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Final report

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Project title: ***Excellence Centre of Advanced Material Research and Technology at the Institute of Solid State Physics, University of Latvia***

Acronym: CAMART

Key words:
materials, technology, research

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Executive summary

The objectives of the project

The ultimate goal of the planned package of measures was to contribute to restructuring of the science and technology sector of Latvia by putting the capabilities of the Institute of Solid State Physics of the University of Latvia (ISSP) better to the service of the economic and social needs of the region, in conformity with the development priorities of Latvia and the European Union.

Material science is one of five scientific priorities in Latvia, however the national support is small. Development of Centre of Excellence will contribute to restructuring the Material Science and Technology sector of industry, by implementing new materials (in particular, with predicted characteristics) and technologies for optics, microelectronics and vision science. The aims of the Centre were approached via attracting talanted young researchers, enhanced exchange of scientific and technological information and know-how (workshops, conferences, work visits) and networking the Centre with other European research centres of the analogous profile. Aditional goal is enhanced participation of Centre in other areas of the 5^{th} and 6^{th} Framework Programme.

The objectives of Centre match with the following priorities of the 5^{th} Framework Programme:

1.1.2. – 4.8.4. Advanced optoelectronics and microelectronics;

1.1.3. – 5.2. Advanced functional materials.

The Centre endevoured to develop the following thematic objectives (fig.1)

- computer modelling of the advanced materials, exspecially ABO_3 type perovskites and catalytic surface reactions;
- development of functional disordered materials for radiation energy detectors and photonics;
- development advanced ferroelectric materials for memory and electrooptic applications;
- new materials and devices for vision science;
- new materials and devices with ionic conductivity.

All these objectives have been really advanced during the work on the project.

Activities and methodologies

Different, often complementary methods of modern theoretical and experimental physics have been applied during the work on the project. Theoretical includes ab inito methods of the atomic and electronic structure calculations, semi-empirical methods of quantum chemistry as well as kinetic Monte Carlo and celluar automata techiques. Experimental modern optical, electrical, photoelectrical as well as structural methods were used, including scanning point microscopy, optical and electron spectroscopy, EPR spectroscopy. In particular ceramic technology, including hot pressing, crystal growth as well as laser ablation and CVD methods were used to create the thin film objects.

All kinds of activities (conventional tokens V 1-3, VR, WS, CF), foreseen by the EC, have been implemented.

The activities were organized by 27 work packages, divided in 5 Networks (see Fig.1). In the following, the major results are presented as a short summary for each Network.

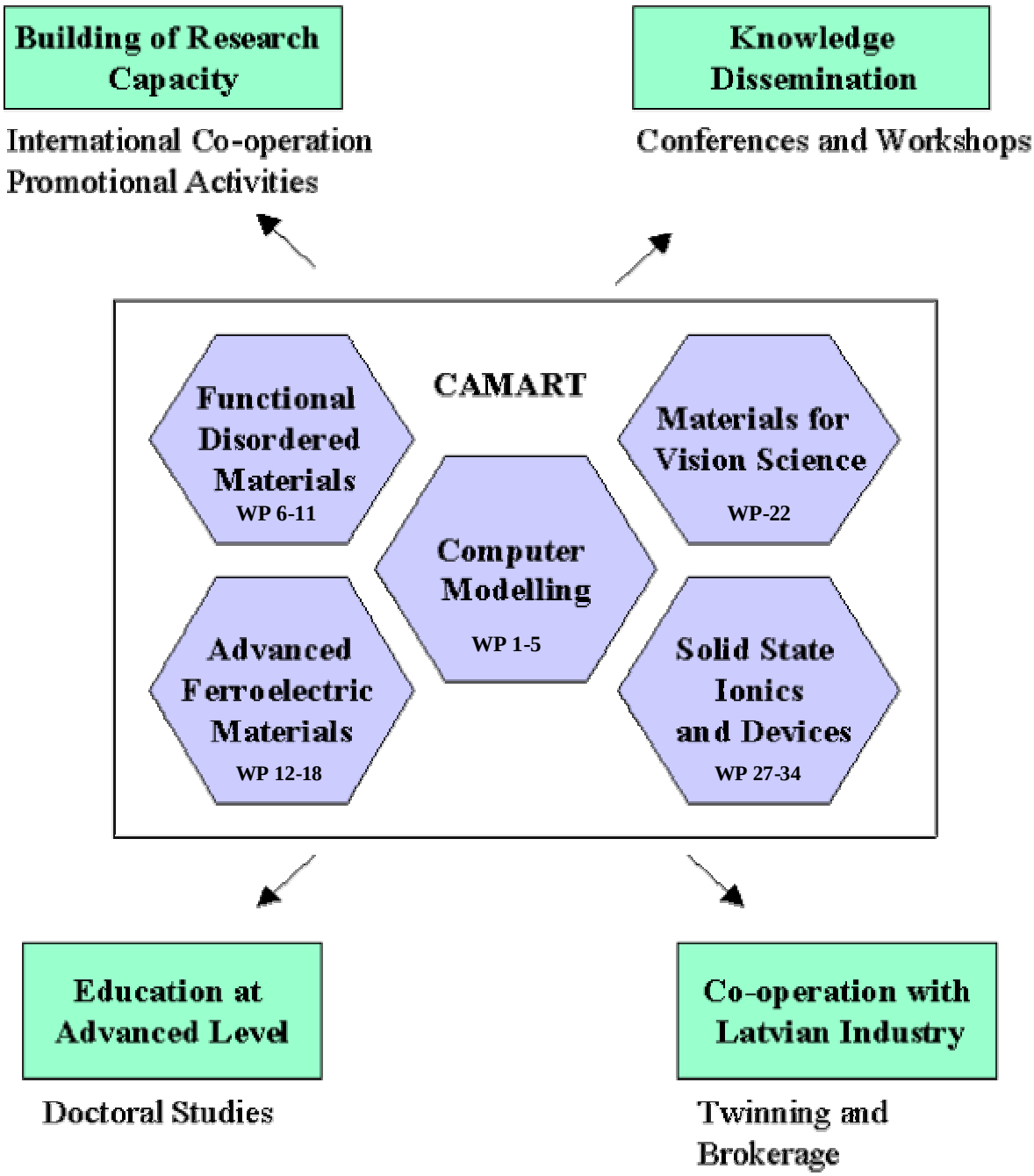

Fig.1. Main activities of CAMART project

Major results obtained and their applications

Network 1. WP 1-5

Computer Modelling of the Advanced Materials (Prof. Dr.E.Kotomin)

We performed large-scale first principles and quantum chemical calculations using parallel computing for a number of perovskite materials, including $SrTiO_3$, $BaTiO_3$, $KNbO_3$, $KTaO_3$, $LaMnO_3$ and their solid solutions, widely used in technological applications. In these materials we modelled O vacancies (*F* type centers), electron and hole polarons, common metal impurities (e.g., Fe) and hydrogen, with a special emphasis on the calculation of defect optical properties. We used these results for identification of basic defects in these materials studied experimentally.

Another activity was focused on the quantum effects in nanoscopically thin perovskite films. For this purpose, we modelled different types of surfaces (neutral 100 and polar 110) with emphasis on near-surface atomic relaxation and reconstruction, formation of surface defects, surface-induced polarization and ferroelectric properties. Quality of these surfaces are extremely important for many applications, e.g. for catalysis and a growth of qualitative high-T_c superconductors. We have established the energetically most stable surfaces and suggested their reconstruction. We predicted increase of a chemical bond covalency near polar surfaces, which is important for the applications in catalysis and fuel cells.

At the next stage, we studied diffusion-controlled defect processes. In particular, we performed large-scale modelling and developed the first *atomistic model* of primary defect aggregation and the metal colloid formation process in insulating solids exposed to irradiation. This opens the way to many important technological applications including safe disposal of radiactive waiste, effective ion implantation, and stability of prospective materials for the first wall of neutron reactors**.**

We have got also a sound understanding of essential processes for the surface reconstruction in catalytic surface reactions on single crystal surfaces. Our theory explains the most important experimental phenomena. As a result of comprehensive computer simulations and theoretical analysis, we described the atomistic mechanisms of initial low-temperature oxidation of Al and Mg as well as formation of metallic coatings on various surfaces of alumina and magnesium oxide.

Network 2. WP 6-11; WP-19

Functional Disordered Materials (Prof. Dr.L.Skuja)

Materials for scintillators for applications in environmental monitoring, medical X-ray and positron emission imaging, neutron and UV dosimetry, based on tungstate, nitride and fluoride compounds were developed and the physical processes in these materials were elucidated. High performance glasses for deep UV and high-power laser optics were studied and the relations between their performance and synthesis parameters established. A solid immersion holographic technique for recording refractive and surface-relief based regular nanostructures in chalcogenide semiconductor films for information storage. Phenomena in nonlinear niobate and titanate crystals, which are detrimental to

optoelectronic applications of these materials, were studied and ways of their improvement were elaborated. Infrastructure for producing advanced thin films by metal-organic molecular vapor deposition was developed and instrumentation for their analysis was constructed.

Network 3. WP 12-18

Advanced ferroelectric materials (Prof. Dr.A.Krumins)

Ferroelectric ceramics and thin films represent a fascinating and challenging class of materials. Along with the revolutionary development of electronics and optoelectronics, integrated devices in areas such as information technology as well as transducer technology are introduced.

The diffused phase transitions and structure peculiarities of complex lead – containing perovskite oxides with the chemical formula $Pb(B^{1}_{1/2}\ Nb^{11}_{1/2})_3$ are studied, where B^{1} – rare-earth elements (Lu, Yb, Tm, Er). Due to ferroelectric – antiferroelectric character of dipole ordering special piezoelectric properties have been obtained.

The nonequilibrium thermodynamics approach was applied to multicomponent dielectrics in presence of paraelectric – ferroelectric phase instability. It was possible to describe theoretically hysteresis, polarization swithing and finite size effects.

Experimental studies of the size effects with regard to material composition-deposition related parameters and obtained structure-property relationships were carried out in thin ferroelectric films and heterostructures. Compounds under investigation included highly oriented perovskite structure PZ, PZT, PLZT, PMNT, $(Ba,Sr)TiO_3$, PLuNT and other thin films of various compositions formed by rf sputtering, pulsed laser ablation and by the sol-gel process.

Propogation and scattering of electromagnetic radiation in electrooptic PLZT ceramics is described theoretically and studied experimentally. Devices for controlling the coherent and incoherent light transmittance were designed. Solid state pulsed medical laser systems emitting radiation in the midinfared spectral region (2-3 μ) were development, using in these systems pasive and active elements of PLZT ceramics.

Network 4. WP 22

Materials for vision science (Prof. Dr.Ozolinsh)

Experimental studies of the newest optical materials and lenses usable for vision correction devices. Model studies of the optical system eye+corrective element for evaluation of the human adaptation ability to different geometry construction of the vision correction devices and influence of unfavourable environmental and physiological factors on visual performance.

New electrophysiology equipment “Neurosoft” to measure electrical brain response of visual stimuli was set up and approved

Network 5. WP 27-34

Solid state ionics and devices (Dr.A.Lusis)

In-situ X-ray absorbtion studies of transition metal oxides (WO_3, NiO, IrO_2) thin films have been performed. It was observed that a nanocrystallinity of the thin films results in strong modification of the Ni-O and W-O interactions, which affect both local atomic and vibration structures.

Development of new experimental techniques for nanomaterials investigation via combination of Scanning Probe Microscopies and Scanning Near-field Optical Microscopy with XAS were started in strong collaboration with scientist from other EU countries.

The catalytic properties of hydrogen injection phenomena in tungsten trioxide (hydrogen storage media) were studied. The model for performance of thin film electrochromic cells was developed. New knowledge and experience in preparation of electrodes and solid electrolytes for ionic devices (batteries, capacitors, sensors).

Different application technologies for electronic nose are developed based on food control and the tests of goods in customs. The test bench of sensors is elaborated and new method developed for gas sensor calibration.

Activity report

The data are provided by Networks of work packages (Fig.1)

Network 1, WP 1-5

Computer Modelling of the Advanced Materials (Prof. Dr.E.Kotomins)

Visitors

Prof. A. Lushchik, Tartu University, Estonia (1-31 May, 2001), „The Kinetics of Metal Colloid Formation under Irradiation of Prospective Materials“
Ph.D. student B. Herschend, Uppsala University, Sweden (2-31 May,2001), „Self-Organization in Surface Catalytic Reaction“
Prof. K. Hermansson, Uppsala University, Sweden (7 May-4 June, 2001), „First Principles Modelling of Metal Oxidation and Corrosion“
Ph.D student S. Piskunovs (Osnabrueck University, Germany, 1 July-31 August, 2001), “Defects and Surfaces of Advances Perovskites“
Ph.D student B. Herschend, Uppsala University, Sweden (29 August – 28 September, 2001), „Self Organization in Surface Catalytic Reaction“
Prof. Ch. Lushchik, Tartu University, Estonia (1-31 October, 2001), „Defect Properties of Prospective Oxide and Halide Materials“
Prof. Dr. K. Schwartz (GSI, Darmstadt, Germany, 15 January--14 February, 2002), „The Kinetics of Metal Colloid Formation under Irradiation of Prospective Materials“
Dr. T. Jansen, Eindhoven University, the Netherlands (18 March – 16 April, 2002), „Self-Organization in Surface Catalytic Reaction“
Dr. R. Salazar Tio, Eindhoven University, the Netherlands (20 March – 19 April, 2002), „First Principles Modelling of Metal Oxidation and Corrosion“
Prof. V. Fomin (Antwerpen University, Belgium, 4 August--3 September, 2002), „Defect Properties of Prospective Oxide and Halide Materials“
Prof. S. Dorfman (Technion, Haifa, Israel, 16 November - 15 December, 2002), “Defects and Surfaces of Advances Perovskites“
Prof. O. Dumbrajs (Helsinki University of Technology, Espoo, Finland, 15 March - 14 April, 2003), „Self-Organization in Surface Catalytic Reaction“
Prof. F. Illas (University of Barcelona, Spain, 13 June - 12 July, 2003), „First Principles Modelling of Metal Oxidation and Corrosion“
Prof. R. González (University of Carlos III, Madrid, Spain, 15 June - 14 July, 2003), “Defects and Surfaces of Advances Perovskites“
Prof. C. Wilkinson (King's College London, UK, 12 October-11 November, 2003), „Defect Properties of Prospective Oxide and Halide Materials“
Prof. V.A. Trepakov (Institute of Physics, Charles' University, Prague, Czech Republic, 21 November - 20 December, 2003), „The Kinetics of Metal Colloid Formation under Irradiation of Prospective Materials“

Visits

MS student V. Kashcheyevs (Oslo University, Norway, 3 short visits to the Graduate Course during February-June,2001), „The Kinetics of Metal Colloid Formation under Irradiation of Prospective Materials“

Prof. V.N. Kuzovkov (Eindhoven University, The Netherlands, 1-30 June,2001), „Self-Organization in Surface Catalytic Reaction“
Dr Yu.F. Zhukovskii (Uppsala University, Sweden, 5 June –2 July, 2001), „First Principles Modelling of Metal Oxidation and Corrosion“
Dr. Yu.F. Zhukovskii, Max Planck Institute für Festkörperforschung, Stuttgart, Germany (March 2002), „Self-Organization in Surface Catalytic Reaction“
Dr. A.I. Popov, Institute of Laue and Langevin, Grenoble, France (April, 2002), “Defects and Surfaces of Advances Perovskites“
Prof. Dr. E.A. Kotomin, Max Planck Institut für Festkörperforschung, Stuttgart, Germany (1-30 July, 2002), „The Kinetics of Metal Colloid Formation under Irradiation of Prospective Materials“
Prof. Dr. V.N. Kuzovkov, Fachbereich Physik, Osnabrück Universität, Germany (15 January – 14 February, 2003), „Self-Organization in Surface Catalytic Reaction“
Dr. Yu.F. Zhukovskii, Fachbereich Physik, Osnabrück Universität, Germany (1-30 April, 2003), „Defect Properties of Prospective Oxide and Halide Materials“
Prof. Dr. E.A. Kotomin, Max Planck Institut für Festkörperforschung, Stuttgart, Germany (1-31 May, 2003), “Defects and Surfaces of Advances Perovskites“

Network 2. WP 6 - 11; WP –19

Functional Disordered Materials (Prof.Dr.L.Skuja)

Visitors

Dr.h. H.-J. Fitting, Univ. of Rostock, Germany, 01.06-30.06 2001. Investigation of EPR and optical characteristics of GaN films: Light absorption spectra; photoluminescence excitation spectra. Impurity – related phenomena: photoluminescence(PL) and cathodoluminescence (CL) spectra.

Dr.h. S.Jursenas, Inst. Material Sci. & Applied Res., Vilnius Univ. Lithuania, 07.07-05.08.2003. Lectures/ Workplan for spectroscopy of InGaN multi quantum well structures).

Dr. J. Rosa, Inst. of Phys. Czech. Acad.Sci, Praha, Czech Rep., 05.03-03.04,2004 Joint research: defect spectroscopy of CVD diamond grown in Czech. Acad. Sci.

Dr. J. Rosa, Inst. of Phys. Czech Acad Sci,Praha,Czech Rep., 01.06-30.06.2001. Joint research: defect spectroscopy of CVD diamond grown in Czech. Acad. Sci. Lectures/ exchange of the experience in investigation of d-group elements in wide gap materials. Agreement for the joint research with IP of Czech Academy of science.

Dr.h. S. Zazubovits, Inst. of Phys. Estonian Acad. Sci, Tartu, Estonia, 20.05-18.06. 2002. Lectures/ Research Spectroscopy of $CsPbX_3$ nanocrystalline quantum dots in CsX:Pb.

Dr. J. Rosa, Inst. of Phys. Czech. Acad.Sci, Praha, Czech Rep, 30.05-29.06.2003; 19.07-17.08.2003. . Joint research. Trapping defect spectroscopy studies of CVD diamond films.

Prof. J. Bok, Charles University, Praha, Czech Republic, 20.01.2001 -20.02.2001. Software design for time-resolved luminescence measuring.

Dr. V. Nagirny, Institute of Physics, University of Tartu, Tartu, Estonia, 08.10.-05.11.2002. Influence of impurities on $ZnWO_4$ scintillation efficiency.

Ph.D. student K. Lenguel, Inst. for Solid State Physics and Optics (Centre of Excellence KFKI), Hungarian Academy of Sciences, Budapest, Hungary, 18.03. – 17.04.2002. Study of luminescence of $LiNbO_3$:OH.

Prof. G. Corrady, Institute for Solid State Physics and Optics (Centre of Excellence KFKI), Hungarian Academy of Sciences, Budapest, Hungary, 26.08-24.09.2002. Free and bound polaron states formation in LiNbO3.

Dr. P.Hlidek, Charles University, Praha, Czech Republic, 07.01 -05.02.2002. Study of narrow-band scintillators based on CdZnTe compounds.

Ph.D. student P. Potera, Institute of Physics, University or Rzeszow, Poland, 2 visits, 15.01 – 13.02.2001 and 11.11 – 10.12.2002. A study of novel single-crystal GaGd garnet scintillators.

Dr. A.Watterich, Inst. for Solid State Physics and Optics (Centre of Excellence KFKI), Hungarian Academy of Sciences, Budapest, Hungary, 21.10-20.11.2002. Electronic processes in tungstate single crystals ($ZnWO_4$, $CdWO_4$).

Dr. M. Cannas, University of Palermo, Italy, 12.06 – 12.07.2001. Spectroscopic studies of point defects in oxide glasses.Vacuum ultraviolet studies of oxygen-deficiency-related defect centers in silica glasses.

Dr. B. Poumellec, Universite Paris Sud, Orsay, France, 12.05-20.05.2002. Study of mechanisms of photoinduced Bragg grating formation in oxide glasses.

Dr. B. Güttler, Physikalisch-Technische Bundesanstalt Braunschweig, Germany, 07.09-13.09.2002. Raman and infrared emission techniques for detection of molecular oxygen species in glassy silicon dioxide and related materials.

M.Sc. Agnieszka Opalinska, Warsaw University of Technology, Faculty of Materials Science and Engineering 27.01-26.02 2003. Luminescence of ZrO_2 nanocrystals: size dependent effects.

Dr. S. Agnello, University of Palermo, Italy, 08.07 -07.08.2003. Native and radiation-induced point defects in pure and doped silica glasses.

Dr. phys. Alfonsas Peckus, Institute of Physics, Vilnius, Lithuania – December 17.12.2001 - 24.01.2002. Holographic recording in amorphous semiconductor films

Prof. M. Reichling, Ludwigs-Maximillian University, München, Germany; 13.11.-13.12.2002. Spectral characterization of wide band gap materials: alkali earth fluorides, aluminium nitride, and calcium fluoride.

Prof. R.Tomasiunas, Vilnius University, Lithuania; 27.10- 27.11.2004. Spectral studies of boron nitride and its modifications.

Visits

M.Sc. L. Dimitrochenko, (to AIXTRON, Germany) 29.07-08.08.2002. Enchancement of scientific competence for nitride thin film growth.

Dr.h. V. Ziraps (to Techn. Hochschule Aachen, Germany) 21.07-27.07.2002. Consultations on nitride thin film deep level spectroscopy.

M.Sc. M. Piesins, (to Berlin, Germany).07.07-17.07.2003. Consultations on the deep level transient spectroscopy of wide gap semiconductors at Techn. Hochschule Berlin.

Dr.h. I.Tale (to Univ. Vilnius, Lithuania) 26.04-28.04.2004. Consultations on joint research programme in optical and electrical characterization of GaInN quantum well and quantum dot structures.

Dr.h. I.Tale (to Univ. Rostock, Univ. Paderborn, Univ. Erlangen) 16.09-09.10.2004. Consultations on joint research programme in optical and electrical investigation of new AlGaN, AlN-BN and BN nanostructured materials.
Dr.hab. B. Berzina (to Lisbon, Portugal).) 01.09.-09.09.2001. Spectroscopic studies of ceramic dosimetric AlN materials.
Dr.h. I.Tale (to Univ. Rostock, Germany). 03.12-19.12.2003. Research. Time-resolved spectroscopy of thin ZnO films, grown in ISSP.
Dr.h. U. Rogulis, Dr. M. Springis, A. Sarakovskis (to Prague, Czech. Rep). 01.09-05.09.2003. Participation in International Conference on Luminescent detectors & Transformers.
Dr.h. I.Tale (to Wienna, Austria) 19.11-23.11.2003. Consultations and Seminar in Atomic Institute of Austrian Universities (Atominstitut der Österreichischen Universitäten) on development of Li- based slow neutron imaging materials.
Dr.h. I. Tale (to Univ. Erlangen, TU Munich, Germany) 05.11-24.11.2004. Lecture/ Preparation of collaboration on investigation of nanostructured radiation imaging and wide-gap semiconductor functional structures.
Dr.h. L. Grigorjeva 6-th European Conference on Applications of Polar Dielectrics, Aveiro, Portugal, (02.09-05.09.2002); Dr.habil.phys. D.Millers EMRS Fall Meeting, Warsaw, Poland, (14.09-18.09.2002); Dr.h. L.Grigorjeva International Conference LUMDETR03, Prague, Czech Rep., (01.09-05.09.2003);
Dr. habil. phys. L. Grigorjeva to the Institute of Physics, Charles University, Praha, Czech Republic (04.04 - 03.05.2002) Infrared Fourier transform spectroscopy of $LiNBO_3$:OH.
Dr. habil. phys. D. Millers, to the European Material Research Society (EMRS) Fall Meeting, Warsaw, Poland, (06.09-10.09.2004).
Prof. A. Silins, to XIX International Congress on Glass, Edinburgh, England, (02.07-06.07.2001).
Prof. A. Silins, 6th European Glass Society (ESG) Conference Montpellier, France, (02.06-06.06.2002).
Dr. A. Truhin, Internat. Conf. on Luminescent Dosimetry (LUMDETR) Prague, Czech Republic, (31.08-08.09.2003).
Dr. L. Skuja X International Conference on the Physics of Non-Crystalline Solids, Parma, Italy, (13.07-17.07.2003).
Dr. J. Teteris, to 19^{th} Nordic Semiconductor Meeting, 20.05-23.05.2001, Copenhagen, Denmark
Dr. J. Teteris, to 19^{th} International Conference on Amorphous and Microcrystalline Semiconductors, (27.08-31.08.2001), Nice, France.
Dr. J.Maniks - International Conference NANO-7 and ECOSS-21, (24.06-28.06.2002), Malmo, Sweden.
Dr. J.Teteris – XIIIth International Symposium on Non-oxide Glasses and New Optical Glasses**,** (09.09-13.09.2002), Pardubice, Czech Republic.
Dr. J. Maniks - European Materials Research Society Fall Meeting. Symposium "Interfacial Effects and Novel Properties in Nanomaterials" and Workshop of the Network "NANO-structured Materials",Warsaw, Poland, September (14.09-18.09.2002).
Dr. J. Teteris – Int. Conf. Northern Optics 2003. (16.06-18.06.2003) June, Espoo, Finland.
Dr.J.Teteris – ICO Topical Meeting on Polarization Optics (30.06- 03.07.2003), Joensuu, Finland.

Dr. I. Manika - VIII International Conference "Hydrogen Materials Science and Chemistry of Carbon Nanomaterials (ICHMS'2003)", Crimea, Ukraine, (14.09-20.09.2003).
Dr. M. Reinfelde - The 20th Nordic Semiconductor Meeting, (25.08-27.08.2003), Tampere, Finland.
J. Teteris - International Conference on Diffractive Optics 2003, Oxford, (17.09-20.09.2003), United Kingdom.
Dr. B. Berzina (Ludwigs-Maximillian University, München, Germany; 17.07.-07.08.02.), Peculiarities of oxygen-related defect structures in CaF_2 crystals for heavy-duty vacuum UV laser optics.
Dr. L. Trinkler (Copenhagen, Roskild, Denmark) 26.08. - 07.09.02. Characterization of dosimetric properties of AlN ceramics.

Problems

Given the well known limitations due to underfunded and in part obsolete scientific infrastructure in East-European countries, the strongest emphasis during the visits to Latvia by senior researchers was on exchange of ideas, planning of joint studies, discussions on the obtained data and on the perspective research directions, less on the purely experimental data gathering. In this context, the most serious hindrance was the limited access to library or to the latest online data sources because of the poor subscription coverage in locally available libraries. This drawback, was, however, in part offset by a good broadband internet connection and by a help from colleagues in partner institutions. There was more emphasis on the experimental work during the visits of younger researchers, particularly those from other former East-block countries, which usually have similar infrastructure problems at their homes. They were generally able to capitalize on the original features of the in-house custom-built instrumentation at CAMART laboratories, not available in standard commercial instruments, and in this way to obtain meaningful new experimental data.

Network 3, WP 12 - 18

Advanced ferroelectric materials (Prof. Dr.A.Krumins)

Workshops, Conferences

- The 3rd International Conference "Advanced Optical Materials and Devices" Riga, August 19 – 22, 2002; purpose: summarizing and discussion of the results in new optical materials and devices; 130 participants from 21 countries; 57 oral and 88 poster presentation; the Proceedings were published in two special issues of International journal "Proceedings SPIE", vol. 5122 and vol. 5123, 2003.
- meeting of International Advisory Board of the Institute at August 18, 2002; the recommendations see at appendix.

Visitors

1. Dr.A.Fuith, Institute of Experimental Physics, University of Vienna, Austria, June 23 – July 21, 2002; investigation of diffuse phase transitions (WP – 12);
2. Dr.Barbara Garbarz-Glos, Institute of Physics, Pedagogical Academy, Krakow, Poland; May 29 – June 30, 2003; studies of ferroelectric solid solutions for piezoeletric applications (WP – 12);
3. Prof. R.Rotomskis, Vilnius University, Lithuanai, July 6 – August 7, 2001; studies of the switching speed and induces birefringence in PLZT electrooptical ceramics (WP – 16);
4. Dr.J.Hlinka, Institute of Physics, Czech Rep.; July 1 – August 1, 2001; theory of electroclastic interactions (WP – 13);
   August 1 – August 31, 2002; paraelectric – ferroelectric phase instability (WP – 13);
   October 16 – November 11, 2003; stochastic approach to phase instability (WP – 13);
5. Dr.P.V.Susho, University College London, November 12 – December 12, 2002; ab inito interpretation of ferroelectric phase instability (lectures) (WP – 15);
6. Mr. Carlos Zieber, University of Saarland, Germany, March 1 – April 8, 2001; RF sputtering of ferroelectric thin films (WP – 14);
7. Dr.M.Tjunina, Microelectronics and Materials Physics Lab., University of Oulu, July 1 – August 15, 2001; March 15 – April 15, 2003; November 20 – December 20, 2003; dielectric properties of ferroelectric relaxors, model of ferroelectric thin films;
8. R.Bittner, Atominstitute aus Osterreichische Universitäten, Vien, Austria, August 20 – September 20, 2001; neutron irradiation effects on sol – gel PLZT thin films;
9. Dr.S.Katholy, Institute of Physics, University of Postdam, Germany; May 17 – June 18, 2002; characterization of thin films by optical elipsometry;
10. DR.J.Banys, Vilnius University, Lithuania, November 5 – December 5, 2002; high frquency dielectric response measurments of ferroelectrics; lectures;
11. Dr. C.Harnagea, Max – Plank – Institute of Microstructure Physics, Halle, Germany; November 17 - December 17, 2002; development of piezoelectric response measurement mode of Scanning Probe Microscopy;
12. Dr.A.Kholkine, Department of Ceramic and Glass Engineering, University of Aveiro, Portugal, July 7 – September 15, 2003; characterization of ferroelectric domains by atomic force microscopy;
13. Dr.Raivo Jaaniso, Institute of Physics, Tartu University, November 15 - December 15, 2004; pulsed laser ablation of polar dielectric thin films.

Visits

1. Prof. M.Ozolinsh, Lund University, Sweden, 27.12.2001. – 14.01.2002; experiments with liquid crystals for vision science;
2. Dr.E.Klotins, Institute of Physics, Chech Rep., 31.03.2003. – 19.04.2003; research in configurational representation for metastable systems;
3. Dr.E.Klotins, University of Aveiro, Portugal; 18.08.2003.-18.09.2003; developments in symplectic integrators; lectures

4. Dr.E.Klotins, University of Saarbrűcken, Germany; 26.04.2001. – 13.05.2001; research in long range interactions;
5. Dr.E.Klotins, Institute of Physics, Chech Rep.; 28.11.2001.-24.12.2001; library search;
6. Dr.V.Zauls, Postdam University; 24.10.2001. – 08.12.2001; optical second harmonic investigation of polar thin films;
7. Mg.K.Kundzins, Institute for Solid State and Materials Research Dresden; 7.10.2001.-8.11.2001; pulsed laser deposition of ferroelectric thin films;
8. Dr.M.Dambekalne, Pedagogical University Crakow, 2.06.2002. – 29.06.2002; technology and properties of ceramic ferroelectric materials;
9. Dr.V.Zauls, Postdam University, Germany; 23.06.2002. – 14.07.2002; ellipsometric measurements of thin transparent films;
10. Mg. K.Kundzins, Institute for Solid State and Material Research Dresden, Germany, 27.04.2003. – 21.05.2003; pulsed laser deposition of ferroelectric thin films;
11. Dr.V.Zauls, Microelectronics Lab., University of Oulu, Finland; 22.04.2003. – 01.05.2003; dielectric spectroscopy of ferroelectric thin films.

Network 4, WP – 22

Materials for opthalmology and vision science (Prof. Dr.M.Ozolinsh)

Visitors

1. Prof. S.Vilani (Firenze, Italia) – 28.09. – 03.11.2001; 28.05. – 27.06.2003.consultations and setting of the new electrophysiology equipment "Neurosoft" and carrying out the evoked visual potential (EVP) measurements; and giving lectures modulus "Electrophysiology methods" for Latvian University Optometry department students.

2. Prof. H.M.Bueno (Murcia, Spain) – 25.10.-25.11.2004; carrying out the polarization elipsometry measurements for the model eye with artificially induced cataract

Visits

PhD.student D.Racene – 14.06.-25.06.2001. München: report in *Europ. Conf. on* ***Biomedical Optics.***
PhD.student R.Paeglis – 14.06.-25.06.2001. München: report in *Europ. Conf. on* ***Biomedical Optics.***
Prof. M.Ozolinsh – 30.08.-10.09 Madrid: report in ***10th International Meeting on Ferroelectrics*** **(IMF-10)**.
Prof. M.Ozolinsh – 5.11.-12.11.2001 Turin, Firenze, Italy: report in *16th Int. Congress of Laser Medicine* ***Laser Florence 2001.***
PhD. student J.Berzinsh – 5.11.-12.11.2001 Turin, Italy: report in ***European Conference "Human factor in Transportation"***.

PhD. student I.Supe – 8.04.-22.04.2002. München: report in ***International Meeting of American Academy of*** **Optometrists- 2002.**
PhD. student A.Svede – 8.04.-22.04.2002. München: report in ***International Meeting of American Academy of*** **Optometrists- 2002.**
PhD. student R.Paeglis – 12.05.-27.05.2002. Murcia, Spain: experiments of point spread function and modulation transfer function of eye with simulated cataract.
PhD. student J.Petrova – 22.08.-31.08.2002. Tampere, Finland: report in
PhD. student G.Papelba – 24.08.-30.08.2002. Glasgow, Scotland: report in
PhD. student A.Svede – 1.07.-5.07.2003. Dublin, Ireland: report in **The Conference of Irish Association of Orthoptists**.
Prof. M.Ozolinsh – 1.08.-10.08.2003. Cambridge, England: report in ***10th European Meeting on Ferroelectrics EMF-10***,
PhD. student G.Krumina – 31.10.-30.11.2003 Utrecht, The Netherlands, studies of stereo visual perception using scattering obstacles.
PhD. student A.Svede – 4.12.-17.12.2003. Dortmund, Germany: studies of visual ergonomics for different stimuli.
Prof. M.Ozolinsh – 31.08.-14.09.2003. Paris, Granada: report in ***European Conference of Visual Perception*** **ECVP-2003** (Paris, September), ***Vision in Vehicles*** **VIV-10** (Granada, September).

Network 5, WP 27 – 34

Solid State Ionics and Devices (Dr.A.Lusis)

Regional seminar on Solid State Ionics (RS-SSI 2001)
The seminar "RS-SSI 2001" (which was in Jurmala, Sept.22-26, 2001, Latvia) attanded 53 scientists and students from Byelorussia (1), Estonia (2), Germany (1), Latvia (29), Lithuania (3), Poland (8), Russia (7) and Sweden (2). On seminar had been presented 39 papers (9 of them was invited). The papers have been published in special issue of " Journal of Solid State Electrochemistry", Vol.7 Nr.2, 2003.

Organization of 10th International Symposium on Electronic Nose (ISOEN'03)
93 participants from 22 countries come together to discuss the main results in sensor and sensor array technologies, e-nose minituarisation, odour description in electronic files and unified description language formation, e-nose application in different fields, making emphasis on product adultaration and environment pollution problems. Latest developments and new results were reported in 49 oral and 28 poster presentations, as well as in many discussions through out the symposium. Manuscripts of the best reports are published in special issue of International Journal from Elsevier "Sensors and Actuators", B: chemical sensors

Visitors

Prof. A.Czerwinski, Warsaw University, Poland

1) 14.05.- 15.06.2001: "Modern problems of solid state batteries and interfacies" started research and training course “Electrochemical Impedance Spectroscopy of solid electrolytes and interfaces”;
2) 20.09.-21.10.2001: "Modern problems of chemical current sources", did teaching work;
3) 09.05.-13.06.2003: "Hydrogen adsorption in electrodes of catalytic metals" did research work on hydrogen adsorption in electrodes of catalytic metals and Sorption in Limited Volume Electrodes of Palladium Alloys.

Prof. A.Orliukas (Vilnius University) did teaching and research work

1) 22.11.-21.12.2001: "Investigation of the pecularities of the ion transport of the solid electrolytes in the microwave region";
2) 11.11.-12.12.2002: "The ion transport in the solid electrolyte ceramics",
3) 13.10.-12.11.2004: “Superionic conductors”

Prof. Enn Lust (Institute of Physical Chemistry of University of Tartu) 05.11.-06.12.2002: “Electrode problems for supercapacitors” did teaching and research work.

Prof. Francesco Rocca (Istituto di Fotonica e Nanotecnologie del Consiglio Nazionale delle Ricerche, Sezione "CeFSA" di Trento,)30.06.-30.07.2003: "X-ray absorption spectroscopy of nanosized materials", did teaching and research work.

Dr. Janius Sinius (Vilnius University) 17.122001-23.01.2002: “Application of super ionic conductors in batteries and sensors”, did training and research work

Dr. Stefan T.H. Strathmann (Institute for Health and Consumer Protection (European Commission Joint Research Centre) 16.07.-16.08.2002: "Chemical gas sensors and sensor array characterization" did teaching and research work.

Dr. Arunas SETKUS (Semiconductor Physics Institute in Vilnius, Lithuania) 03.06.-03.07.2002: “Adjustment of metal oxide thin film gas sensors to an electronic device for odours recognition” did teaching and research work.

Dr.Andris Azens (Angstrom laboratory, Uppsala University) 01.-31.07.2002: “Functional coatings on glass”, did teaching and research work.

Postdoc Nikos Papamichail (University of Tuebingen, Institute for Physical Chemistry, Germany) 04.06.–03.2003: "Application of e-nose: sampling, measurements and data analyses” did training and research work.

PhD student Z.Rogulski (Warsaw University) 15.06.-15.07.2001: “Electrochemical impedance of solid electrolytes and interfaces”, did research work.

Ing. D. Pailharey (University of Marseille II) 20.05.-20.06.2002: “AFM and application for study of thin films”, did training work.

Visits

Dr. A.Lusis attended

1) Moscow Energetic Institute and Institute of Problems of Chemical Physics of RAS to discuss with content of INTAS project for development application technologies of e-noses and sensors in June, 2002.
2) kick-off meeting for setting up consortium for collective research project of the system on chip for SME in Oct.31, 2002, Copenhagen (Denmark);

3) consortium meeting Munich (Nov.14, 2003) for preparation contract FP6 Collective research project "Removal of Hazardous Substances in Electronics: Processes and techniques for SMEs (GreenRoSE)". From that point of view to visit this meeting was very important for WP32, WP33 and WP34 in part material research;
4) Board meeting of project "SoC-SME" coordination activities, which important for development intelligent sensor systems for application of our research results obtained in WP34 and for instrument design.

Dr. J.Purans research visits at

1) Synchrotron facility on LURE (Paris, France) according plans of WP31 in Sept. 03-09, 2002. Aim: establishing of a collaboration for the use of UV and IR beam lines at new DAFNE storage ring
2) University of Trento (Italy) in Sept.2003. Aim: use of UV and IR beam lines at new DAFNE storage ring.

Dr. A.Kuzmin research visits at

1) University of Trento (Italy) in Sept.2003. Aim: use of UV and IR beam lines at new DAFNE storage ring
2) Synchrotron Center at LNF INF, March 05-10, 2002, Frascati, Italy. Aim: use of UV and IR beam lines at new DAFNE storage ring.

MS student L.Grinberga attended

1) First NorFa Summer School *"New materials and technologies for low temperature fuel cells"* for MS and PhD students at Chalmers University of Technology, Gothenburg, Sweden, Sept.5-7, 2002. Topics of Summer School cover thematic of WP32.
2) NORFA summer school for Ph.D. students ''Infrastructure for the Hydrogen Society", June 10-14, 2003, Reykjavik, Iceland

Dr.V.Eglitis did training and research visit for investigaion of glass fiber surfaces with AFM at Kaunas Technical University (Lithuania).

PhD student G.Veveris did training and research visit at

1) Kaunas Technical University (Lithuania) for investigaion of glass fiber surfaces with AFM;
2) Department of Chemistry of Warsaw University and did research work on ion distribution in glass fiber.

Consolidated scientific report

Objectives

The principal objective of the project has been development of the functional material science at the Institute of Solid State Physics (ISSP) University of Latvia, thus in Latvia and whole EU. The efforts are mainly focused on the thin film materials(ceramics) for sensors, actuators, radiation dosimetry and imaging, particle detection, energy storage, for optical wavequides and high power laser optics, materials for deep – ultraviolet lithography and thin film compounds for holographic recording media. The goal was finding of new materials and improving the properties of the existing ones for the currently emerging applications.

The second aim was to perform detailed theoretical studies of the basic properties, intrinsic and radiation – induced defects in technology important ABO_3 type perovskites and development of the a computer aided design of catalyst.

The materials under study included binary and ternary crystaline compounds, wide band-gap oxide glasses, based on silicon dioxide, thin semiconducting films based on amorphous chalcogenides, fullerene, ferroelectric ceramic solid solutions and thin films, as well as films and heterostructures with ionic conductivity.

In achieving the objectives the opportunities, opened by the EC financing to the Centres of Excellence, was used in full: invitation of outstanding scientists and postdocs as well as visits of own scientist to the leading research centres, participation in scientific meetings, organization of conferences. Due to cofinansing of Centre of Excellence from Latvia governmevt new scientific equipment was purchased, thus the infrastructure of ISSP was improved and new researchers from University of Latvia were attracted.

All objectives of the project were really achieved.

Research methods

A number of different but complementary methods and techniques were used in our large-scale computer modelling of advanced materials and defects therein, including ***ab initio*** methods of the atomic and electronic structure calculations (Hartree--Fock with the electron correlation corrections, and Density Functional Theory), semi-empirical methods of quantum chemistry (Shell Model and INDO) as well as kinetic Monte Carlo and cellular automata techniques. Combination of a wide range of methods and techniques permits us to get a reliable information on the atomic, electronic structure and optical properties of material properties and basic impurities therein.

In contrast to Network 1, the tasks of other Networks were solved basically by experimental methods. These included optical absorption spectroscopy spanning infrared to vacuum ultraviolet spectral ranges, different luminescent spectroscopies, dielectric and electrooptic measurements, electron paramagnetic resonance and magnetooptic methods, refractometry, mechanical property studies, X-ray diffraction and holographic recording tests. The materials under study were either locally developed and processed or obtained from partners. In course of the project, essential improvements to analytical instrumentation were performed and the infrastructure for growing thin films and heterostructures were built. The locally missing experimental analytical or material preparation capabilities were supplemented by collaboration and coordination with network partners and within the preexisting international collaborations. The advances in Scanning Probe Microscopy (SPM) and further development should be specially mentioned.

Results and achievements

In the following we present the main results, together with the lists of principal publications for each Network (Fig.1). The achieved deliverables, according to the Technical Annex, are also provided for each Network. All outlined deliverables have been attained.

Network 1. Computer Modelling of Advanced Materials

Deliverables achieved:
***D1* - Research report for each half-year of CAMART activity which includes short information about achievements, scientific contacts and publications for this period.**
***D2 - Publications (new knowledges)* 30-35 papers annually (WP1-5) in high-rating International journals.**
***D3 - Proceedings of various conferences and meetings* 30-40 presentations annually (WP1-5) at local and International scientific conferences as well as numerous discussions and contacts.**
***D4 - Dissemination of achievements* regular seminars in the leading scientific centers and laboratories (25-30 annually in the framework of WP1-5), regular upgrade of actual information in our website: http://www.cfi.lu.lv/teor .**
***D5 – Information about current state in appropriate sector of RTD works* regular discussions with collaborators on joint projects and public presentation of the research reports.**
***D7 - Knowledge transfer* training of young bachelors and magisters for PhD studentships and participation in joint scientific projects.**
***D8 - Enhance competence and expertise* regular participation in the referiing of scientific projects and papers.**
***D12 - New materials* active participation in those scientific projects which focus on advanced technological materials.**
***D13 - New method or technology* elaboration, realization and testing of new theoretical methods and programs for further application in scientific researches.**

WP-1. Defects and surfaces of advances perovskites

According to planned deliverables *1D1/1D2/1D3/1D7/1D12/1D13,* we performed large scale parallel calculations for a number of perovskite materials, including $SrTiO_3$, $BaTiO_3$, $KNbO_3$, $KTaO_3$ and their solid solutions, widely used in numerous technological applications. We obtained the atomic, electronic structure and optical properties of basic impurities in these materials, including O vacancies (*F*-type centers), electron and hole polarons, metal impurities (e.g., Fe) and hydrogen. This was used for defect identification in these materials. We studied also quantum (confinement) effects in nanoscopically thin perovskite films terminated by 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-T_c superconductors.

The main results of this WP were understanding of the nature of the *F* centers, interpretation of the green luminescence observed in most perovskites under photoexcitation and considerable covalency of chemical bonding near polar surfaces.

WP-2. The kinetics of metal colloid formation under irradiation of prospective materials

According to planned deliverables *2D1/2D2/2D3/2D4/2D7/2D8/2D13,* we performed large-scale modelling of insulating solids under irradiation and developed the first *atomistic model* of primary defect (*F* center) aggregation and the metal colloid formation process. This opens the way to many important technological applications including safe radiactive waiste disposal, effective ion implantation, and stability of prospective materials for the first wall of neutron reactors**.**

The main results of this WP were interpretations of numerous experimental data on metal colloid formation in three different types of experiments.

WP-3. Self-Organization in Surface Catalytic Reaction

According to planned deliverables *3D1/3D2/3D3/3D7/3D8/3D13,* we developed models for **c**atalytic surface reactions, which are of enormous importance in industrial (synthesis of NH_3, H_2SO_4, cracking and reforming processes) and environmental chemistry (catalytic control of emission CO, SO_2). In particular, optimisation of the $CO+O_2$ and the CO+NO catalytic reactions is very important for the automotive industries, and 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.

The main results of this WP were interpretations of experimental data on several catalytic surface reactions which permit their optimization.

WP-4. First Principles Modelling of Metal Oxidation and Corrosion

According to planned deliverables *4D1/4D2/4D3/4D4/4D7/4D8***,** we performed comprehensive quantum chemical modeling of different stages of the initial oxidation of light metals (mainly aluminum). We modeled the metallic substrate interaction with molecular oxygen, its further dissociative chemisorption, surface diffusion of adatoms and their absorption inwards substrate, up to formation of the first oxide units in the O/Me interface. To study possibilities of initial oxidation deeper we considered steps on the metal surface and vacancies of metal atoms. When modeling all the stages of initial oxidation, we simulated both relaxation and reconstruction of the metal surface. The calculated properties of both interface energetics and its electronic structure for the systems under consideration were compared and analyzed, in order to interpret various stages of the initial oxidation. The analogous methodology was applied for theoretical study of different densely-packed Me/MeO interfaces: Ag/α-Al_2O_3, Ag/MgO, $Cu/BaTiO_3$ and Cu/MgO when varying coverage of oxide substrates and considering different kinds of defects. Combining results of *ab initio* calculations on metal/metal oxide interfaces with thermodynamic theory (taking into account the lattice mismatch), we show that the metal cluster formation becomes predominant growth mode already at low coverages, in agreement with experiment.

The main results of this WP were prediction of atomistic mechanisms for thin films growth on metallic and metal oxide substrates based on first principles

calculations on the interface combined with statistical thermodynamic treatment of interatomic potentials extracted from those calculations.

WP-5. Defect Properties of Prospective Oxide and Halide Materials

According to planned deliverables *5D1/5D2/5D3/5D5/5D7/5D13*, we studied experimentally basic defects in a number of technologically important materials, including scintillators, ceramics, dosimeters, storage phosphors. In particular, storage phosphor imaging plates (IP) are widely used as two-dimensional integrating position-sensitive detector based on the effect of photo-stimulated luminescence (PSL). By admixture of Gd_2O_3 the storage phosphor can be sensitised to thermal neutrons utilizing the extremely high absorption cross section of gadolinium in this energy range. In collaboration with *European Molecular Biology Laboratory, Grenoblé, France,* and *King's College London, UK,* we have studied neutron sensitive image plates in combination with a suitable scanning system, which exhibit excellent characteristics. We have performed comparative measurements PSL recorded using a Molecular Dynamics 'Storm' scanner (635 nm) after neutron irradiation of a number of new combinations of converter/storage phosphors. Measurements have been made for a number of advanced materials, in order to characterize the intrinsic fading of the PSL signal with time after neutron irradiation. The X-ray sensitivity and fading of several of these compounds have also been measured.

The main results of this WP: we made the image plates by layering Eu^{2+} doped BaSrFBr phosphor alternately with Gd_2O_3 converter. Prototype image plates have been constructed and tested using a spraying technique for the phosphor/converter. The method has the potential to produce large image plates with good uniformity.

Problems

It was forbidden to invite visitors/experts from Russia, even those who are important for our project.
Another problem was that duration of visits of guests could not be shorter than one month, which is inconvenient for many very busy foreign professors.

Principal scientific papers published in 2001-2004

1. J.T. Devreese, V.M. Fomin, E.P. Pokatilov, E.A. Kotomin, R.I. Eglitis, and Yu.F. Zhukovskii, Theory of bound polarons in oxide compounds. - *Physical Review B*, 2001, **63**, 184304 (p. 1-6).
2. V.N. Kuzovkov, A.I. Popov, E.A. Kotomin, M.A. Monge, R. González, and Y. Chen, The kinetics of F-center aggregation in thermochemically reduced MgO single crystals. - *Physical Review B*, 2001, **64**, 064102 (p. 1-5).
3. E.A. Kotomin, V. Kashcheyevs, V.N. Kuzovkov, K. Schwartz, and C. Trautmann, Modeling of primary defect aggregation in tracks of swift heavy ions in LiF. - *Physical Review B*, 2001, **64**, 144108 (p. 1-7).
4. E. Heifets, R. I. Eglitis, E. A. Kotomin, J. Maier, and G. Borstel, *Ab initio* modeling of surface structure for $SrTiO_3$ perovskite crystals. - *Physical Review B*, **64**, 235417, p.1-5, (2001).
5. V.N. Kuzovkov, O. Kortlüke, and W. von Niessen, Comment on "Surface restructuring, kinetic oscillations, and chaos in heterogeneous catalytic reactions". - *Physical Review E*, 2001, **63**, 023101 (p. 1-5).
6. G. Zvejnieks and V.N. Kuzovkov, Monte-Carlo simulations for Lotka-type model with reactant surface diffusion and interactions. - *Physical Review E*, 2001, **63**, 051104 (p. 1-10).
7. V. Kashcheyevs and V.N. Kuzovkov, Global oscillation mechanism in the stochastic Lotka model. - *Physical Review E*, 2001, **63**, 061107 (p. 1-8).

8. Yu.F. Zhukovskii, E.A. Kotomin, S. Dorfman, D. Fuks, and A. Gordon, Hartree-Fock study of adhesion and charge redistribution on the Ag/MgO(001) interface. - *Surface Science,* 2001, **482-485**, p. 66-72.
9. S. Dorfman, D. Fuks, A. Gordon, E.A. Kotomin, and P. Wyder, Some nonlinear properties of ferroelectric smart materials. - *Physica B*, 2001, **304**, p. 339-347.
10. A.I. Popov, M.A. Monge, R. González, Y. Chen, and E.A. Kotomin, Dynamics of F-center annihilation in thermochemically reduced MgO single crystals. - *Solid State Communications,* 2001, **118**, p. 163-167.
11. B. Savoini, C. Ballesteros, J.E. Muñoz-Santiuste, R. González, A.I. Popov, and Y. Chen, Copper and iron precipitates in thermochemically reduced yttria-stabilized-zirconia crystals. - *Philosophical Magazine Letters*, 2001, **81**, p. 555-561.
12. V. S. Vikhnin, R. I. Eglitis, S. E. Kapphan, E. A. Kotomin and G. Borstel, A new phase in ferroelectric oxides: The phase of charge transfer vibronic excitons. - *Europhysics Letters*, **56**, p. 702-708 (2001).
13. R.I. Eglitis, E.A. Kotomin and G. Borstel, Quantum chemical modelling of polarons and perovskite solid solutions. - *Computational Materials Science*, 2001, **21**, p. 530-534.
14. V.S. Vikhnin, R.I. Eglitis, S.E. Kapphan, G. Borstel, and E.A. Kotomin, Polaronic-type excitons in ferroelectric oxides: Microscopic calculations and experimental manifestation. - *Physical Review B*, 2002, **65**, 104304 (p. 1-11).
15. V.N. Kuzovkov and G. Zvejnieks, Reply to "Comment on 'Monte Carlo simulations for a Lotka-type model with reactant surface diffusion and interactions' ". - *Physical Review E*, 2002, **65**, 033102 (p. 1-4).
16. V.N. Kuzovkov, O. Kortlüke, and W. von Niessen, Kinetic model for surface reconstruction. – *Physical Review E*, 2002, **66**, 011603 (p. 1-10).
17. V.N. Kuzovkov and G. Zvejnieks, Model of the catalytic A+B -> 0 reaction with surface reconstruction. – *Physical Review E,* 2002, **66**, 021109 (p. 1-9).
18. O. Kortlüke, V.N. Kuzovkov, and W. von Niessen, Internal spationtemporal stochastic resonance in the presence of weak noise. – *Physical Review E*, 2002, **66**, 036139 (p. 1-7).
19. D. Fuks, S. Dorfman, Yu.F. Zhukovskii, E.A. Kotomin, and A.M. Stoneham, Theory of the growth mode for a thin metallic film on an insulating substrate. - *Surface Science*, 2002, **499**, p. 24-40.
20. E. Heifets, R.I. Eglitis, E.A. Kotomin, J. Maier, and G. Borstel, First-principles calculations for $SrTiO_3$(100) surface structure. - *Surface Science*, 2002, **513**, p. 211-220.
21. Yu.F. Zhukovskii, E.A. Kotomin, B. Herschend, K. Hermansson, and P.W.M. Jacobs, The adhesion properties of the Ag/α-Al_2O_3(0001) interface: an *ab initio* study. - *Surface Science*, 2002, **513**, p. 343-358.
22. R.I. Eglitis, E.A. Kotomin, and G. Borstel, Qunatum chemical modelling of electron polarons and charge-transfer vibronic excitations in $BaTiO_3$ perovskite crystals. – *Journal of Physics: Condensed Matter*, 2002, **14**, p. 3735-3741.
23. R.I. Eglitis, E.A. Kotomin, S.E.Kapphan and G. Borstel, Qunatum chemical modelling of electron polarons and "green" luminiscence in $PbTiO_3$ perovskite crystals. - *Journal of Physics: Condensed Matter*, 2002, **14**, p. L647-L653.
24. V.N. Kuzovkov, W. von Niessen, V. Kashcheyevs, and O. Hein, Exact analytic solution for the generalized Lyapunov exponent of the two-dimensional Anderson localization. - *Journal of Physics: Condensed Matter*, 2002, **14**, p. 13777-13797.
25. J.R. Kalnin, E.A. Kotomin, and J. Maier, Calculations of the effective diffusion coefficient for inhomogeneous media. - *Journal of Physics and Chemistry of Solids*, 2002, **63**, p. 449-456.
26. R.A. Evarestov, S. Piskunov, E.A. Kotomin, and G. Borstel, Single impurities in insulators: *ab initio* study of Fe-doped $SrTiO_3$. – *Physical Review B*, 2003, **67**, 064101 (p. 1-9).
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28. Yu.F. Zhukovskii, P.W.M. Jacobs, and M. Causá, On the mechanism of the interaction between oxygen and close-packed single-crystal aluminum surfaces. – *Journal of Physics and Chemistry of Solids*, 2003, **64**, p. 1317-1331.
29. G. Borstel, R.I. Eglitis, E.A. Kotomin, and E. Heifets, Modelling of defects and surfaces in perovskite ferroelectrics. – *Physica Status Solidi (b)*, 2003, **236**, p. 253-264.
30. E.A. Kotomin, V.N. Kuzovkov, G. Zvejnieks, Yu.F. Zhukovskii, D. Fuks, S. Dorfman, and A.M. Stoneham, The kinetic MC modelling of reversible pattern formation in initial stages of thin metallic film growth on crystalline substrates. – *Solid State Communications*, 2003, **125**, p. 463-467.

31. R.I. Eglitis, V.A. Trepakov, S.E. Kapphan, and G. Borstel, Quantum chemical modelling of “green” luminescence in self activated perovskite-type oxides. – *Solid State Communications*, 2003, **126**, p. 301-304.
32. R.A. Evarestov, E.A. Kotomin, E. Heifets, J. Maier, and G. Borstel, *Ab initio* Hartree-Fock calculations of $LaMnO_3$(110) surfaces. – *Solid State Communications*, 2003, **127**, p. 367-371.
33. E.A. Kotomin, E. Heifets, J. Maier, and W.A. Goddard III, Atomistic simulations of the $LaMnO_3$(110) polar surface. – *Physical Chemistry and Chemical Physics*, 2003, **5**, p. 4180-4184.
34. A. Gunhold, L. Beuermann, K. Gömann, G. Borchardt, V. Kempter, W. Maus-Friedrichs, S. Piskunov, E.A. Kotomin, and S. Dorfman, Study of the electronic and atomic structure of thermally treated $SrTiO_3$(110) surfaces. – *Surface and Interface Analysis*, 2003, **35**, p. 998–1003.
35. V.S. Vikhnin, S.E. Kapphan, I.L. Kislova, R.I. Eglitis, and P.A. Markovin, Manifestation of polaronic states in ferroelectric relaxor PMN. – *Ferroelectrics*, 2003, **285**, p. 291-302.
36. E. Heifets, W.A. Goddard III, E.A. Kotomin, R.I. Eglitis, and G. Borstel, Ab initio calculations of the SrTiO3 (110) polar surfaces. – *Physical Review B*, 2004, **69**, 035408 (p. 1-7).
37. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, Resonance approximation and charge loading/unloading in adiabatic quantum pumping. - *Physical Review B*, 2004, **69**, 195301 (p. 1-9).
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41. V.N. Kuzovkov, V. Kashcheyevs, and W. von Niessen, Reply to Comment on 'Exact analytic solution for the generalized Lyapunov exponent of the two-dimensional Anderson localization'. - *Journal of Physics: Condensed Matter*, 2004, **16**, p. 1683-1685.
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43. G. Zvejnieks, V.N. Kuzovkov, O. Dumbrajs, A.W. Degeling, W. Suttrop. H. Urano, and H. Zohm, Autoregressive moving average model for analyzing edge localized mode time series on Axially Symmetric Divertor Experiment (ASDEX) Upgrade tokamak - *Physics of Plasmas*, 2004, **11**, p. 5658-5667.
44. O. Kortlüke, V.N. Kuzovkov, and W. von Niessen, Forced oscillations in a self-oscillating surface reaction model. - *Physical Chemistry and Chemical Physics*, 2004, **6**, p. 1227-1229.
45. L. Grigorjeva, D.K. Millers, V. Pankratov, R.T. Williams, R.I. Eglitis, E.A. Kotomin, and G. Borstel, Experimental and theoretical studies of polaron optical properties in $KNbO_3$ perovskite. - *Solid State Communications*, 2004, **129**, p. 691-696.
46. A.V. Sidorenko, A.J.J. Bos, P. Dorenbos, C.W.E. van Eijk, P.A. Rodnyi, I.V. Berezovskaya, V.P. Dotsenko, and A.I. Popov, Storage properties of Ce3+ doped haloborate phosphors enriched with 10B isotope. - *Journal of Applied Physics*, 2004, **95**, p. 7898-7902.
47. S. Piskunov, E. Heifets, R.I. Eglitis, and G. Borstel, Bulk properties of $SrTiO_3$, $BaTiO_3$ and $PbTiO_3$ perovskites: an ab initio HF/DFT study. – *Computational Materials Science*, 2004, **29**, p. 165-178.
48. Yu.F. Zhukovskii, E.A. Kotomin, and G. Borstel, Adsorption of single Ag and Cu atoms on regular and defective MgO(001) substrates: an *ab initio* study. - *Vacuum*, 2004, **74**, p. 235-240.
49. V. Kashcheyevs, A. Aharony, and O. Entin-Wohlman, Quantized charge pumping by surface acoustic waves in ballistic quasi-1D channels. - *European Physical Journal B*, 2004, 39, p. 385-396.
50. A.W. Degeling, J.B. Lister, Y.R. Martin, and G. Zvejnieks, Were the chaotic ELMs in TCV the result of an ARMA process? - *Plasma Physics and Controlled Fusion*, 2004, 46, p. L15-L21.

Network No 2. Functional Disordered Materials

Deliverables achieved:

D1- Research report for each half-year of CAMART, includes the activities completed, short information of results achieved, scientific papers published and submitted.

D2 – **Publications (new knowledge, dissemination of knowledge)** on average 20-30 papers yearly published by members of Network 2 in acknowledged international journals.

D3 – Presentations at scientific conferences and workshops (dissemination of knowledge) on average 20 yearly over the network.

D4 - **Dissemination of achievments at conferences and meetings**

D5 – Information about current state of RTD problems in the area of materials for scintillators via regular contacts with regional enterprises Anda Optec (manufacturer of fiber-optic cables) and Baltic Scientific Instruments (fabrication of radiation detectors and related equipment) and participation at network ‘’Interfacial effects, novel properties and technologies of nanostructured materials” meetings.

D7 – Knowledge transfer via training of master and Ph.D. students. PhD thesis, based on the results of collaborative work within the network, were successfully defended. The education capacity of University of Latvia in basic, doctoral and post doctoral studies in nanophysics and nanotehnology has been improved.

D8 – Enhance competence and expertize – the participants of the network served on a semi-regular basis as referees for the general physics journals (e.g., Phys. Rev. Letters, Physical Review and similar) and as well for field-specific journals (e.g., Nuclear Instruments and Methods in Physics Research, J. Non-Crystalline Solids) and advisory boards/ program committees of various international scientific conferences and meetings

D12 – New materials. An active media for imaging of slow neutron flux based on Li-containing fluoride based perovskite (ABF_3) materials have been developed for selective detection of slow neutron flux.

D14 – New devices or instruments The development of infrastructure for chemical vapour deposition (CVD) growth of nitride and oxide thin film structures, infrastructure for investigation of optical and electrical, characteristics in cooperation with EU partners.

D15- Education – Lectures in a number of specialized seminars and in summer schools for M. Sc. and PhD level students. Local students of University of Latvia and other institutions obtained international experience and benefited from the numerous lectures by visiting scientists.

In the folllowing, the summaries of the specific results by each work package within Network 2 are listed.

Work package WP6 - Third group nitride thin films (Prof. I. Tale).

Infrastructure for producing thin films and heterostructures by metal-organic chemical vapor deposition (MOCVD) method was developed and the instrumentation for the characterization of their optical and electrical properties was built. Nitride and oxide thin film structures were grown and their optical and electrical charactreristics were explored in collaboration with the partner universities from Rostock, Paderborn, Vilnius, and St.-Petersburg. Such films are promising in the light emitting devices and sensor applications. The results allow essentialy better understanding of the nature of defects, transport and radiative electron recombination processes in wide gap semiconductor nitride structures up to 6 eV.

Work package WP7- Radiation energy detectors and storage-readout materials (Prof. I. Tale)

Solid state materials, developed as radiation storage and readout media for radiation imaging systems have been studied. The nature of centers, responsible for energy accumulation and optical readout were investigated in collaboration with universities of Paderborn, Tartu, Rostock, Vienna. Active media for imaging of slow neutron flux based on Li-containing fluoride materials have been developed. Within collaboration with partner universities, a program of investigation of nanostructured radiation imaging and wide-gap semiconductor functional structures has been elaborated .

Work package WP8 – Materials for photonics (Dr. hab. D. Millers)

Ways to improve the efficiency of non-linear optical elements used for frequency-doubling in photonic applications were studied by time-resolved spectroscopy. Crystals of lithium- and potassium niobate were grown by partner Excellence Centre KFKI in Budapest, Hungary, and strontium titanate was prepared by Univ. of Osnabrueck, Germany. It was established that the bound polarons created by high-energy excitation pulse are one of the main physical reasons, responsible for the reduction of frequency doubling efficiency, and that the observed ultrafast luminescence is due to creation of weakly separated electron- and hole-polaron pairs.

Work package WP9 –Materials for storage media and scintillators (Dr. D. Millers)

Materials for fast and radiation-resistant scintillators for applications in environment monitoring and imaging in X-ray computer tomography and positron-emission tomography were developed and the physical processes taking place in these materials under excitation by electron pulses were studied. Details of scintillation formation mechanisms in tungstate single crystals ($PbWO_4$, $ZnWO_4$, $CdWO_4$, $CaWO_4$) were elucidated and nanostructured transparent ceramics as a material for advanced scintillators was proposed.

Work package WP10- Defects in oxide glasses and related materials (Dr. L. Skuja)

Optical properties and their stability upon laser irradiation were studied in glassy SiO_2 (g-SiO_2), which is currently the most important glassy material for vacuum ultraviolet and for high power laser optics. The diffusion parameters of oxygen interstitials in g-SiO_2 were established, their role in defect processes was demonstrated by interconversion between oxygen dangling bond (≡Si-O$^\bullet$) and peroxy radical (≡Si-O-O$^\bullet$) defects. A new vacuum ultraviolet optical absorption band around 6.8 eV of oxygen dangling bonds was experimentally identified and confirmed by calculation. This band interferes with applications involving ArF excimer laser (e.g., high-resolution lithography). The photolysis of silanol (≡Si-O-H) groups by F_2 excimer laser photons was studied and the diffusion parameters and reactions of released interstitial hydrogen atoms and molecules were established. A highly efficient defect formation channel involving secondary photoreactions with interstitial atomic hydrogen was elucidated. The effect of fluorine doping on the transparency at the ultraviolet absorption edge was studied and it was shown that increase in transmission is due to reduction of the number of strained SiO bonds by fluorine doping. Fluorine doped g-SiO_2 is considered as optical material for fluorine excimer lasers.

Work package WP11- Photo- and e-beam induced processes in amorphous chalkogenide semiconductor and fullerene C_{60} thin films (Dr. J. Teteris)

A solid immersion holographic method for the recording of refractive-index and surface-relief modulated regular nanostructures in amorphous chalcogenide semiconductor thin films has been developed and studied. This method can be applied in nanotechnology and information technology for holographic recording and storage of information with ultrahigh density

Work package WP19 – Defects and their dynamics in alkali earth fluorides (Dr. B. Berzina

The luminescence mechanisms of native defects in aluminum nitride ceramics and cubic boron nitride ceramics were established. The dosimetric characteristics of AlN ceramics were obtained and it was shown that it is a promising medium for ultraviolet light dosimetry. Applicability of synthetic diamonds in UV light dosimetry was established as well.

Narrowing of the band gap of hexagonal boron nitride (h-BN) nanotubes in comparison with that of the h-BN macromaterial is demonstrated.

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Network 3. Advanced ferroelectric materials

Deliverables achieved:

D1 - **Research report** for each half – year of CAMART
D2 - **Publications** (new knowledge) annually in high – rating international journal
D3 - **Presentations at scientific conferences and workshops** on average 20 yearly over the network
D4 - **Dissemination of achievments** trough organization International conference AOMD – 3
D5 - **Increased networking** between centres – participation at network "Interfacial effects, novel properties and technologies of nanostructured materials"
D7 - **Knowledge transfer** via training of master and PhD students as well as at the scientific seminar of ISSP
D8 - **Enhanced participation in other areas of the 5th or 6th Framework programme:** Research Network "Polar Electroceramics", supervisor Dr.V.Zauls; Network of Excellence "Multifunctional and Integrated Piezoelectric Devices", supervisor Dr.V.Zauls
D9 - **New devices;** designed and tested electrooptic ceramic elements with integrated functions for Q-switching and output coupling; dedigned and tested Fabry – Perot type dielectric laser output couplers for midinfrared medical lasers

In the following , the summaries of the specific results by each work package within network 3 are listed.

WP 12 – Investigation of diffused phase transitions and processing new ferroelectric perovskites for electromechanical applications (Dr.habil. L.Shebanovs)

A series of antiferroelectrics with chemical formula $PbB^{3+}_{1/2}Nb_{1/2}O_3$ were synthesized by solid state reaction from oxides and carbonates. Ceramic samples were produced by hot pressing sintering. The data of X-ray diffraction and differential thermal analysis were used to select optimal conditions for solid state reaction of compounds. According to the X–ray analysis the ceramic samples of $PbB^{3+}_{1/2}Nb_{1/2}O_3$ with B^{3+}= Lu, Yb, Tu, Er were mainly single-phased with little amount of pyrochlore phase and had the perovskite structure characterized by monoclinic distortion and sharp phase transition from paraelectric to antiferroelectric phase near 300 ^{0}C. They belong to complex perovskites with highly ordered arraengement of B–site cations. It should be noted that the compounds with B^{3+} = Ho, Tb and etc. were not obtained as a mixture of perovskite and pyrochlore phases. As it was found from literature studies the compounds with B^{3+} = Ho, Sm and etc. of rare-earh ions with larger radius can be synthesized by solid state reaction under high pressure up to 6300 kN. The investigation of $PbHo_{1/2}Nb_{1/2}O_3$ showed a failure of the synthesis. The nearly dense packing of the crystallographic structure in the $PbB^{3+}_{1/2}Nb^{5+}_{1/2}O_3$ accounts the geometric peculiarities in the composition line B=Lu, Er, Ho causing a gradual ''hardening''of parameters of synthesis in the compositions. By use of the ion radius 0.93 Å, 0.96 Å and 0.97 Å of Lu^{3+}, Er^{3+} and Ho^{3+} accordingly, the tolerance factor is calculated. The gradually decreasing low values of t = 0.83; 0.82; 0.81 become critical for the perovskite structure revealing a remarcable B–O bond strain in

BO_6 octahedron. Apparently, in the case of $PbHo_{1/2}Nb_{1/2}O_3$ the overstrain of bonds in the ABO_3 perovskite structure becomes thermodynamically unstable. The PHoN is located at the far end of the region of perovskite structure formation in the series of isomorphous substituents Lu →Er→Tu →Ho.
The processing of electroceramics by means of chemical solutions has become increasingly important especially in the producing transparent $Pb_{1-x}La_x(Zr_{0.65}Ti_{0.35})O_3$ (PLZT) ceramics of large size. We have worked out original two-stage co-precipitation method from mixed solution of inorganic salts, as follows: $ZrOCl_2 \cdot 8H_2O$, $TiCl_4$, $La(NO_3)_2 \cdot 6H_2O$, $Pb(NO_3)_2$, which are commercially easy available and cheap. At the first stage hydroxopolimer of TiO_2-ZrO_2-La_2O_3 is obtained by co-precipitation from mixed solution of corresponding metallic salts by 10% NH_4OH. In result "dry" curds, snow-like deposit was obtained (without any liquid phase). After it thermal decomposition at 1000 ^oC for 4 h white powder of above mentioned oxides was obtained.
At the second stage PbO was introduced in powder produced at the first stage of reaction by milling in $Pb(NO_3)_2$ solution for 10 h. After co-precipitation of obtained suspension by mixture of NH_4OH and H_2O_2 the deposit of peroxohydroxopolimer was produced. After filtration the deposit by waterpump and thermal decomposition at 600 ^oC for 4 h we have obtained PLZT powder of desired composition with perovskite structure.
Transparent PLZT ceramics of large size were produced by two-stage hot pressing sintering. The first stage was performed at 930 ^{o} – 980 ^oC for about 1 h in vacuum at 20 MPa pressure. The second stage was performed at 1150^o-1200 ^oC for 1 ÷ 40 h depending on size (15 ÷ 90 mm of diameter) at pressure 20 MPa in air or rich in O_2 atmosphere. The optical transmittancy of ceramic plates (thickness 0.3 mm) measured at wavelength λ= 630 nm reached 67 - 69 %.

WP 13 – Nonequilibrium thermodynamics of multicomponent dielectrics in presence of paraelectric – ferroelectric phase instability (Dr.E.Klotins)

Objective of this WP was time propagation of polarization response under alternate driving being a challenge for technological applications of advanced electronic materials and for theoretical modeling as well. In context of the CAMART project this objective harmonizes with WP15 (Computer modeling of the Advanced Materials).
As a method the theory of complex systems was used.
Principal activities include:

- An extension of standard thermodynamical approach toward a globally/locally coupled model representing the kinetics of polarization by a Schrödinger – type relation sufficient for numerical solutions.
- Statistically decomposition within spatial-polarization mesh resulting in original computing codes for the first nonlinearly and nonstationary model of thermodynamic phase instability.
- Test calculations focused on hysteresis, polarization switching and finite size effects.

Results and achievements

- The major result is a nonlinearly and nonstationary model for thermodynamic phase instability.

§ Particular results include: remnant polarization exhibiting itself at overcritical coupling, time propagation of polarization switching under arbitrary pulse, and finite size effect on the remnant polarization. This opens a way to model electroelastic interactions, multiple dimensions, and allows connections with first principle results.

WP 14 – Finite size effects in ferroelectric thin films (Dr.V.Zauls)

Studies of the size effects with regard to material composition-deposition related parameters and obtained structure-property relationships were carried out in thin ferreolectric films and heterostructures. Compounds under investigation included highly oriented perovskite structure PZ, PZT, PLZT, PMNT, (Ba,Sr)TiO_3, PLuNT and other thin films of various compositions formed by rf sputtering, pulsed laser ablation and by the sol-gel process working jointly with University of Saarland, University of Oulu and Jozef Stefan Institute, Institute for Solid State and Materials Research, Dresden and Tartu Institute of Physics.

Dielectric studies of various nanostructured ferroelectric (FE) or relaxor thin films and heterostructures have been made using newly developed Fourier-analysis of dielectric response under sinusoidal ac-drive supported by traditional LCR bridge and impedance analysis in the wide spectral range up to 1 GHz in collaboration with Oulu University and Vilnius University.

Optical spectral reflectometry and multiple angle null ellipsometry were developed jointly with Potsdam University as an efficient nondestructive tools for measuring thickness and refractive index of transparent or reflective thin films and heterostructures, revealing surface roughness and electrode passive layer effects.

The basic technologically important parameters for application of ferroelectric and relaxor thin films such as local piezoresponse and polarization state can be probed with nanoscale resolution using atomic force microscopy (AFM) introduced in our laboratory. Various AFM operation multi-pass regimes allow us direct poling of the nanoregions in a voltage lithography mode and immediate testing local piezoresponse. These domain manipulation and imaging techniques were developed together with colleagues from MPI Halle and Aveiro University.

WP 15 – Electromagnetic radiation in ceramics in presence of paraelectric – ferroelectric phase instability

Objectives of this work was (a) elaboration of a new type of laser with electrically controllable radiation, and (b) eraseable holographic recording pilot model designs for industrial and life – science applications.
The ceramics for investigation and application was commercially available lanthanum modified lead zirconate titanate electrooptic ceramics (PLZT) transparent to electromagnetic radiation over visible and infrared region.

Principial activities in objective (a)comprise:

- Full scope theoretical modelling (in Mueller matrix representation)of the electromagnetic radiation determined by microscopic scale inhomogeneous structure controllable by electric driving and/or mechanical stress.

- Elaboration of a guide for analysis, material specification, and device design based on electrooptic ceramics.
- Design of active elements for a new type of spatio-temporal-frequency modulated laser for space applications (in partnership with Dr.phys. V. N. Alekseev, Research Institute for Complex Testing of Optooelectronic Devices and Systems, Sosnovy Bor, Russia).

Principial activities in objective (b)comprise:

- Electroooptic PLZT ceramics with large electrooptic effect, holographically induced birofringence and remarkable electrically controlled light scattering were synthesized and devices for controlling the coherent and incoherent light transmittance were designed.
- On studies of writing of holographic pattern in PLZT ceramics modulators using Ar^+ laser radiation a device for physics education laboratory work "Writing of the holographic patterns in the solid state photorefractive media" (using rewritable PLZT ceramics school modulator as a photorefractive media) is designed.

Main results and achievements:

- Propagation and scattering of electromagnetic radiation in electrooptic ceramics is described, first time, in terms of the chaotic phase screen model recovering the anisotropic nature of scattering and explaining discrepancies between experimental evidences and conventional approaches.
- Users guide: Electooptic ceramics: material specifications and test methods. The scope and framework is addressed to technologists and manufacturers and covers grey scale, interferometric, intercavity applications and life science.

WP 16 – Development of midinfared medical laser systems with transparent ceramics passive and active optoelectronics elements (Prof.Dr.M.Ozolinsh)

PLZT ceramics with composition within the range PLZT 8,75-9.25 are manufactured using different synthesis parameters to obtain efficient electrooptic material for use in 2-2.5 micrometer wavelength range. Dielectric and electrooptical investigation and ranging of materials within the coordinates: electrooptic effect/optical phase shift at laser irradiation wavelength/temperature were perfomed for these materials.
Laser resonator configuration was tested for the Er:Cr:YSGG - 2.79 mm, and Er:YAG - 2.94 mm pulse midinfrered lasers; new designs of Q-switching are developed - incorporating the PLZT ceramics elements in the resonator as Brewster plate as an element to obtain polarized laser emission and as plane parallel plate instead a dielectric mirror as an resonator output coupler.
The high refractive index (2.25 at 3 mm) of PLZT ceramics Brewster plate inside the laser resonator was used to obtain efficient laser polarization needed for electrooptical modulation (for Er:YAG laser the output of the linear polarized emission was up to 500 mJ at pump energy 338J) and a PLZT plate was used also as a passive resonator output coupler in a configuration allowing to obtain the laser output up to 400mJ for Er:YAG laser).
Main result – active elements for systems of medical diagnostics and treatment were developed and tested**.**

WP 18 – Organization of 3rd International Conference (AOMD-3) and Supervisory Board meeting of CAMART (Prof. Dr.A.Krumins)

The Conference was organized at August 19 – 22, 2002 by the Institute of Solid State Physics in collaboratorion with the Baltic Chapter of SPIE and Institute of Physical Energetics LAS. 130 participants alltogether from 21 countries come together to discuss the main results in this field. Latest develpoments and new results were reported in 57 oral and 88 poster presentations, as well as in many discussions trough out the meetings.

The main sections covered during the Conference were:

- theory of optical materials;
- organic optical materials;
- inorganic optical materials and radiation effects;
- semiconductor optical materials, nanostructures and SPM technique;
- ferroelectric optical materials and applications;
- holographic materials and optical recording;
- electrochromic devices, wavequides, sensors and laser technoloqies;
- optical devices and methods for vision science and medicine

The Conference abstracts were published before the meeting. Manuscripts of the prepared reports were edited during the Conference and is published in 2003 in two special issues of International journal "Proceedings SPIE":

- vol. 5122 "Advanced optical materials"; editors A.Krumins, D.Millers, I.Muzikante, A.Sternbergs, V.Zauls.
- vol. 5123 "Advanced optical devices", editors J.Spigulis, J.Teteris, M.Ozolinsh, A.Lusis.

The sponsors of the Conference were European Community (5th Framework programme), SPIE – The Internacional Society for Optical Engineering, European Office of Aerospece Research and Development, Latvian Council of Sciences, Stora Enso Packaging SIA.

The meeting of International Supervisory board takes place August 18 2002. The recomendations of the meeting see at the appendix.

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Network 4. WP-22
Materials for vision science (Prof. Dr.M.Ozolinsh)

Deliverables achieved:

D2 – **results reported in conferences**
D3 – **results published in scientific journals**
D7 and 22D8 – knowledge transfer between partner institutes and enhancement of competence (***PhD*** degree obtained – G.Krumina, expertise of workpackage staff members, new courses for Optometry departments students – "Electrophysiology")
D12 – optical active materials for dynamic occlusion devices are studied (PLZT ceramics and PDLC liquid crystals) and devices for vision science experiments developed
D13 – **visual perception and vision quality characterization techniques** are designed, psychophysical and objective perception techniques are developed and installed for visual performance studies of system eye+appliances: lenses, progressive ophthalmic lenses, light scattering obstacles (characterization parameters: visual acuity, contrast sensitivity, colour discrimination, stereovision acuity, etc.)
D14 – new devices to control optical visual information and simulate eye cataract designed

Objectives
- to develop and to study new bulk and thin film optical materials applicable for vision correction aids and for vision science investigations in order to characterize visual performance in different model and real life conditions;
- to study aberration effects and image quality of the eye optical system using optical appliances and inducing unfavourable side effects;
- development and use of advanced materials in new optical and pshychophysical testing and training technologies (for proper fitting of vision correction tools, in diagnostics of vision characteristics and defective vision - orthooptics, binocular, stereovision, ambliopia, low vision and other vision insufficiencies).

Research methods
We used in our studies commercially available optical materials, lenses and appliances and specially developed optical smart materials with dynamically controllable properties (partially with different degrees of light scattering – ***PLZT ceramics and PDLC liquid crystals***). Research methods were based on available in the ISSP scientific equipment for spectral colour analyse of optical materials transmittance, visual stimuli emittance and reflectance colour analysis (***Ocean Optics*** fibber spectrometer); special for the workpackage designed computer presented colour, 3D-stereo, dynamic visual stimuli software package; new installed vision electro physiology equipment "***Neurosoft***" for an objective characterization of the visual response; besides equipment to measure aberration characteristics, image point spread function and modulation transfer functions of the partner institute (*University of Murcia*).

Results.
A number of optical passive materials used in advanced eye appliances and new active materials allowing to control image flow through the system ***appliance+eye*** forming the retinal image are studied to characterize the visual performance.

New technique based on the cross-cylinder method using a subject drive eye aberration pattern alignment with a computer simulated reference pattern on a PC display developed.
Eye model with simulating eye lens cataract, studies of visual stimuli image formation on artificial retina on dependence of the lens scattering degree.
Studies of optical transfer and point spread function using double pass method for a model eye system.
Psychophysical vision experiments were set to measure vision acuity, stereovision, colour perception in combination with coloured selective filters, eye corrective devices and occluders modelling scattering. Conditions to improve colour discrimination using coloured selective filters are determined.
Studies of optical retroreflective materials and illumination conditions in order to optimise ergonomics of vehicle drivers at night to avoid vision loss during the glare creating by oncoming vehicles.
New electrophysiology equipment to measure electrical brain response of visual stimuli was set up and approved.
The main aim of this workpackage 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 to different geometry construction of the vision correction devices and influence of unfavourable environmental and physiological factors on visual performance.

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Tagung der Deutsche Ophthalmologische Geselschaft-2001, Berlin, 2001.
European Conference “Human factor in Transportation,” Turin, 2001.
Int. Meet. of American Academy of Optometrists “Academy in Alps-2002”, Munich, 2002.
IXth Int.Conf. ”Laser Applications in Life Sciences”, Vilnius Univ., 2002.
12th General Conf. Of the European Physical Society “Trends in Physics”, Budapest, August 26-30, 2002.
The 3rd International Conference “Advanced Optical Materials and Devices”, Riga, 2002.
The ***25th European Conference on Visual Perception***, August 2002, Glasgow.
ICO Topical Meeting on Polarization Optics (ICOPO) , Polvijärvi 2002.
The ***10th European Meeting on Ferroelectrics EMF-10***, Cambridge, 2003..
The ***26th European Conference on Visual Perception (ECVP),*** Paris, 2003.
The 10th International Conference “Vision in Vehicles” VIV-10, Granada, 2003.
Meet. of ***American Academy of Optometrists***, Dallas, 2003.
The ***4th Conf. “Ocular Biomechanics-2004”***, Moscow, 2004.
ECVP-2004, Budapest, 2004.
The ***3rd International Conference on Traffic & Transport Psychology***, Nottingham, 2004.
The ***II EOS Topical Meeting on Physiological Optics***, Granada, 2004.
«Basic Problems of Optics», Topical Meeting on Optoinformatics, St.Petersburg, 2004.
Conference OSAV-2204 Optical Sensing and Artificial Vision. St.Petersburg, 2004.

Network 5. Solid state ionics and devices

Deliverables achieved:

D1 - **Research report** for each half – year of CAMART
D2 - **Publications** (new knowledge) annually in high – rating international journal
D3 - **Presentations at scientific conferences**
D5 - **Increased linkage** with economic and social environment; joint RTD projects with enterprise for development prototypes of devices
D7 - **Knowledge transfer** via training of master and PhD students
D12 - **New materials** for sensors
D14 - **New devices** and methods for food quality control and fight against fraund
D15 - **Enhanced participation of centres in other areas of the 5th and 6th EC Framework** programme:

- § STRP "Nanoscale chemical mapping and surface structural modification by joined use of x-ray microbeams and tip assisted local detections", supervisor Dr.habil. J.Purans
- § Collective research project "Removal of hazardous substances in electronics", supervisor Dr.A.Lusis

In the following, the summaries of the specific results by each work package within Network 5 are listed.

WP 27- Organization of Regional seminar on Solid State Ionics (RS-SSI 2001)(Dr. A.Lusis)

The objectives of seminar "RS-SSI 2001" had been achieved. Within this activity for 11 invited speakers on seminar were covered full expenses. Part of papers presented on seminar has been published special issue of "Journal of Solid State Electrochemistry, vol.7, Nr.2, 2003, guest editor A.Lusis, which collected new knowleges in Ionics and Functional coatings, Batteries and Fuel Cells, Materials and Technologies, Intercalation electrodes and Electrode reactions, Fast ion conduction phenomena and Solid electrolytes, and Sensors

WP 28 - Participation of researchers in conferences and research visits (Dr.A.Lusis)

Totally 14 scientific events (conferences, symposiums, workshops, seminars, coordination meetings) and 11 visits (research, training and networking) had been attended by researchers from Semiconductor Material Department of ISSP. The preference for research visits and participation in conferences had been given for students and young researchers (MS student L.Grinberga, PhD student G.Veveris and Dr. A.Kuzmin). Visits are listed at the Activity report

WP 29 - Organization of 10th International Symposium on Electronic Nose (ISOEN'03) (Dr.J.Kleperis)

The initial activity of WP29 was "Organization of International Meeting on Solid State Electrochemistry" in 2002, but it had been changed to "Organization of 10th International Symposium on Electronic Nose (ISOEN'03)" in 2003 and was organized by ISSP of UL in Riga, June 25-28, 2003. Within this activity for 10 invited speakers as well as for 10 participants on seminar were covered expenses. The symposium was excellent place for local scientific and engineering community to give awareness new emerging technologies. 93 participants from 22 countries come together to discuss the main results in sensor and sensor array technologies, e-nose minituarisation, odour description in electronic files and unified description language formation, e-nose application in different fields, making emphasis on product adultaration and environment pollution problems. Latest developments and new results were reported in 49 oral and 28 poster presentations, as well as in many discussions through out the symposium. The Symposium Abstracts were published before the meeting in special book on 281 pages (A4 format). Manuscripts of the prepared reports were edited during 12 months after meeting and will be published in 2004 in special issue of the International Journal from Elsevier "Sensors&Actuators, B: chemical sensors"; editors J. Kleperis and A. D`Amico.

WP 30 - Visiting fellows for teaching and training (Dr.A.Lusis)

The objectives of WP-30 have been achieved by inviting professors and researchers which are represented excellent groups in solid state ionics and device area. Within this activity 16 visits of partners were paid by project (see Activity report)

WP 31- In-situ X-ray Absorption Study of Transition Metal Oxides (Dr.habil.J.Purans)

The objectives of using of large scale facilities (synchrotron radiation) in France and Italy for characterisation of atomic structure and properties of mixed RE:TM, TM:TM oxide thin films have been realized and develop new mixed RE:TM, TM:TM oxide thin films with optimum optical and electrical properties for electrochromic devices by using of the multi-magnetron and laser technologies. In-situ XAFS, XRD and IR study of local atomic and electronic structure have been done, which provides new insights in to the local structure of amorphous and nanocrystalline electrochromic oxides, nature local atomic and electronic due to the small polaron formation and Jahn-Teller effect in the mixed valence TM oxides and insertion (electrochromic process) of electrons and ions into TM oxides and electrochromic (gasochromic) devices.

WP 32 - Synthesis and characterization of materials for fuel cells (FC) and metal hydride batteries (MHB) (Dr.A.Lusis)

Objectives to obtain new knowledge and to analyze the state of the art in the area of fuel cells as well as of solid electrolytes and electrodes have been done. That is realized by study properties of solid electrolytes and electrodes and their degradation during ion

insertion and extraction as well as approved preparation technology of H-ion insertion and catalyst electrodes layers based on Ni. There have been sated co-operation and exchange of researchers and Ph.D. students plan with Department of Chemistry of Warsaw University for study interfacial phenomena, finished review article about metal hydrides and started to prepare advance teaching course "Solid State Batteries" for graduate students. The obtained results lead us to new conclusions concerned with catalysis, storage of hydrogen and new conceptions of fuel cells. There have been worked out model for performance of thin film electrochemical cells, which helps to solve the problem of cycling capacity for ionic devices or electrochemical cells (ECC) with intercalation electrodes. The multi layer thin and thick film technologies allow miniaturization of electrochemical cells for FC and MHB.

WP 33 - Study of high temperature super conductors (HTSC), solid state batteries (SSB) (Dr.A.Lusis)

Objectives of research of HTSC to clarify the relationship between the rearrangement in the first, second and next coordination shells of TM and RE metal and change of their electronic structure during the cooperative effects in different compounds with TM and RE metals have been done. To learn and pick up new knowledge and experience in preparation and research of electrodes and solid electrolytes as new material for ionic devices (batteries, capacitors, sensors) have been performed. The common research work (Department of Chemistry of Moscow State University, Institute of Experimental Cardiology, Moscow, Institute of Problems of Chemical Physics Russian Academy of Science) on UHF magnetic effects on HTCS was base for preparation project proposal "Mercury cuprates: superconductivity, ions pairs and electron spin resonance" for INTAS program. Application of super ionic conductors of $Li_{1+x}M_x\ Ti_{2-x}(PO_4)_3$ and $Li_{1+x}Ge_{2-x}M_x(PO_4)_3$ in batteries have been worked out based on common work. The lithium cell – prototype – was built up based on such new materials and charge-discharge properties investigated. New conception is developed how to apply the Li/polymer foil in preparation of Li-ion electrode based on polymer substrate and application such coatings for Li ion electrochemical cells. The lithium electrode for Li/polymer batteries and for supercapacitors was investigated. The Li-ion thin film coatings (made in a/s "SIDRABE") have been tested for supercapacitors. Particularly Li_2CuO_2 shows high initial charge capacity.

WP 34 - Practical application of artificial olfaction in the control of quality and adequacy of goods (Dr.J.Kleperis)

Objectives of this twining project are to arrange the cooperation with center in Europe (Tubingen University) and for preparing joint research and implementation project of "electronic noses". New intelligent instruments and especially artificial olfaction technologies and in particular 'electronic noses' are emerging technology. The laboratory prototypes of e-noses have been used for research odors of food, beverages, alcohol, textiles etc for development application technologies how to control quality them. Odors from different production facilities as well in Industry, as well as in Agriculture and also in Oil transport enterprises are causing problems throughout the world. During last 3 years complaints on odours in Latvia grew exponentially. Obtained new knowledge on nature of odors and application technologies for intelligent instruments was base to help

Latvian government to implemented European Standard EN 13725 “Air Quality – Determination of Odor Concentration by Dynamic Olfactometry”, which was accepted on April, 2003.

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Concluding remarks

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

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

Due to EC funding, **four international scientific events and scientific seminar of Institute** were organised by the Centre. These meetings upgraded the level of education in the scientific field of the project and were stimulating for the Institute's staff, as well for the visitors from European partner institutions. The CE project stimulates attracting of **young researchers** and modernisation of study programms in physics.

Centre of Excellence funds enabled to **improve the scientific infrastructure** of the Institute. Due to financial support from Latvian government, on condition that a part of expenses is covered by CE funds, in 2002 – 2004 was purchased scientific equipment by 200 000 EUR.

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

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

Prof. Dr.A.Krumins
scientific coordinator
of CAMART

Annex 1

EVALUATION REPORT
of the International Supervisory Board
on Research, Education and Development activities
of the Institute of Solid State Physics, University of Latvia

Overview

Institute of Solid State Physics (ISSP), University of Latvia was established on the basis of the University's two Problem Laboratories: Semiconductor Physics and Ferro- and Piezoelectric Physics – in 1978. Since 1986 the ISSP has the legal status of an independent organization of the University. The research activities of ISSP include:

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

The highest decision-making body of the ISSP is the Council of 23 members elected by the employees of the Institute. The total staff number of the ISSP is 175, including 31 Habilitatus Doctors of Sciences, 46 Doctors of Sciences and 52 students.

The research activities of the ISSP in 2001 were reflected in 210 publications in the internationally recognised scientific journals. The staff of the Institute has succeeded in 31 national science grants and one national co-operation project with total financing in 2001 (maintaining the same in 2002) of 238.8 thousand lats (LVL). Contracts and market orientated research in 2001 was for sum – 116.5 thousand LVL. Other financing -79 thousand LVL.

The ISSP carries out RTD projects in co-operation with Latvian enterprises (Joint Stock Companies Sidrabe, Alfa, Alfa Pro., Baltic Scientific Instruments, Valmieras stikla skiedra), as a spin-off of some other projects two SMEs (Hologramma Ltd., Dardedze Holografija Ltd.) are established at the Institute.

In order to improve the energy efficiency of the building a large scale reconstruction work in the framework of the State investment project, comprising the total sum of 418 thous. LVL, has been carried out in the laboratory part of the house during the last four years (change of thermal insulation of outer walls and windows, building of double-pitch roof, a partial renovation of the interior), making the stay in the Institute more comfortable and conserving energy.

From the beginning of 2001 the ISSP has the status of the European Commission (EC) Centre of Excellence for Advanced Material Research and Technologies (CAMART) with the following main tasks:

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

The research activities in the CAMART are carried out on:

- functional disordered materials;
- advanced ferroelectric materials;
- computer modelling;
- materials for vision science;
- solid state ionics and devices.

In 2001 these activities were supported by the EC financing - 158 thousand LVL. In addition several other EC projects (EURATOM, POLECER) are going on in the ISSP which give total international funding 183 thousand LVL.

The total financing for the ISSP in 2001 thus comprised 617.3 thousand LVL (the international funding making 30%).

ISSP has developed different kinds of wide-scale international collaboration and has submitted more than 10 "Expressions of interest" for the Integrated Projects and Networks of Excellence in 6 FP.

The ISSP has recently intensified its teaching activities. Three research staff members of the Institute have been elected as professors of the University of Latvia, and other three - as professors of Riga Technical University, and the University of Daugavpils. Postgraduate and graduate curricula are offered in solid state physics, material science, chemical physics, physics of condensed matter, semiconductor physics, and in experimental methods and instruments.

Achievements and Problems

1) Most of the research activities of the ISSP have high internationally recognised scientific quality (publications, good citation, active participation in the international projects, etc.), but the average salary of scientific staff (120 LVL/month) is lower than the average salary in Latvia (157 LVL/month) in 2001. The low salaries make it hard to attract young researchers to work in the ISSP.
2) Up to now the ISSP is accomplishing its research in a satisfactory way, but there is an urgent need for modern scientific infrastructure.
3) Large concentration of high quality scientific staff in important fields of solid state physics and material sciences is the basis for good scientific perspectives of the ISSP, but there is an urgent need for a new generation of researchers, because the average age of research staff in the ISSP is around 52 years.
4) The ISSP has increased its share in the higher education at the universities of Latvia, but special requirements for the election to the academic staff of the universities make the participation of the ISSP researchers in the teaching activities rather difficult.
5) Active participation of the ISSP in the international projects is welcomed, but long delays of the payments from EC and small co-financing from Latvia's side (only ~25%) make it hard to fulfil these projects.

Recommendations

1) To guarantee the internationally competitive level of scientific research in the ISSP, in the future it is necessary to allocate additional financial resources from the State budget of Latvia for the ISSP.
2) The ISSP must play a more active role to stimulate the start of the National Programme of Materials Science with appropriate additional financial resources from the budget.
3) Development of modern scientific infrastructure (equipment, e.g., SEM with EDX, IR Fourier spectrometer; multicluster computer; technologies, e.g., MOCVD reactor, PLD system, improved library facilities included online access to international journals etc.) estimated to costs of 2 Mio. LVL is urgent in the ISSP.
4) International projects must have appropriate co-financing in agreement with the rules of the European Commission from the State budget. Delays of EC payments

for the projects must be avoided. If this is not possible national resources must be available as a buffer.

5) For successful work in future the ISSP must have the legal status of a self-governing organization of the University of Latvia.
6) It is recommended that a sound long-term recruitment plan for staff members is made.

Signed (approved) by the International Supervisory Board:

18.08.02

Prof. Gunnar Borstel, University of Osnaebrueck, Germany

18.08.02

Prof. Niels E.Christensen, University of Aarhus, Denmark

18.08.02

Prof. Claes-Goran Granqvist, Uppsala University, Sweden,

18.08.02

Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia

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Prof. Sergei Tuituinnikov, Joint Institute for Nuclear Research, Dubna, Russia

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Prof. Juris Upatnieks, Applied Optics, USA

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Prof. Harald W.Weber, Atomic Institute of Austrian Universities, Vienna, Austria