5 provided an interdisciplinary forum for the presentation of the most recent development in polar dielectric materials research, basic research of device oriented physical properties, device research and processing technologies. There were 80 registered participants in ECAPD-5 from 21 different countries. The scientific program included 17 invited presentations, 47 oral contributions and 57 posters in 10 sessions. During the Conference 72 manuscripts were submitted for Proceedings and reviewed. The Proceedings will be published in two separate volumes of the international journal *Ferroelectrics*.

Prof. A. Krumins  
Chairman of ECAPD-5



## Introduction/Background

Computer simulation is now having a major impact on almost all areas of physical, biological and engineering sciences. One of the most significant and successful areas of application of computer modelling techniques has been in materials science, especially relating to understanding and predicting the structures and properties of complex materials at the atomic level, and increasingly at the mesoscopic level. The excitement and impact of the field continues to grow with the constant expansion in computer power and with the development of new techniques and algorithms. Computational materials science is also having a growing impact on applied and industrial science, ranging from electronics to catalysis. The expansion and diversification of the field makes it necessary and timely to hold an Advanced Study Institute, which will survey both fundamental and applied aspects of the field and will look to future developments and opportunities. No NATO school has been held in this or a closely related field for several years, making the proposed ASI particularly timely.

The school will provide a comprehensive survey of atomistic modelling of materials and of the link between micro- and meso-scale modelling. It will have three major components:

- **Fundamentals**, which will survey the essential techniques, including electronic structure methods (Density Functional Theory; Hartree-Fock methods; tight binding methodologies) and interatomic potential (or forcefield) based methods (including minimization, Monte Carlo and Molecular Dynamics methods).
- **Applications**, which will describe the different classes of simulation, including: Crystal structure, modelling and prediction; simulation of defects (including point, line and plane defects) and diffusion; modelling of amorphous materials; simulation of phase transitions; calculation of mechanical properties; models of surface and interface structures, properties and reactivities.
- **Systems**, which will explore the use of modelling methodologies in the main classes of materials, including metals/alloys; semiconductors; ceramic/ionic materials; silicate/phosphate systems; molecular materials and polymers. Strong emphasis will be given to systems of industrial importance.

The above topics will be covered by lectures (followed by discussion) supported by workshops. The latter format will be used to introduce and discuss the increasingly important area of mesoscopic modelling and its interaction with atomistic techniques. Special seminars will highlight key contemporary application areas such as colossal magneto resistance, new catalytic materials and mantle minerals.



The field is an interdisciplinary one. The lectures and topics have been chosen to reflect the contributions to the field of different areas of physics, chemistry and materials science. The field is active worldwide and the school will offer a good opportunity for interaction between lectures and participants from NATO and partner countries. The school will therefore provide a balanced overview of this exciting and growing field. The resulting publication will provide a definitive, up-to-date survey of the field.

## **Directors**

[Professor C.R.A. Catlow](#), The Royal Institution of Great Britain, 21 Albermarle St., London W1X 4BS, UK

[Professor E.A. Kotomin](#), Institute of Solid State Physics, University of Latvia, 8 Kengara Str., Riga LV--1063 LATVIA

## **Scientific Organizing Committee**

**Professor I. Abarenkov**, St. Petersburg University, St. Petersburg, Russia

[Professor A.N. Cormack](#), NYSCC at Alfred University, Alfred, NY, USA

**Professor S. Yip**, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

## **Lecturers**

Dr. V. Antonov, Institute of Metal Physics, Kiev, Ukraine

Professor P. Deak, Technology University, Budapest, Hungary

Dr. R. Dovesi, University of Turin, Italy

Professor R.A. Evarestov, St. Petersburg University, Russia

Dr. N. Harrison, Daresbury Lab, UK

Professor F. Illas, University of Barcelona, Spain

Dr. A.I. Milchev, Bulgarian Academy of Sciences, Sofia, Bulgaria

Professor C. Noguerra, Université Paris-Sud, France

Professor A.V. Postnikov, Institute of Metal Physics, Yekaterinburg, Russia

Dr. D. Wolf, Argonne National Lab, USA  
Dr. G.M. Zhidimirov, Institute of Catalysis, Novosibirsk, Russia

To view programme timetable and organization, [click here](#).

### **Registration Information**

**For more information, please contact:**

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## First Announcement

### First Regional Seminar on Solid State Ionics, (RS-SSI)

to be held in Jurmala, Latvia, 22-26 September, 2001

#### Related conferences:

- XII Russian Conference on Solid State Electrolytes, Nalchik (Georgia), September 17-23, 2001
- Baltic Conference "Materials Engineering&Balttrip 2001", Jurmala (Latvia), September 27-28, 2001

**Oct 28-Nov 2, 2001.** Lake Louise, Canada [3rd Int. Conf. on Composites](#)

Details from: [Pat. Nicholson, McMaster University](#)

#### Dear Colleague!

Solid State Ionics is based on the phenomena of ion insertion/extraction and fast ion transport in solids, which is comparable to that of liquid electrolytes. These phenomena offer many opportunities for new technologies – light (solar) and thermal radiation intensity control, information display and storage, renewable energy, energy conversion and storage, sensorics and battery cells.

In the University of Latvia researches in the field of Solid State Ionics started on 1972, but the first All-Union (USSR) seminar (in those times – Vsesojuznij Seminar Joniki Tverdovo Tela) was firstly organised in Riga on 1981. During next ten years this Seminar was organised every year, and Riga appeared strongest centre in previous USSR of investigations of electrochromic materials (transition metal oxides with mixed – ion and electron – conductivity and solid electrolytes) and devices. It is important for us to renew the tradition from Soviet times: to organise an annual seminars on Solid State Ionics in Riga like it was in years 1981-1990

The aim of Regional seminar is to get together researchers, engineers and users from Baltic region for presentation state of art in SSI and discussion. An interchange of information and dissemination of knowledge about new fast ion conducting materials and their properties will give additional stimulus in development of new applications (batteries, ion/gas pumps, chemical and electrochemical sensors, fuel cells)..

Jurmala, literally "the seaside", is a cluster of former fishing villages along the southern shores of the Gulf of Riga, some 25 km from the capital of Latvia Riga (established in 1201). The seaside resort is a favourite summer place for residents and guests of Riga. Pine tree wood, fresh air, the calm flow of the river, and the golden sandy beaches provide the finest conditions for enjoyment of nature, relaxation and creative work.

**The following topics will be intensively discussed:**

- A. Solid electrolytes and intercalation electrodes
- B. Sensors
- C. Electrochromics
- D. Fuel and Hydrolysis Cells
- E. Batteries
- F. Supercapacitors
- G. Electrochemically Promoted Solid State Reactions
- H. Functional coatings and new technologies
- I. Other Applications

### **International Advisory Board:**

Nadjezda Bukun (Chernogolovka, Russia)  
Edwards Peter (University of Birmingham, United Kingdom)  
Czerwinski Andrzej (Warsaw University, Poland)  
Granquist Claes-Goran (Uppsala University, Sweden)  
Lusis Andrejs (University of Latvia, Latvia)  
Murin, Igor V. (University of St.Petersburg, Russia)  
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Orliukas Antanas (University of Vilnius, Lithuania)  
Scholz Fritz (University of Greifswald, Germany)  
Weppner Werner (Kiehl, Germany)

### **Local organizing committee:**

1. A. Lusis - Chairman
2. J. Kleperis - Secretary
3. G. Vaivars
4. A. Vitins
5. A. Jozepa
6. J. Grabis
7. E. Serdiene
8. R. Siatkovskis

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Please, complete [Application form](#) and return to facilitate the planning of the RS-SSI