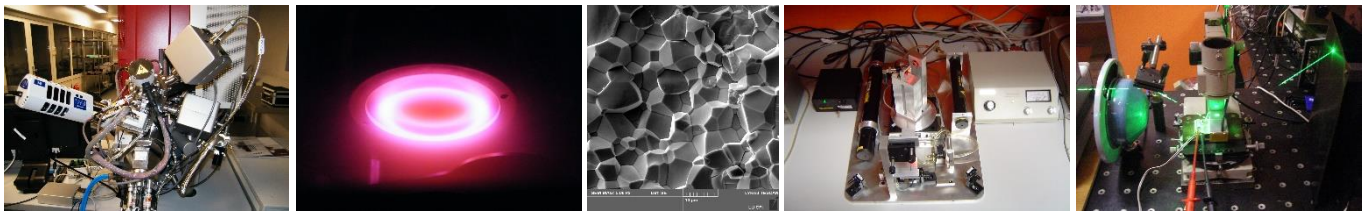




**INSTITUTE OF SOLID STATE PHYSICS
UNIVERSITY OF LATVIA**

RESEARCH PROGRAMME 2019 - 2023



**Riga
2019**

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Executive Summary

The present Research Programme formulates the practical implementation of the mission of the Institute of Solid State Physics University of Latvia (further ISSP UL) in the years 2019-2023 following its general strategy: *To transfer excellence in material science into highly educated people and innovation.*

The first part of this document is devoted to an assessment of the present state of the scientific activities at the ISSP UL and followed by a second part, which outlines the principal directions of further development in the period 2019-2023 with the goals to enhance the efficiency of the research and technological innovation activities of the institute and to increase its competitiveness at both national and EU levels.

The Research Programme of ISSP UL puts emphasis on four top Priority Directions. These Priority research Directions have been strategically established for increasing strong international scientific capacity and are further elaborated and implemented within four interdisciplinary and inter laboratory mission-oriented Domain groups.

I. Theoretical and experimental studies of materials structure and properties

Domain: Functional materials theory & modelling;

II. Nanotechnology, nanocomposites and ceramics

Domain: Sensors & actuators;

III. Functional materials for electronics and photonics

Domain: Photonics & micro & nanoelectronics;

IV. Energy

Domain: Energy

1. Strategic context

ISSP UL research programme uses the instructions and recommendations of Europe 2020 strategy, EC recommendations for development R&D strategy of Latvia, strategy for smart specialisation (RIS3), priority directions in science and regional development plans. The gained information is linked with investigations of the national and regional situation and future perspectives to define the roadmap to transform ISSP UL into a new competitive European level scientific centre where research, education and business will work together and complement each other.

Guidelines for Science, Technology Development, and Innovation 2014-2020 (Cabinet of Ministers of the Republic of Latvia order No 685, 28 December 2013) state that for the transformation of national economy to the knowledge and innovation-based model it is necessary to form globally competitive Latvian science, technology and innovation industry that could support the needs for development of the national economy and society¹. It is clear that successful impact of research and innovations on economic development depends not only on the results of activities, but also on cooperation, infrastructure, environment and regeneration of human resources.

The goal of the ISSP UL research programme and strategic development plans is to maintain and increase the fundamental research level (that is highly evaluated in the International research assessment exercise from Technopolis group²) but also to promote further development of research and industry connection by offering infrastructural and intellectual support.

¹ https://www.em.gov.lv/files/nozares_politika/2014ino.pdf

² http://www.izm.gov.lv/images/zinatne/ZISI/Latvia-systems-review_2014.pdf

The research programme foresees to promote the general public understanding of the "Europe 2020" priority "For Smart, Sustainable and Inclusive Growth", which aims to improve the quality of education and to strengthen the research performance, to foster innovation and knowledge transfer, ensuring that innovative ideas can be turned into new products and services. Any new smart material, methodology or know-how, that can be used to improve the product, allows one to understand better the processes or to develop technology and thus support the achievement of economic growth.

The foundation of the ISSP UL research programme maintains the compliance not only with European directives but also with the Priority Directions in Science for 2014-2017 "Innovative and advanced materials, smart technologies (multi-functional materials and composite materials, nanotechnologies and photonics, computing, computer science, information and communications technologies, signal processing technologies)", in accordance with Section 13, Paragraph two, Clause 3 and Section 34, Paragraph four of the Law On Scientific Activity. All corresponding research areas smoothly overlap since scientific and research activities at the ISSP UL are multi- and interdisciplinary as well as take into account all respective priorities of Key enabling technologies (KET - Advanced Materials, Photonics, Nanotechnology and Micro- and Nanoelectronics) and RIS3.

Based on knowledge, experience, cooperation and competences of ISSP UL, the research programme promotes various scientific and educational activities in material research and nanotechnology, alternative energy sources (solar & hydrogen energy), energy efficiency (LED and OLED, heat loss reduction) and nuclear (fusion) energy, photonics and electronics, which are related to such RIS3 directions as advanced materials, technologies, and engineering, smart energy, biotechnology, information and communications technology (ICT) development.

ISSP UL research programme includes different actions to stimulate and support productive research of new materials and technology creation, meaningful use and diversification of already known materials and processes, paying intensified attention to the studies of material pre-treatment, creation and modification of products and services with high scientific added value. The performed activities also contribute to the continuation and expansion of cooperation with the Latvian industries by promoting investment in the R&D&Innovation, thus supplementing EC growth strategy and reaching Europe 2020 objectives.

Upgraded advanced science laboratories, an established appropriate development programme, well-equipped technical environment, experimental workshops and pilot plant elaboration possibilities, which are open for each respective scientific project or business research, are the most favorable conditions to promote cooperation between entrepreneurs, scientists and students. The created base of high-quality knowledge and expertise will serve for preparation and training of highly skilled research institution, academic or innovative company employees that in return will increase public and business investment in research and innovation, which are crucial elements of the strategy "Europe 2020" and the National Reform Programme of Latvia for the Implementation of the "Europe 2020" objectives. Such activities will strengthen ISSP UL position locally and internationally, will create new jobs and global competitiveness that after all will lead to the economic growth of Latvia³ to reach EC recommended 3% of GDP level for R&D investments in every Member State.

Much attention in the ISSP UL research programme is devoted to the education and sustainable renewal of professional and highly qualified scientific personnel. The research programme is not focused exclusively on local interests. A lot of attention is paid to the

³ http://ec.europa.eu/europe2020/pdf/nrp/nrp_latvia_en.pdf

potential cooperation with regional institutions of higher education, training of students and specialists as well as to attract regional entrepreneurs and their possible investments. Latvia is a geographically small country; therefore, the education, science and research activities in the framework of the common use of equipment, research co-operation and sharing of knowledge cannot and should not be separated in specific regions.

Territorially ISSP UL is located in the Riga planning region and the institute's strategic objectives as well as the developed research programme are consistent with the long-term goal of Sustainable development strategy of Riga until 2030 (approved by the Riga City Council 10.22.2013. Decision No. 302), which states that the development of Riga city as the administrative, cultural, higher education and research centre is a prerequisite for innovative, open and export capable economics. By increasing infrastructural and human potential of scientific institutions it is planned to strengthen business and science cooperation in order to improve competitiveness, innovation level and new product development to promote all Riga economic sectors and businesses. ISSP UL research programme includes also feasibility studies of industrial development, improvement of cooperation with universities and scientific institutes operating in Riga, in order to create new jobs and economic growth.

Moreover, the ISSP UL research programme activities are in line with all Latvian territorial specializations, where science, education and industry cooperation is considered as a priority. One of the aims of the research programme is a linkage of innovative business, excellent research and higher education and promotion of cooperation between all regions in Latvia and beyond. ISSP UL already has a good collaboration with Latgale and Kurzeme regional higher education institutions (Daugavpils University and Ventspils University College) within state research programs and with several entrepreneurs.

Therefore, open scientific laboratories equipped with modern infrastructure, competent researchers 'on demand', and an easy-to-access system are the best conditions to create and maintain long-lasting cooperation and mutual support between entrepreneurs, scientists and students. A great attention is paid to students that will accordingly be prepared for the scientific, academic or entrepreneur research laboratory employee's careers.

In the framework of the ISSP UL strategy and institutional development plan there shall be elaborated a system for monitoring of scientific and innovation results that will reflect R&D&I intensity and influence of public/private/state funding on the outcome. This system shall work together with advanced resource management system thus increasing funding/tasks/rewards for each person of the scientific staff in accordance with the investment, results and skills. Such approach will stimulate efforts to provide high-quality science, to improve and transfer knowledge and skills to students, companies or technical personnel. This type of management system will also help to register statistics and to demonstrate the interdependencies between funding, skills, results and investment to maintain the dialog with society and funding institutions.

The long term mission of the research programme and strategic development plan is to identify and develop power of ISSP UL in the actual situation, to integrate in the European Research Area and an involvement in the creation of joint research programmes with the Member States and regions, especially in the Baltic Sea region.

2. Priority research directions

I. Theoretical and experimental studies of materials structure and properties

Domain: Functional materials theory & modelling

The main task will be further development of existing and novel theoretical and experimental tools, combined with computer simulations, to predict how molecules form particular crystallographic structures. Quantum chemistry and molecular dynamics study of fine structural effects and the next mesoscopic modelling will be valuable in studying of nanomaterial structural, electronic, magnetic and optical properties. Experimental tools include high power computing, x-ray absorption and optical spectroscopies, scanning/electron/optical microscopy and structural methods.

Research and development of novel complex functional materials require deep understanding and characterization of their structural, electronic, magnetic and optical properties. This task becomes even more challenging when applied to nano- sized and/or nanostructured systems. A successful solution to this problem involves a combined use of (i) advanced and conventional experimental techniques, providing local information on the atomic and nanometre scales as well as those that provide ensemble-average measurements, and (ii) advanced theoretical methods, able to describe the material properties at different time and length scales. Strong interconnection between theory and experiment is of key importance for acquiring new knowledge and obtaining a complete picture of material properties.

Nowadays, the availability of high-performance computing (HPC) infrastructure makes modelling and simulations an integral component of research process helping the experimentalists to access information that would not be available otherwise and interpret the experimental results. Moreover, modelling of the evolution of a system is often a quicker and/or cheaper way than with trial and error method, thus allowing speeding up the R&D activities at reduced cost. Since a description of real materials and phenomena is always simplified within a model, its validation becomes the most crucial issue to obtain realistic and reliable results.

To address the challenges faced, a set of measures will be implemented at ISSP UL, including

- maintenance and future development of experimental and computational infrastructure and methods for investigation, better understanding and improving of processes and materials having technological and industrial importance,
- an increase in the **number of staff** and its competence, attracting preferably young and promising researchers,
- strengthening of collaboration with leading research centres to gain an access to unique or large scale (synchrotron and neutron radiation sources) facilities as well as to specific competence.

The successful implementation of these measures during next five years will significantly strengthen the position of the Institute in the R&D fields at the National and EU levels in terms of both research infrastructure and personnel qualification.

Realization of above mentioned measures will drive the science at the ISSP UL within the following five research themes, which were identified based on the institute recent achievements and local market requests:

- I. Theoretical Materials Science
- II. X-ray Absorption Spectroscopy

- III. Optical Spectroscopy
- IV. Microscopy and Structural Methods

The description of each theme, its current state of the art, future prospects, needs and expected results are given below.

Theoretical Materials Science

Modelling is a powerful tool which drives materials research providing the key information for identifying, tailoring and designing of materials and structures. The interpretation of experimental data as material properties relies on models as well. The multi-scale modelling (Density Functional Theory, Molecular Dynamics, Monte Carlo, Hybrid simulation approaches, etc.) allows one to deal with the time and length scale of the processes and determines the size of the studied systems depending on available computing resources. Reliability, transferability and linking of models are the issues to solve.

The activities within the computational materials science address (i) a large-scale electronic structure modelling of various prospective functional materials with perfect and defective 3D, 2D and 1D morphologies [1,2], which are important for a wide range of high-tech applications, e.g., in new sources of energy, catalysis, nanoelectronics, sensorics, spintronics, etc. as well as (ii) self-assembled systems with static and dynamic ordering (nanoparticles in soft matter, radiation defects and colloids in solids), which can serve as prototypical building blocks of nanoscale “switches” and machines [3].

Future developments in the field will require development of new efficient computational algorithms for long-time modelling of large-scale systems of mobile charged nano-particles with a focus on self-assembling and development of new methods in ab initio thermodynamics of advanced technological materials for energetics.

These research activities at the ISSP will be supported by EUROfusion project, EC FP7 GREEN-CC project and ERA.Net RUS.Plus WATERSPLIT project as well as by Latvian funding within National programs and Latvian Science Council grants. The support from ERA.Net project on electromechanical properties of nano-sized ferroelectrics (submitted) is planned in the future.

Current experience and advantages

For atomic/electronic structure calculations, we use massive parallel computations based on ab initio methods, e.g., plane wave (PW) and localized atomic orbitals (LCAO) formalisms within density functional theory (DFT) or state-of-the-art hybrid approach DFT-HF (partly incorporating exact Hartree-Fock exchange) [2]. The electronic properties of various materials are also studied using scattering theory formalism, within the effective medium approximation based on cluster approach, within which we develop semi-empirical formalism of „effective bonding”, for better description of different edge interfacial effects [4]. Cooperative effects in kinetics of bimolecular reactions in condensed matter are studied based on a novel formalism of many-particle densities described in our book [5]. We study also surface-induced reactions in heterogeneous catalysis with emphasis on such fundamental phenomena as pattern formation, reactant self-assembly, regular and irregular reactant concentration oscillations as well as chaotic behaviour. Another activity deals with the defect-controlled growth modes of thin metallic films on oxides and diffusion in ceramics, composites and heterogeneous media which is of great importance for the interpretation of numerous experimental data in the ISSP UL and its partners.

Detailed description of ISSP Theoretical department current activities is available at www1.cfi.lu.lv/teor. The Department is one of leaders in the area of computational materials science in Eastern Europe, publishing annually 20-25 research papers accompanied with 50-60 conference presentations [1-5]. This activity is based on recently upgraded high-performance computing (HPC) infrastructure (Latvian SuperCluster - "LASC") with the theoretical peak-performance about 11 TFlops.

Future RDI prospect

The expected results of our activities will address but will be not limited to

- Development of new methods for first principles calculations of 0D and 1D inorganic nanostructures (nanoclusters, nanotubes and nanowires) as well as their heterostructures. Prediction of basic physical and chemical properties of nanotubes and nanowires based on ABO_3 perovskites.
- First principles predictions of catalytic properties of advanced reducible oxides. Search for new materials for fuel cells and permeation membranes based on $(La,Ba,Sr)(Co,Fe)O_3$ type perovskite solid solutions.
- Improvement of theory of diffusion-controlled reactions taking into account short- and long-range interactions of nano-particles and their self-assembling. Application to pattern formation in organic and biological systems.
- Theoretical modelling of the kinetics of radiation defect accumulation and annealing, including metal colloid formation in non-metallic solids under irradiation, with application to Al_2O_3 , MgO , alkali halides, and binary oxides.
- The main results of our studies will include understanding of the fundamental microscopic mechanisms of self-assembling in condensed matter, in general, as well as increase of the radiation stability of advanced construction and functional materials for fusion reactors and predictable construction of nanoparticle self-assemblies in organic systems with applications in nanoswitches, in particular.

Two prototypes are also feasible:

1. Prototype of electronic nanodevices containing two types of interconnects: CNT-Me (CNT = carbon nanotube) as well as GNR-Me (GNR = graphene nanoribbon).
2. Prototypes of FET-type nanodevices as prospective nanosensor systems: (a) physical nanosensors, *i.e.*, a conducting threshold can be altered when CNT or GNR is bent; (b) chemical nanosensors, this threshold can be altered when the amount of free charges on CNT or GNR surface is increased or decreased by the presence of donor or acceptor molecules of specific gases or composites; (c) biological nanosensors: monitoring of bimolecular processes such as antibody/antigen interactions, DNA interactions, etc. [4].

Enabling resources, technology, infrastructure

Successful implementation of the proposed tasks will require the qualified staff of 20 researchers including 10 young researchers, PhD, MSc and BSc students, and improved (up to at least 100 TFlops) high-performance computing (HPC) infrastructure at ISSP, as well as an access to computational centres abroad (Germany, Japan, Russia and USA).

X-ray Absorption Spectroscopy

Optical spectroscopy is an indispensable tool in many areas of research and technology, providing with the information on the nature of defects and electronic excitations. Two levels may be singled out. First, an availability of *reliable and robust basic spectroscopic tools* and services creates a benign environment for many technology areas, which can count on the help from the regional research centre. Second, *high-level advanced optical spectroscopy tools* help researchers to perform internationally acknowledged work, and in this way provides contact, cooperation and idea-generation opportunities with more advanced institutions in EU and worldwide. The presence of optical spectroscopy know-how and equipment both on the basic and advanced levels in university-related research centre helps student training in science and engineering fields.

The trends in basic optical spectroscopy involve transition to instruments based on multichannel detectors/spectral imaging or Fourier analysis; fibre-optic based light guiding and sampling accessories, an increasing use of solid-state laser and LED-based light sources. The trends in advanced optical spectroscopy involve usage of tuneable and/or high-power lasers for nonlinear spectroscopy (e.g., Coherent anti-Stokes Raman spectroscopy (CARS), 2nd harmonics spectroscopy etc.), optically detected magnetic resonance (ODMR), usage of ultrashort time domain (ps and fs lasers), other advanced light sources (synchrotron), super-

high spectral resolution (Fourier) and sensitivity (advanced detectors, single-molecule spectroscopy), improved spatial resolution on micrometer scale (microscope and confocal microscope-based spectrometers) and nanoscale (tip-based near-field spectroscopies, e.g., SNOM, TERS etc.).

The intricate knowledge in technical details of research-grade optical spectroscopy helps to generate ideas on innovative or improved optical elements for optical instrumentation. Due to their relatively small market they are usually not targeted by large companies or institutions and their development by smaller participants is realistic, in particular, if the necessary know-how in material synthesis, thin film coatings and planar or fibre waveguides is available. The National funding (National programs, Latvian Science Council Grants and collaboration projects) is considered as primary source of required budget for R&D activities. The collaboration with local small and medium-sized enterprises (GroGlass, Light Guide Optics International, Ceram Optec, SIDRABE) are feasible.

Current experience and advantages

ISSP has internationally recognized expertise in different luminescence spectroscopies and know-how in building non-standard equipment. The present capabilities include luminescence spectroscopy in the spectral range from near-IR to vacuum-ultraviolet, thermostimulated luminescence (TSL), time-resolved luminescence down to picosecond time range, luminescence excitation spectroscopy up to vacuum UV range and under x-rays, equipment for determining quantum yield, the electron paramagnetic resonance (EPR) and optically detected magnetic resonance (the only one in the Baltic states) spectrometers. Absorption measurements are possible from vacuum UV to far-IR range, in the latter case using high-resolution Fourier transform spectrometers, magneto-optic effects can be studied both in absorption and luminescence. Raman spectroscopy is well-developed with excitation at several wavelengths and spatial resolution provided by confocal-microscope-based spectrometer. Optical methods applicable for thin films, e.g., ellipsometry, cathodoluminescence (CL) are available. The institute staff has also considerable experience in synchrotron radiation-based optical spectroscopy, including high-pressure experiments.

Future R&D&I prospect

The future challenges in development involve consolidating the block of basic spectroscopic methods available to ISSP staff and to outside industrial and academic clients. On advanced level, the most important tasks are: (i) improving of the available light (laser) sources, which are critical for developing nonlinear, high spectral-, temporal- and spatial-resolution spectroscopy, (ii) improving the presently insufficient spatial resolution capabilities by developing tip-related nanoscale spectroscopies [10], (iii) developing/acquiring new spectroscopic methods with a particular emphasize on the field of nanoplasmonics, which is one of the most important growth areas of this century [11]; (iv) development of the spectroscopic methods at extreme conditions (high-pressure and high temperature); (v) improvement of EPR/ODMR setup sensitivity for investigation of nanoparticles and thin films.

Enabling resources, technology, infrastructure

Successful implementation of the proposed tasks will require the qualified staff of 10 researchers and up to 10 MSc and BSc students. The infrastructure upgrade will include (i) laser sources; (ii) deep-cooled (down to -100°C) CCD camera(s) with single-photon-sensitivity for significant improvement of signal-to-noise ratio and a reduction of acquisition time for Raman/TERS/TSL/CL signal detection; (iii) nano-positioning sample stage(s) for development of TERS mode, allowing significant spatial resolution improvement down to nanoscale; (iv) optical low-temperature cryostat and high-temperature furnace for micro-Raman measurements; (v) high-pressure setup with diamond anvil cells (up to 20 GPa); (vi) upgrade of EPR/ODMR setup to high microwave frequencies range (93 GHz (W-band) to

enhance the sensitivity of the EPR/ODMR spectrometer in the case of nanoparticles and thin films.

Optical Spectroscopy

The progress in material science is directly related to the increased availability of sophisticated physical methods, allowing determination of material atomic and electronic structures, elemental composition, morphology and other important properties [12,13]. These techniques include electron microscopy and scanning probe microscopies, x-ray and neutron diffraction, small angle scattering, total scattering, x-ray absorption and fluorescence spectroscopies, x-ray photoelectron spectroscopy, atom probe tomography, nuclear magnetic resonance and various spectroscopies. While determination of the materials structure for the case of bulk crystals is rather straightforward, as far as the average atomic positions are concerned, this is not so for nanomaterials. The principal difficulty is related to the fact that, in general, any one technique does not contain sufficient information to constrain a unique structural solution. Therefore, a coherent strategy is required for combining input from multiple experimental methods and theory.

Besides the size effect, surfaces and interfaces play also an important role on the properties of advanced functional materials. Therefore, the characterization of surfaces, thin films, nanostructured materials and nanocomposites is of particular interest. In particular, the following topics of research are actual for the present project: (i) effects of surfaces and interfaces on mechanical behaviour and functional properties; (ii) problems of contact interaction (adhesion, wetting, environmental effects) of metals with metals and non-metallic materials; (iii) surface and bulk modifications of functional materials (oxides, alkali halides, etc.) induced by irradiation, including irradiation with swift heavy ions and lasers.

To address these challenging problems the ISSP UL provides an infrastructure for National Research Centre for Nanostructured and Multifunctional Materials, design and technology as well as for two competence centres in the fields of microelectronics and biotechnology. National funding (National programs, Latvian Science Council Grants and collaboration projects) and EU funding (Horizon 2020) are considered as primary sources of required budget for R&D activities. The collaboration with local small and medium-sized enterprises (GroGlass, SIDRABE and Schafler) is also continuously realized.

Current experience and advantages

ISSP UL possesses the best equipment and highest resolution electron microscopes in Latvia and have strong experience in solid state material crystallographic structure and element composition analysis. In particular, a list of modern equipment to address increasing demands for materials characterization in the bulk and at the surface down to micro, nano and atomic scale includes:

- A new transmission electron microscope (TEM) Tecnai G20 (FEI) is equipped with optional features like energy dispersive x-ray fluorescence (EDX) detector for element analysis, precise holder stage to perform tomography, STEM detectors for bright field and dark field STEM.
- Scanning electron microscope Lyra (Tescan) equipped with Focused Ion Beam (FIB) column, Gas Injection System (GIS), EDX detector and manipulator.
- Scanning electron microscope EVO 55 (Zeiss) for electron lithography.
- X-ray diffractometer PANalytical X'Pert Pro equipped with Cu long fine focus X-ray tube accompanied with PixCel multichannel detector and utilized for high resolution powder diffraction, phase identification and quantitative phase analysis, analysis of thin films and coatings, crystallite size and strain determination, kinetic and non-ambient experiments.
- Energy-dispersive X-ray fluorescence microanalyzer with multicapillary focussing optics (EDAX Eagle III) for express-analysis of elemental composition ($Z > 10$) of different materials and devices without special sample preparation.

- Two atomic force microscopes (NT-MDT "Smena" and Veeco Digital Instruments CP-II) for surface imaging studies, nano-spectroscopy, magnetic force microscopy and nanolithography.
- Confocal optical microscope with spectrometer "Nanofinder-S" for simultaneous surface imaging and Raman/luminescence spectroscopy with a resolution down to 300 nm.
- Surface profile measuring systems in contact (Veeco Dektak 150) and non-contact (Zygo NewView 7100) modes for thickness, roughness and surface quality studies.
- Nanoindenter G00 (Keysight [Agilent], USA) for investigation of micromechanical properties of functional materials using nanoindentation technique, which allows one to perform measurements of hardness, Young's modulus, work of plastic and elastic deformation on a micro- and nano-scale.

The actual research at ISSP UL on most of complex material components and crystal grains is in nanometer scale, therefore there is an increasing demand for high resolution microscopes in combination with other research methods. This topic is mostly aimed to implement novel research methods. ISSP UL already has some experience and was involved in research and development of new nanoscale research methods like "X-TIP" [6], combining x-rays spectroscopy with scanning probe microscopy, within the framework of EC FP6 Specific Targeted Research Project NMP4-CT-2003-505634.

Future R&D&I prospect

To maintain the leading positions and address new demands in functional material characterization we plan to upgrade existing equipment with new possibilities for nanoscale chemical mapping and nanomanipulation. In particular, the electron energy loss spectroscopy (EELS) will be used with available TEM to perform element analysis and to detect element distribution over sample with precision and flexibility far exceeding currently present EDX technology. Moreover, the existing expertise in theoretical x-ray absorption spectroscopy will significantly extend the amount of information on the local electronic and atomic structure provided by EELS through the detailed analysis of the fine structure above the element inner inner-shell ionization edges. The upgrade for SEM microscope with the atom force microscope (AFM) module and nanomanipulators will offer new possibilities for measuring surfaces and nanostructures with simultaneous control of exact positioning of the AFM tip. The cathodoluminescence detection option for SEM will extend possibilities of available luminescence spectroscopy techniques, the field where ISSP UL has historically strong background, to study distribution of luminescent centres in non-homogeneous samples with nanoscale resolution. This will extend the research possibilities into the field of nanotribology and mechanical properties of nanowires, currently realized at partner institution [14]. The surface and interfaces studies will provide with the knowledge on effects of surfaces and interfaces on micromechanical properties of thin film systems and materials with nanoscale dimensions; understanding of the mechanisms of size effects in micromechanical properties; contribute into solving the problems of contact interaction (wetting, corrosion and compatibility) related to application of magnetohydrodynamic technologies in fusion reactor projects.

Enabling resources, technology, infrastructure

Successful implementation of the proposed tasks will require the qualified staff of 10 researchers and up to 10 MSc and BSc students. The infrastructure upgrade will include (i) the EELS module for TEM, (ii) AFM-SEM and nanomanipulators for tribological and nano-mechanical studies, (iii) cathodoluminescence detection setup for use with SEM, (iv) the upgrade of Nanoindenter with new software and indentation head DCM II for the testing of ultra-thin films. For general development of the surface physics in ISSP, the acquisition of a vacuum atomic force microscope with STM mode for performing experiments under controlled atmosphere and a Time-of-Flight Secondary Ion Mass Spectrometry unit (TOF-SIMS) for elemental analysis/mapping and depth profiles studies are required.

Microscopy and Structural Methods

The progress in material science is directly related to the increased availability of sophisticated physical methods, allowing determination of material atomic and electronic structures, elemental composition, morphology and other important properties [12,13]. These techniques include electron microscopy and scanning probe microscopies, x-ray and neutron diffraction, small angle scattering, total scattering, x-ray absorption and fluorescence spectroscopies, x-ray photoelectron spectroscopy, atom probe tomography, nuclear magnetic resonance and various spectroscopies. While determination of the materials structure for the case of bulk crystals is rather straightforward, as far as the average atomic positions are concerned, this is not so for nanomaterials. The principal difficulty is related to the fact that, in general, any one technique does not contain sufficient information to constrain a unique structural solution. Therefore, a coherent strategy is required for combining input from multiple experimental methods and theory.

Besides the size effect, surfaces and interfaces play also an important role on the properties of advanced functional materials. Therefore, the characterization of surfaces, thin films, nanostructured materials and nanocomposites is of particular interest. In particular, the following topics of research are actual for the present project: (i) effects of surfaces and interfaces on mechanical behavior and functional properties; (ii) problems of contact interaction (adhesion, wetting, environmental effects) of metals with metals and non-metallic materials; (iii) surface and bulk modifications of functional materials (oxides, alkali halides, etc.) induced by irradiation, including irradiation with swift heavy ions and lasers.

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The actual research at ISSP on most of complex material components and crystal grains is in nanometer scale, therefore there is an increasing demand for high resolution microscopes in combination with other research methods. This topic is mostly aimed to implement novel research methods. ISSP already has some experience and was involved in research and development of new nanoscale research methods like "X-TIP" [6], combining x-rays spectroscopy with scanning probe microscopy, within the framework of EC FP6 Specific Targeted Research Project NMP4-CT-2003-505634.

Future R&D&I prospect

To maintain the leading positions and address new demands in functional material characterisation we plan to upgrade existing equipment with new possibilities for nanoscale chemical mapping and nanomanipulation. In particular, the electron energy loss spectroscopy (EELS) will be used with available TEM to perform element analysis and to detect element distribution over sample with precision and flexibility far exceeding currently present EDX technology. Moreover, the existing expertise in theoretical x-ray absorption spectroscopy will significantly extend the amount of information on the local electronic and atomic structure provided by EELS through the detailed analysis of the fine structure above the element inner inner-shell ionization edges. The upgrade for SEM microscope with the atom force microscope (AFM) module and nanomanipulators will offer new possibilities for measuring surfaces and nanostructures with simultaneous control of exact positioning of the AFM tip. The cathodoluminescence detection option for SEM will extend possibilities of available luminescence spectroscopy techniques, the field where ISSP has historically strong background, to study distribution of luminescent centres in non-homogeneous samples with nanoscale resolution. This will extend the research possibilities into the field of nanotribology and mechanical properties of nanowires, currently realized at partner institution [14]. The surface and interfaces studies will provide with the knowledge on effects of surfaces and interfaces on micromechanical properties of thin film systems and materials with nanoscale dimensions; understanding of the mechanisms of size effects in micromechanical properties; contribute into solving the problems of contact interaction (wetting, corrosion and compatibility) related to application of magnetohydrodynamic technologies in fusion reactor projects.

Enabling resources, technology, infrastructure

Successful implementation of the proposed tasks will require the qualified staff of 10 researchers and up to 10 MSc and BSc students. The infrastructure upgrade will include (i) the EELS module for TEM, (ii) AFM-SEM and nanomanipulators for tribological and nano-mechanical studies, (iii) cathodoluminescence detection setup for use with SEM, (iv) the upgrade of Nanoindenter with new software and indentation head DCM II for the testing of ultra-thin films. For general development of the surface physics in ISSP, the acquisition of a vacuum atomic force microscope with STM mode for performing experiments under controlled atmosphere and a Time-of-Flight Secondary Ion Mass Spectrometry unit (TOF-SIMS) for elemental analysis/mapping and depth profiles studies are required.

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M.F. Hoedl, E. Makagon, I. Lubomirsky, R. Merkle, **E.A. Kotomin**, and J. Maier.

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DOI: [10.1016/j.actamat.2018.08.042](https://doi.org/10.1016/j.actamat.2018.08.042)

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D. Fuks, D. Gryaznov, **E.A. Kotomin**, A. Chesnokov, and J. Maier.

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Solid State Ionics, 2018, **325**, pp. 258-264.

DOI: [10.1016/j.ssi.2018.08.019](https://doi.org/10.1016/j.ssi.2018.08.019)
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A. Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, L. Nataf, F. Baudalet, T. Irifune,
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II. Nanotechnology, nanocomposites and ceramics

Domain: *Sensors & actuators*

The R&D activities will cover novel nanomaterials and nanostructures, crystals, glasses, nanoceramics, polymer nanocomposites, and hybrid structures. Application areas: dosimeters and sensors using thermoluminescence (TL) and optical stimulated luminescence (OSL) in nitrides and oxides, scintillators for high-energy physics and medical applications, sensors for diagnostics and bioimaging, persistent short wave infrared phosphor for bioimaging low temperature persistent phosphors sensors, transparent nanocomposite oxyfluoride materials for optical applications, nanostructured upconversion luminescent environmental sensors, high values electrocaloric effect in ferroelectric perovskites for refrigerators, ferroelectric NBT composition ceramics for electromechanical actuators.

Nanotechnology is the undisputed 21st century science and technology paradigm. Nanotechnology is currently in the transition to integrated systems and fundamentally new products, ranging from passive nanostructures with stable characteristics to active structures, including three-dimensional nanosystems. Therefore, ISSP UL is constructing the open access laboratory LATNANO-C already equipped with new features, like Transmission Electron Microscopy and Scanning Electron Microscopy with Focused Ion Beam accessory. The share of nanotechnology-related research at ISSP UL scientific production increases year by year.

Nanostructured materials such as nanoparticles, nanostructured ceramics and glasses with certain predictable and tailored characteristics are under investigation at ISSP UL. The possibility to engineer, control and modify the material properties at the nanoscale is of fundamental and applied importance for the EU and Latvian economies, going towards a more knowledge-intensive manufacturing.

This direction of research includes the following research themes:

- I. Nanomaterials and nanostructures
- II. Nanoceramics and polymer nanocomposites
- III. Ferroelectric ceramic materials

Nanomaterials and nanostructures

Nanomaterials are extremely interesting from both scientific and technological point of view, and contain tremendous commercialization potential. They can be applied in electronics, energetics, photonics, biology and medicine, and many other fields. It is well known, that due to their small size and large surface to volume ratio, their properties differs considerably from and are superior to their bulk counterpart. Traditionally, nanomaterials can be divided into three general groups: 0D (quantum dots, nanoparticles, nanocrystals), 1D (nanotubes, nanowires, nanofibers) and 2D (layered materials like graphene, etc.).

There are many nanostructure synthesis methods, starting from milling and etching of bulk materials into nanostructured ones (top-down methods) and ending with bottom-up methods. They are grown atom by atom via physical or chemical routes. It is worth to mention that nanostructures can be produced as powders and suspensions or alternatively as ordered 2D planar or vertical networks or arrays, and 3D arrays on solid substrates.

Silver nanowire's coating has transparency and conductivity comparable or better than ITO transparent coatings, while manufacturing costs of silver nanowire coatings is significantly smaller. Spray coating or metal nanowires printing are technologies, which can be easily adopted for mass production.

Current experience and advantages

Several groups at ISSP UL work currently on synthesis and characterization of nanoparticles, nanocrystals, nanowires, nanotubes and other nanomaterials [1]. Variety of nanomaterials are produced by colloidal chemistry methods, which have proved to be flexible and powerful routines for synthesis of different nanostructures (metal nanowires and nanoparticles, metal oxides, fluorides, sulfides, selenides, etc.) allowing to control their morphology, shape and size. Sol-gel chemistry is combined with colloidal chemical methods to synthesize various hybrid materials. Related chemical methods are hydrothermal and microwave assisted synthesis methods. All these methods can be easily scaled up for mass production. Ball milling and pulsed laser ablation are flexible nanoparticle production methods for scientific application from bulk materials. However, related methods - focused optical evaporation - can be used to synthesize nanomaterials from corresponding bulk material and adapted for large-scale production. All the above-mentioned methods produce powders or suspensions of nanomaterials. Swift-ion-induced formation of bulk nanostructures and modification of optical and micromechanical properties of functional materials (oxides, alkali halides, etc.) is studied using irradiation at large accelerator facilities. High-fluence irradiation with MeV-GeV ions leads to the formation of defect nanoclusters and extended defects (ion tracks, dislocations, grain and subgrain boundaries) [2].

Main application areas of nanomaterials produced at ISSP UL are white light sources and light up-convertors, nanomaterials for hydrogen and solar cell energetics, catalyzers, gases and other sensors, NEMS nanocomponents, photodetectors, transparent conductive electrodes, photonics and plasmonics, biological and biomedical applications, etc. Few examples of nanomaterials applications: metal nanowires (Ag, Cu, etc.) are real candidates for printable electronics and transparent conductive coatings [3, 4].

ISSP UL has the infrastructure and the instruments to characterize and optimize produced nanomaterials using many experimental and theoretical methods. There are scanning and transmission electron microscopy, optical spectroscopy in different range of wavelengths, X-ray diffraction and analysis methods, electron paramagnetic resonance spectroscopy to be continued. Moreover, full spectrum of theoretical modelling and calculations are available to simulate and interpret the obtained experimental results.

Future R&D&I prospect

- Synthesis of metal nanowires and nanotubes as main component of conductive inks for inkjet printing on polymer films, plastics and other flexible substrates.
- Production of semiconducting, metal and magnetic nanoparticles for catalysis, bio labeling and water filtering.
- Synthesis of fluoride based rare-earth doped core-shell nanocrystals for up-conversion luminescence applications, particularly, bio labeling.
- Development of hybrid heterostructured core-shell nanoparticles and nanowires with tunable functional properties using combination of chemical and physical methods. Possible implementations of these nanostructures are sensors, photocatalytic, electrochromic and other applications.
- Synthesis of metal, metal oxides, nitrides, sulfides and other nanowires on different solid substrates by CVD/MOCVD methods for electrochromic, thermochromic applications and sensors. CVD methods allow to grow nanowires epitaxially, providing excellent electrical contact of nanowire and substrate, precisely optimize key parameters, change dopants and doping level along nanowire length.
- Development of electrochemical anodization methods to produce nanotube arrays or porous membranes for nanowire template synthesis for energy applications. Electrodeposition inside nanoporous template membrane allows producing mainly metallic nanowires with variable diameter and length, which are determined by template dimensions at room temperature.
- Synthesis of nanostructures and improvement of physical and micromechanical properties of functional materials (oxides, alkali halides, etc.) by irradiation with beams of swift (MeV-GeV) heavy ions.

Enabling resources, technology, infrastructure

It is necessary to update and expand the infrastructure necessary for nanostructures synthesis. Ultracentrifuges are required for nanoparticles washing procedure. Variable pressure CVD reactors are needed for better control and reproducibility of nanostructure synthesis. Microwave assisted hydrothermal reactors are tools to improve and enhance already existing sets of nanostructures synthesis methods. X-ray photoelectron spectroscopy is absolutely necessary for the characterization of their surface chemistry of synthesized nanostructure. A compact UV-VIS-NIR optical spectrometer is needed for express analysis of nanoparticles during synthesis process. Nanoparticle size analyzer is required for a fast estimation of the produced nanoparticles size. Glovebox with inert atmosphere is needed for oxygen sensitive synthesis of nanomaterials.

Nanoceramics and polymer nanocomposites

The nanosized materials are known in various forms, however more appropriate for application are nanoparticles embedded in some matrix. The composite material (shortened term - composite) is a combination of two or more materials and in the simplest case the composite reveals a combination of the individual properties of the materials incorporated, however new properties can appear also [5]. The origin of these new properties is based on the interaction of different materials as well as on forming interfacial layers between nanosized grains. Since interactions could be complicated it is an object of intense study. The appropriate combination of materials in composites can introduce new materials with properties meeting requests for a particular application.

Current experience and advantages

The composites studied at ISSP UL include glass-metal hydride composites for hydrogen storage [6], glassy organic components embedded in polymers [7], as well as inorganic nanoparticles embedded in polymers [8], rare-earth doped oxyfluoride silicate glass-ceramics [9], combined different titanates and zirconates ceramics, including optically transparent ceramics [10], metal covered nanoparticles (core-shell composites) [11],

nanostructured oxide ceramics [12], persistent phosphors [13]. The methods used for studying these properties cover a wide range - volumetric PCT (hydrogen sorption), EPR, ODMR, optical methods (luminescence, absorption), including time-resolved measurements down to sub-nanosecond range, electric methods, microscopy (AFM, SEM, TEM), XRD, EDX.

The research of composites carried out at ISSP UL results in new knowledge; it is confirmed by a number of papers in refereed scientific journals and by presentations at international scientific conferences. The new knowledge obtained is promising for application, e.g., inorganic nanoparticles embedded in polymer could be used for lighting applications [8]. Joint research [14], carried out with producing firm ZRF RITEC, SIA result in production of more efficient radiation detectors. ISSP UL has collaborations with a number of devices and equipment producers (e.g. Baltic Scientific Instruments, ISP Optics Latvia; Ekoosta), thus the new knowledge is disseminated and the search for possible applications is a hot topic.

Future R&D&I prospect

- Synthesis and characterization of optically transparent luminescent glass ceramics for efficient mercury-free lighting applications.
- Synthesis and characterization of optically transparent glass ceramics for laser active medium.
- Nanocomposites: glass - ceramics for efficient IR up-conversion luminescence applications like visualization of IR radiation and solar cell efficiency enhancement.
- The study of nanoceramic layers obtained by plasma electrolytic oxidation process.
- Search for nanoporous ceramics for gas sensors.
- Development of efficient persistent phosphors embedded in polymer matrix.

Enabling resources, technology, infrastructure

Isostatic hot pressing equipment is required for processing nanomaterials and synthesis of optically transparent ceramics. The advanced techniques and appropriate tools for fast luminescence signal detection like high dynamic range streak camera in picoseconds-nanosecond range are necessary. Powerful light source for steady state luminescence excitation is also required.

Ferroelectric ceramic materials

NBT-containing materials represent a large group of lead-free ferroelectrics mainly attracting interest as a replacement for lead-containing ones in applications exploiting electromechanical properties. This group of materials can also be modified to have a large dielectric permittivity, temperature-independent in a wide temperature range, and high values of induced polarization, perspective for application in energy harvesting [15, 16]. NBT-containing samples are essential for the study of relaxor properties related to non-regular distribution of Na^{1+} and Bi^{3+} ions in A-sublattice of ABO_3 perovskites.

Modifications with 3d metals are essential for tailoring properties of ferroelectrics with perovskite ABO_3 structure. In spite of the similar electronic configuration, they influence the ferroelectric properties in a different way, which is not fully understood yet.

Current experience and advantages

Studies of NBT and NBT-containing solid solutions, including novel compositions are in progress at in ISSP UL. Structure and complex physical properties are studied for a new family of ferroelectric materials exhibiting a wide range of stability of relaxor properties and a pronounced electrocaloric effect [17]. The materials have excellent luminescence and nonlinear optical properties. The role of Nb doping in lowering the phase transition temperature is studied [18].

The influence on local structure and dielectric properties of transparent PLZT ceramics modified by 3d metals (Mn, Fe, Co, Cu) is studied, the change of the nature of the

relaxor state in dependence on valence and replacement position in the crystallographic lattice is determined [19].

ISSP is a founding member of the Piezo institute, a European organization, dedicated to research and application development of piezoelectric materials and devices.

Future R&D&I prospect

- Development of NBT-containing materials with enhanced electromechanical (piezoelectric, electrostrictive, deformation at field induced phase transitions) properties, perspective for replacement of lead-containing counterparts. Studies on the mechanism responsible for “electrostrictive” properties in the relaxor state.
- Development of materials with high values of the electrocaloric effect, requested for cooling devices.
- Study of luminescence and nonlinear optical properties in NBT solid solutions doped with lanthanides, appearance of features of crystalline fields on luminescence.
- Development of microstructure by doping and modifying processing route, possibilities to produce optically transparent ceramics.
- Doping with transition metals to develop multiferroic materials, the role of Jahn-Teller centres (Mn^{3+} , Fe^{4+} (d^4 configuration), Cu^{2+} (d^9 configuration)) in promoting the ferroelectric state. Study of elastically interacting ferroelectric-ferromagnetic composite systems.

Enabling resources, technology, infrastructure

Modern equipment for the measurement of ferroelectric properties of materials, in particular, vibrating sample magnetometer and piezoelectric coefficient d_{33} measurement equipment are required. For advanced synthesis of ferroelectric samples planetary mill, high temperature furnace with controlled atmosphere, hot pressing equipment and equipment for sawing and grinding of bulk ceramic specimens are needed.

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SNIP: 0.79

III. Functional materials for electronics and photonics

Domain: Photonics & micro & nanoelectronics

The R&D activities will address new materials for light emitters, waveguides and sensors, materials for photonic applications in information and communications technologies, oxide based optoelectronics devices, large area nano coatings for application in transparent and flexible electronics, for wide bandgap semiconductor power electronics. The R&D activities will address the so-called Green Thin Film Nanotechnologies based on vacuum technologies such as physical and chemical vapour deposition (PVD & CVD) and pulsed laser deposition (PLD) as well as organic and inorganic spray wet technologies, novel High Power Impulse Magnetron Sputtering (HIPIMS) technology. Innovative infrastructure and technological processes in the field of photonics and electronics could pave a way to prototyping

of photonic and microelectronic devices based on the developed materials in close cooperation with Latvian SMEs in the field, also being of high economical priority for Latvia, which has one of the largest vacuum technology industries among the Baltic countries.

It is believed that in the 21st century the photonics - a multi-disciplinary science and technology sector, defined by the EC as one of the Key Enabling Technologies (KETs) - will acquire a dominant role in the society, leaving electronics behind. The operation of photonic devices is attained by manipulation of photon flux, unlike the electronic devices in which electron currents are manipulated.

Most scientists at ISSP UL conduct research in this thematic area. All steps of material research, starting from design to synthesis, investigation of properties, processing and device application assessment, are covered. More than half of the ISSP LU scientific publications are related to this thematic area. A wide variety of material classes ranging from inorganic single crystals to amorphous polymers are within the scope of ISSP LU research. These materials are designed and investigated for applications like solid state lighting, lasers, sensors, photovoltaic energy harvesting, information storage and transmission, etc. Unfortunately further commercialization of R&D achievements at ISSP UL is limited due to the lack of facilities for prototyping electronic and photonic devices. Development of appropriate infrastructure and personnel skills for prototyping will be in the focus of the research agenda and strategy of ISSP UL. Despite of the fact that the largest part of ISSP UL scientists are already involved in this research direction to achieve the planned goals, an increase in human resources involved in the R&D&I activities is essential. Latvia, among the Baltic countries having one of the largest vacuum technology industry (SIDRABE, Inc., GROGLASS, Ltd., ALFA, Inc.), should provide increasing skills in the thin films materials science and plasma technologies in collaboration with material science centres as the ISSP UL. Vacuum technologies today are considered as *Green Thin Film Nanotechnologies* (PVD, CVD, PLD, etc.) and are a key technologies for many multifunctional coatings (Solar Cells, Transparent Electronics, Transparent Conducting Oxides -TCO, tailored surfaces), innovative glass coatings, and will be the future technology for smart windows production [1,2].

As a next generation technology, ultrasonic spray wet processing is already quickly developing in R&D and pilot lines, it is being proven as a viable alternative to sputtering. The future high efficiency of these wet processes will further decrease the cost per Watt of already profitable wet process manufacturing lines.

The thin films activities will contribute to reducing the greenhouse gas emissions and enable European industry to stay globally competitive and to fulfill the goals of the Lisbon Treaty. Furthermore the Action will strongly contribute to the Action Plan of the European Commission on Sustainable Industrial Policy and on Sustainable Consumption and Production released on 16 July 2008. In addition, this Action will also help Latvian small to medium sized enterprises (SMEs) in creating new market opportunities for innovative plasma technologies to become a truly European success story.

The detailed description of each theme, its current state of the art, future prospects, needs and expected results are given below.

Direction of research activities has subsequent main themes:

- I. Thin films and coating technologies
- II. Materials for light emitters,
- III. Materials for sensors and waveguides,
- IV. Materials for photonic applications in Information and Communications Technologies (ICTs),
- V. Prototyping of photonic and microelectronic devices.

Thin films and coating technologies

PVD, CVD and PLD deposition thin film technologies

The existing hard competition in coating manufacturing requests from producers to improve functionality and quality of thin films as well as coatings. This is the reason for the development of a cooperation between ISSP UL and producers, what is especially efficient with local producers (SIDRABE, Inc., GROGLASS, Ltd., ALFA), where the role of ISSP UL is to work out new and improve existing functionalities, followed by transferring of the corresponding deposition technologies to manufacturing as well as functionalizing of large area glass surface for smart, energy saving windows is one example of area of cooperation. New plasma technologies of High Power Impulse Magnetron Sputtering (HIPIMS) [3-5] and plasma processes (COST action MP0804) bear an enormous potential for manufacturing coatings with properties exceeding by far those of the state of the art. Improvement will be available in the fields of Photovoltaic, Green Buildings (Smart windows), Mechanical Engineering, Automotive, Aerospace, Tribology, Decoration, Displays, Tools, etc. Thus lifetime, reliability, fuel consumption, performance and cost in the named applications can be updated significantly.

Current experiences and advantages

ISSP UL has more than 35 years of expertise in vacuum deposition technologies realized in the strong cooperation with largest vacuum technology industries (SIDRABE, Inc., GROGLASS, Ltd., ALFA, Inc.) that has provided increasing skills in the thin film material sciences and plasma technologies:

- electrochromic thin films (WO_3 , MoO_3 , NiO , IrO_2) [6-10]
- transparent conducting oxides thin films n- and p-type ZnO , $\alpha\text{-In}_2\text{O}_3\text{-SnO}_2$ (ITO)[11-13]
- photocatalytic coatings (ReO_3 , $\text{WO}_3\text{-TiO}_2$, $\text{IrO}_2\text{-NiO}$) [14-16]
- resistive terabit switching memories (ReRAM) for nanoelectronics and functional materials [17-19]
- electrode materials for lithium ion batteries (LiFePO_4) [20-22].

The SAF25/50 multifunctional R&D cluster plant installed at ISSP UL cleanrooms in 2015 is intended for research and development works in the field of thin film technologies. The plant is a multifunctional, expandable, modular and flexible system. The plant comprises an input/output chamber with ion gun, a central substrate transfer chamber with radial telescopic transport arm and up to 7 deposition chambers. The Substrate is positioned horizontally on a holder. Deposition zones are configured for substrate rotation or displacement during upward deposition.

Vacuum plasma deposition technologies developed in the last years at the ISSP UL (PVD, MOCVD) are widely and extensively used for thin films and coatings productions. Magnetron sputtering has become the process of choice in many applications. Especially HIPIMS processes developed at ISSP LU using highly ionised pulse plasmas play an important role for modification of material properties.

Transition metal (TM) oxide based thin films (COST MP 1308) and coating technologies (PVD, HIPIMS, CVD, MOCVD, PLD) are at the core next-generation nanoelectronic, microelectromechanical and macroelectronic devices expected to revolutionize fields of major social relevance as digital information and communication technologies, microactuation/microsensing and energy conversion. Such class of materials is characterized by an unprecedented wealth of functionalities, often being relevant to different fields of applications, found in compounds that are extremely similar to each other in terms of chemistry, crystal structure and fundamental mechanisms. The necessity to

handle the unprecedented complexity of these materials rescales efforts of solid state scientists to a higher level:

- High Power Impulse Magnetron Sputtering (HIPIMS) vacuum sputtering technology;
- In situ characterization plasma HIPIMS technology processes;
- low-cost transparent conducting oxides thin films and technologies;
- electrochromic and thermochromic thin film devices and technologies (Smart windows);
- photocatalytic coatings ($\text{WO}_3\text{-TiO}_2$, $\text{IrO}_2\text{-NiO}$);
- highly oxygen-permeable nano-structured oxygen transport membranes.

PLD is a valuable tool for production of thin films and heterostructures from various materials with complicated stoichiometry. PLD allows a one-to-one transfer of elements from target to substrate, what is a strong advantage for the deposition of multiple element systems. Different atmospheres of deposition allow varying of properties of films in a wide range. ISSP UL has experience in making high-quality thin films of perovskite structures by PLD, studying structure, surface topology (by AFM), dielectric and electromechanical properties. Research is done in cooperation with University of Oulu (Finland) and IFW-Dresden (Germany). The institute has experience in the evaluation of PLD thin films in cooperation with Forschungszentrum Jülich (Germany), working on technology of producing of ReRAM [17-19].

The present MOCVD reactor Aixtron (AIX-200RF) is available for the synthesis of thin films using liquid metal-organic compounds and gaseous non-metal chemical hydride and oxide gases. The equipment is suitable for the synthesis of classic LED structures, as well as for the synthesis of Si, ZnO, and group III nitride 1D nanostructures. There is a possibility to dope the materials, in order to obtain n- or p-conductivity. MOCVD equipment provides wide possibilities to manipulate chemical reactants creating different 1D, 2D, and hybrid structures.

These research activities at the ISSP UL are currently supported by Competence centre projects, Latvian funding within National programs and Latvian Science Council grants.

Future R&D&I prospect

The aim of ISSP UL is the development of the basic thin film material sciences and coating technologies (PVD, CVD, PLD) underpinning the production of new functional TM oxide (TMO) and AIIIBV thin films and heterostructures:

- High Power Impulse Magnetron Sputtering (HIPIMS) vacuum sputtering technology;
- low-cost transparent conducting oxides thin films and technologies (PVD);
- resistive terabit switching memories (ReRAM) for nanoelectronics and functional materials;
- electrochromic and thermochromic thin film devices and technologies;
- highly oxygen-permeable nano-structured oxygen transport membranes;
- functional materials for transparent electronics: p- and n-type metal oxides;
- optical sensors (metal oxide materials) for carbon dioxide, nitrogen or other gasses;
- new green plasma vacuum technologies R&D;
- transition metal oxide thin films R&D for 21st century energetics and buildings (low cost transparent conducting oxide (TCO) coatings, smart windows with electrochromic thin films);
- transition metal oxide thin films for 21st century new terabit memories such as ReRAM
- electrode and solid electrolyte thin films for lithium/sodium ion batteries.

TMO thin films (WO_3 , MoO_3 , NiO , IrO_2 etc.) are used as optical coatings in electrochromic devices (such as “smart windows”) where they change their transmittance upon insertion or extraction of electrical charge. The market of these devices is still limited to niche

applications (mainly in automotive technology) due to the high manufacturing costs. Redox-based resistive switching in TMOs (as NiO, Ta₂O₅, TiO₂, doped SrTiO₃), is under the attention of the industry for the next-generation of nonvolatile memories (resistive RAM) and for the implementation of a new electronic circuit element, the memristor.

Enabling resources, technology, infrastructure

The existing hard competition in coating manufacturing requests from producers to improve functionality and quality of coatings. This is the reason for the development of cooperation between ISSP UL and producers, what is especially efficient with local producers, where the role of ISSP UL is to work out new and improve existing functionalities, followed by transferring of the corresponding deposition technologies to manufacturing. Functionalizing of large area glass surface for smart, energy saving windows is one example of area of cooperation.

For the industrial realization of the HIPIMS processes further improvement and adjustment has to be performed concerning the pulse generation. Today the upgrade of an existing sputtering plant with HIPIMS technology is connected with high service time due to optimization and adjustment of the electrical parameters to get the processes running. Therefore close collaboration and feedback to companies building power supplies has to be realized.

The SAF25/50 multifunctional R&D cluster plant will be further developed for research and development works as well as for feasibility studies and more general academic work. The multifunctional, modular plant will be extended by new chambers for HIPIMS and PLD processes as well as for characterization thin films.

The HIPIMS plasma sputtering technology laboratory will be renovated. The plant comprises a dual HIPIMS magnetron vacuum chamber with plasma regulation and control by an Optical Emission Spectroscopy (OES) system.

The RF-OES multifunctional R&D plant is intended for research and development works as well as for feasibility studies and more general academic work in the field of thin film technologies. The plant comprises a RF magnetron vacuum chamber with plasma regulation and control by Optical Emission Spectroscopy (OES) system.

The necessity to upgrade the sputtering equipment's is related to the main direction of the research Programme by providing direct means of process development for thin film deposition, to the main direction of the Programme by supplying the films for characterization, and by providing the experimental grounds for development of theoretical modelling. In a broader perspective, development of advanced deposition methods will contribute significantly to the accumulation of a critical potential at ISSP UL for successful participation in research activities at EU level in the strategic field of thin film coatings. The HIPIMS package includes purchase and installation of two magnetrons and two power sources. Capitalizing on HIPIMS advantages, this will open new venues for the development of thin film deposition methods even for coatings of more complex compositions and/or layer structures than obtainable with a single deposition source.

In line with the main direction of planned development PLD of ferroelectric materials, the PLD deposited lead-free films will be obtained and their potential for future applications will be studied, paying attention to:

- energy harvesting, MEMS
- capacitors for extended temperature range, high energy density
- elements for photonic devices
- non-volatile memories
- magnetoelectric devices.

Organic and inorganic spray wet technologies

As a next generation technology, ultrasonic spray wet processing is already quickly developing in R&D and pilot lines and is being proven as a viable alternative to sputtering. The future high efficiency of these wet processes will further decrease the cost per Watt of

already profitable wet process manufacturing lines. Although the vacuum-deposition processes are far ahead of the solution processes from the commercialization point of view, the solution or “wet” processes for the fabrication of devices are still fascinating due to their potential advantages for the production of large area photonic (OLEDs and OPV) and other devices at low cost. Cost per Watt of already existing wet manufacturing process lines will further decrease with developments of novel materials and technologies. Large research institutions such as NREL are actively developing wet spray processes and predict that efficiencies as high as 16% (comparable to sputtering) will be reached within a decade using these wet processes. 10.5 % efficiencies have already been proven on large area pilot lines today. Existing cooperation of ISSP UL with domestic companies, which are interested in implementation of technologies and products, like Valmiera Glass Group, EPD is firstly applied to functionalize glass fibers for catalyst and gas sensor applications.

Current experiences and advantages

ISSP UL has more than ten years of experience in thin film preparation by wet coating methods like spin-coating, blade casting, ultrasonic spray wet processing etc. [23-28] These methods are used to prepare samples of original low molecular weight organic as well as inorganic materials which form amorphous, nanocrystalline or polycrystalline thin films. Designed in close collaboration with chemists in Riga Technical University organic materials are targeted for such applications like solar cells, organic light emitting diodes, organic lasers and other photonic and electronic applications. The available equipment allows preparing small area samples useful for material characterization and proof of concept demonstrations.

A large variety of rather different wet methods is used in ISSP UL [23-28]. One area of applications of wet film technologies is creation of porous chemically active media to reach large surface areas, appropriate for electrode materials for hydrogen cells, batteries and supercapacitors. Electrochemical oxidation is a method to prepare oxide and complex oxide coatings. Especially interesting are the anodic and plasma electrochemical oxidation (PEO) methods. Up to now the PEO coatings were prepared to increase the mechanical properties of aluminium and aluminium alloys and to increase the chemical resistivity of magnesia alloys.

In ISSP UL electrophoresis is applied to obtain films from suspensions and sols (pure and Fe(III), W(VI) doped TiO₂, GO and other carbon structures) on electricity conducting substrates and fibreglasses. The obtained photosensitive films are appropriate for filtering of organic impurities. We have expertise in prototypes to demonstrate application possibilities for various types of thin film coatings - smart windows with adjusted reflection, heat transmission, light transmission (coloring-bleaching), gas sensitivity, ion intercalation (energy harvesting), water splitting in oxygen and hydrogen, water treatment etc., as well as in prototypes of solid state lithium or sodium ion battery. Together with Elgootech Ltd PEO method was applied to produce luminescent coatings for the first time. During this cooperation the first successful attempt to prepare luminescent coatings was achieved.

Spray coating is appropriate method for preparation of nanoparticles and nanowires thin films. Metal oxide ITO, ZnO and TiO₂ nanoparticle films, as well as metal nanowire and nanoparticle films (Cu, Ag) can be prepared by spray coating methods [29-31]. Post-processing such as laser or flash lamp annealing can be applied for nanoparticle films on low temperature flexible substrates, such as paper, cellulose paper, plastics and others. For example, transparent conductive coating can be prepared from ITO nanoparticles through spray coating and sintering in atmospheric conditions without expensive vacuum technologies [30].

These research activities at the ISSP UL are currently supported by Latvian funding within the Latvian Science Council grants, National Research Programs in material science and energy & environment, bilateral and tripartite cooperation (Latvian - France, Latvian-Lithuanian-Taiwan projects); European Regional Development Funds and European Research Funds (FW, H2020), Elgootech Ltd (phosphorescent coatings).

Future R&D&I prospect

The development of organic thin films will be targeted for solar cells, organic light emitting diodes, organic lasers and other photonic and electronic applications. New equipment will allow preparing the medium area samples useful for material characterization and proof of concept demonstrations.

A large variety of rather different wet methods are planned to implement in ISSP UL. One area of applications of ultrasonic spray wet film technologies is creating of porous chemically active media to reach large surface areas, appropriate for electrode materials. Electrochemical oxidation will be developed to prepare oxide and complex oxide large surface areas coatings for hydrogen cells, batteries and supercapacitors including (PEO) methods.

The green routes for coatings will be priority in the Program. We plan to develop tape casting and aerosol deposition of lead-free perovskite films and multilayers appropriate for:

- energy harvesting (MEMS)
- capacitors for extended temperature range, high energy density
- cooling devices by electrocaloric effect
- elements for photonic devices
- magnetoelectric devices.

We plan to increase the experience in making of films and coatings, using spin-coating, blade casting, electrophoresis and electrochemical oxidation as well as to increase the experience and infrastructure for evaluation of the physical properties of coatings including dense single lead-free films and layered structures. We plan to apply the sedimentation of nanoparticles from suspensions and emulsions, sol-gel processing to obtain nanoparticle coating, screen printing for making of anodes and cathodes of Li/Na-ion batteries as well as further development of electrophoretic processing of nanoparticles, including sedimentation on textile. As a result new prototypes and technologies will be obtained. For example, spray pyrolysis coatings will be developed for photo-catalytic electrodes to demonstrate the power of light - decomposition of organic matter in water solutions, as well as water splitting in hydrogen and oxygen.

Laser and flash lamp sintering of nanocrystals thin films is a new direction in ISSP UL. This technology was developed for laser crystallization of amorphous silicon thin films on glass substrates [32-35]. In near future it is planned to apply this method for sintering of metal Cu and Ag nanoparticles, and metal oxide nanoparticles (ZnO, ITO).

Enabling resources, technology, infrastructure

Development of infrastructure and knowledge in flexo, screen, ink-jet and 3D printing for making of large area films of organic compounds, perspective for solar cells, organic light emitting diodes, organic lasers and other photonic and electronic applications. Such development is necessary for prototyping and technology transfer, oriented to Latvian high added value enterprises (EuroLCD, GroGlass), which exploit wet casting methods (flexo, screen and roll to roll printing) for producing of large area functional thin films.

Room equipped for wet film technologies will be developed. Existing cooperation with domestic companies, which are interested in implementation of technologies and products, like Valmiera Glass Group, EPD will be applied to functionalize glass fibers for catalyst and gas sensor applications.

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Materials for light emitters

A large variety of materials is known as “cold” emitters of light [1], among them the most intensively investigated ones are organic as well as inorganic solids having various chemical compositions and forms. Investigations clarify some basic questions concerning electronic and ionic processes in solids. This knowledge was successfully used in applied research and a large number of applications for “cold” light emitters were developed (LED, OLED, economic luminescent light sources, luminescent safety signs, scintillators for ionizing radiation detectors etc.). Despite previous achievements, the current need for efficient light emitting materials is unsaturated. Search for these materials is based on detailed understanding of the electronic - ionic processes. Therefore, investigations into these areas are of great interest and are conducted worldwide.

The R&D activities in this area was supported by Latvia through Latvian National research program IMIS2, Latvian Science Council grants, ESF and ERDF projects.

In relation to this area ISSP LU has collaborations with industrial companies Baltic Scientific Instruments, ISP Optics Latvia, Ekoosta, thus the new knowledge obtained in basic research is disseminated and the search for possible applications is a hot topic.

Current experience and advantages

ISSP UL has developed and characterized a wide range of light emitting materials. These materials include nanosized oxides and nitrides [2,3,4], organic glass-like and polymer materials [5,6], classical semiconductors [7], some other compositions for up-conversion as well as for permanent afterglow [8,9]. More than 14 papers were published on studies devoted to light emitting materials by ISSP LU researchers in refereed scientific journals.

The results were also presented at a number of International Scientific Conferences. Possible applications were developed simultaneously with basic research, e.g., a European patent on new white light emitting material based on AlN nanopowders was obtained [10]. Development of efficient permanent luminescence material is in progress.

Future R&D&I prospect

ISSP UL will investigate electronic-ionic processes of nanosized as well as composite materials with emphasis on interfacial layers properties. The knowledge obtained in these basic studies could result in new applications of light emitting materials. An example could be the realisation of optically transparent luminescent ceramics for lightening. These ceramics can have higher light output since the light back scattering, caused by powder layers, is excluded. On the other hand, the use of these ceramics in mercury-free light sources could be excited by UV from electric discharge in some noble gas or by blue light LED. Other examples - the efficient permanent luminescence of some powder materials are possible [9]. These materials can be excited by light within visible range and their afterglow continues up to 20-30 hours. These powders successfully embedded in polymer matrix could be used to produce warning labels, road signs, advertisements, all operating without electricity - this material accumulates light energy during daytime and emits light during night. Another example is the up-conversion luminescence that could be used for efficiency enhancement of solar panels, since infrared radiation could be transformed to visible light to which the solar panel is sensitive. In the field of communication and sensing organic solid state lasers which can be easily integrated in nowadays technologies have become more attractive. The GaN nano-rods could be obtained by MOCVD process and elaboration of efficient GaN nano-LED would be predicted.

The methods used in research are luminescence spectroscopy, including time resolved methods, EPR, ODMR, thermally stimulated luminescence, fractional glow techniques and transient optical absorption detection, including absorption of short lived excited states. Materials for the study were obtained via collaboration with Institute of Inorganic Chemistry (Riga Technical University institute) and via collaboration with Prof. V. Kampars from the Faculty of Material Science and Applied Chemistry of Riga Technical University. However some materials were also synthesized in ISSP UL.

Enabling resources, technology, infrastructure

Equipment for experiments shall be upgraded and supplemented, e.g., the new streak camera, having wide dynamic range and sub-nanoseconds time resolution, as well as additional sources for luminescence excitation and some other equipment is necessary.

Prototyping facilities are essential.

Materials for sensors and waveguides

With the proliferation of nano- and information sciences in virtually every field of technology and everyday life, sensors and actuators become increasingly important as a bridge between the real world and information processing. Given the rapidly increasing information processing power, the performance of the sensors is often the "rate determining step". Finding new materials, operation principles and designs of sensors and improvement of the existing ones is important in order to meet the environment, energy and health care challenges, addressed by Horizon 2020 program.

The R&D activities within this theme at ISSP UL were supported by Latvian funding within Latvian National research program IMIS2, Latvian Science Council grant, ERA-NET project Metrology at the Nanoscale with Diamonds (MYND).

ISSP UL has existing R&D collaboration with and possible technology transfer to Latvia-based industry like, Light Guide Optics International, CeramOptec, Baltic Scientific Instruments.

Current experience and advantages

Several labs at ISSP UL perform work relevant to the sensor and actuator field. Among the significant past achievements is an extensive investigation of pure and doped zirconium dioxide [2], which resulted in the development of luminescent oxygen sensor based on nanocrystalline zirconium dioxide. Oxygen sensing is an important and intensively studied field [11]. For this sensor, which was developed together with researchers of the High Pressure Physics Institute (Polish Academy of Sciences) an European patent (valid in 37 states), as well as separate USA patent were obtained [12]. Another group of materials which are prospective for oxygen gas optical sensors contains III group element nitride nanopowders (AlN, hBN). A nature of active defects responsible for material optical sensing properties was studied [13]. An European patent application for oxygen gas optical sensors based on AlN nanopowder was submitted [13].

Joint research in collaboration with the company ZRF RITEC was carried out, with the achievement of the more efficient radiation detectors [14]. Interactions of oxygen molecules with SiO₂ matrix, important for sensor applications of this widely used material have been studied in detail [15].

In the past, significant work in thermoluminescent dosimetry materials for ionizing and UV radiation [3] has been accomplished and an experimental technique for thermostimulated luminescence has been developed. Fluoride-based nanocrystalline up-conversion luminescence materials, suitable for luminescent sensing and imaging in biological systems have been developed and studied [8].

Optical sensing often requires fiber optic waveguides to deliver or extract light to or from the area of interest. This puts application-specific requirements on waveguides used, which are very different from those for standard communication fibers. Characteristics like wide spectral transparency, stability against hostile environment - ultraviolet, high energy radiation, lasers, high temperatures are often required. These fibers are based on SiO₂ and related glassy materials. ISSP has performed a number of internationally well-recognized studies of these materials, e.g., [16,17], aimed at increasing their optical transparency and stability under UV or ionizing radiation [18].

Internationally recognised work has been carried out in synchrotron-radiation-assisted studies of perovskite materials suitable for chemical sensors and photocatalysis [19]. Expertise has been acquired in physics of amorphous/glassy materials for optical fibers [17], photoinduced Bragg gratings and holographic recording [20]. Organic semiconductor films suitable for sensing applications have been advanced and characterized [21]. Using the recently improved electron microscopy (SEM/TEM) and nanofabrication (FIB) facilities, ZnO, CuO, TiO₂, PbS, Si nanowires have been synthesized and characterized (e.g. [22]), with the aim to improve their characteristics for selective sensing of chemical species in gas or fluid media.

Future R&D&I prospect

Research and development work will be conducted in search of new luminescent materials, having enhanced sensing performance based on complex nanostructures (nanoparticles, coatings, porous ceramics and heterogeneous structures). Novel concepts of sensing molecular species by their magnetic properties in conjunction with the diamond nitrogen-vacancy magnetic field sensors will be explored, with an emphasis on single oxygen sensing important in cell biochemistry. The feasibility of far-infrared radiation detectors based on organic semiconductor films will be explored. Research will be performed with and aim to elucidate factors causing unwanted light attenuation and to obtain multimode fiber waveguides with improved transmission in near-infrared to deep-ultraviolet regions, suitable for applications in sensor and analytical instrumentation. The synthesis methods of heterogeneous core-shell nanowires, nanotubes and other types of 1D nanostructures will be developed and their applications for the sensors will be explored.

Enabling resources, technology, infrastructure

Prototyping facilities are an essential requirement. The envisaged research mostly concerns materials on micro- and nano-scales, shaped into heterogeneous systems, which are significantly influenced by surfaces. The present research infrastructure, formerly aimed at studying larger scale homogeneous systems at larger scales, must be upgraded by adding capabilities to create and handle micro- and nano-scaled objects, to process and to characterize surfaces under vacuum or under controlled atmospheres. Due to the tight focusing requirements in micro- and nano-sized photonic devices, laser light sources are typically used in their studies, and new sources, additionally to the existing ones should be acquired. The existing equipment for testing of spectral properties, pulsed power guiding reliability and radiation toughness of fiber-optic waveguides should be upgraded and extended. Further, the ability to create and handle planar and in particular, fiber-optic waveguides used in the photonic sensor context should be further explored.

Materials for photonic applications in ICT

It is expected that in the 21st century the dominating role of electronics in the development of information and communication technology (ICT) will be overwhelmed by photonics - a multidisciplinary field of science and technology concerning light emission, transmission, amplification, detection and modulation. The commission of European communities has defined photonics as one of the top five key fields of science and technology for society and economy [23]. Large diversity of devices, like light sources, modulators, switches, Bragg and arrayed waveguide gratings for WDM, optical data storage and etc. are necessary for the transition from the electron to the photon as an information carrier. Development of photonic devices, obviously powered by light and matter interaction, depends on new materials exhibiting the necessary properties. In order to construct the active waveguide elements the Silicon Photonics (SP) workflow and technology could be employed. The SP has many advantages that suggest that it could become a standard for building Photonic Integrated Circuits (PIC). Unfortunately silicon as optical material has some drawbacks, therefore search for materials to complementing SP in developing PIC continues within a R&D community [24]. The R&D activities within this theme at ISSP UL were supported by funding within Latvian National research program IMIS2, ESF and Latvia-Lithuania-Taiwan mutual projects. ISSP UL have existing R&D collaboration with and possible technology transfer to Latvia-based industry like EuroLCDS, Baltic Scientific Instruments, RD Alfa microelectronics, ALFA RPAR, Light Guide Optics International, CeramOptec,.

Current experience and advantages

ISSP UL has been conducting research on materials exhibiting the phenomenon of photoinduced mass transport and novel NLO active organic materials. The first effect is very promising for practical application in material surface relief patterning technologies for lithography and diffractive optical element fabrication [25]. Organic NLO materials could be used in electro optical (EO) and all optical (AO) modulators for high speed data transmission, because of their multiple advantages such as low cost, easy processability, low dielectric constants and high NLO efficiency [26]. Different materials (amorphous chalcogenides, azo-dye containing organic polymers, gelatine and etc.) have been studied. The influence of recording light polarization and intensity on surface relief formation efficiency was studied [20,27,28]. It was shown that surface relief formation efficiency in organic molecular glasses is about 50 times higher than in chalcogenide films [29].

Laboratory of organic materials at Institute of Solid State Physics University of Latvia in collaboration with the Faculty of Material Science and Applied Chemistry at Riga Technical University are conducting research aimed to create novel organic glasses for use in photonic devices. Since 2004 more than 100 novel photonic materials have been developed and have been investigated. Theoretical modelling of the structure, chemical and physical properties of these materials has been done by means of quantum chemistry ab initio and molecular dynamics methods [30]. Since 2011 a major material class under

investigation became the low molecular weight organic glasses that were developed using a novel approach [31]. Novel EO active organic glasses synthesized at Riga Technical university have been studied experimentally [32,33,34] and their capability to use them in photonic devices is evaluated [35]. Remarkable NLO efficiency in combination with high optical quality has been achieved in some of these materials. Unfortunately wide practical application of these materials is limited due to the poor thermal stability - so far no one has met industrial demands i.e. short time exposure to temperature $\sim 170^{\circ}\text{C}$ during the PIC device manufacturing and fulfilled Telecordia standards of long term stability at typical device operational temperature of 85°C .

Future R&D&I prospect

Up to now there is no clear understanding of the photoinduced mass transport [36,37], This demands further research which will be conducted to understand the physical mechanisms. Improvement of light sensitivity of such direct recording media with the aim to develop new types of photoresist exploiting photoinduced mass transport phenomenon is planned. In addition we plan to advance a new optical lithographic process, based on developed resist, for production of diffractive optical elements in photonics integrated circuits (PIC). Investigation will be conducted with the aim to obtain diffractive optical elements like Bragg Reflectors, Arrayed Waveguide Gratings etc. with electrically tunable properties.

Another research activity addresses EO materials meeting industrial demands i.e. short time exposure to temperature $\sim 170^{\circ}\text{C}$ during the PIC device manufacturing and fulfil Telecordia standards for long term stability at typical device operational temperature 85°C . To overcome the problem with so called "PO lattice hardening" after orientation of NLO chromophores incorporated in glassy structure are considered. This can be accomplished by thermo- or photo- initiated crosslinking of polymers or low molecular weight molecules by the presence of coupling groups. We plan to pay more attention to the research in field of materials for "all optical" PIC devices.

Enabling resources, technology, infrastructure

Renovation of existing and purchase of new (excimer) laser systems for holographic recording are necessary. New complex for nonlinear multiphoton excited spectroscopy (TPL, SHG, THG, CARS) investigations of nonlinear optical properties of materials should be established. Equipment for investigations of waveguide PIC elements must be advanced. Prototyping facilities are essential.

Prototyping of photonic and microelectronic devices

For several decades the Institute of Solid State physics has been the leading scientific institute in Latvia specializing in material research and development. Most of the research performed at the ISSP UL is aimed towards creating new materials for application in photonic and micro-electronic devices as described previously. The future development of ISSP UL would depend on the success in prototyping of photonic and microelectronic devices. Based on competences of ISSP UL it is a logic consequence to pursue the challenges in the field of photonics integrated circuits (PIC). Currently the main platform for the development of PIC components is the semiconductor-on-insulator (SOI) platform. Within this approach the PIC components - light sources, waveguides and detectors - are fabricated on a single chip using complementary metal oxide semiconductor (CMOS) fabrication technology. The current status and growth trends indicate that in short time the SOI will become the main tool for developing low cost-per-chip and small footprint commercially available network components, sensors and other devices. However, there are still challenges that should be overcome in order to obtain further reduction of size, increase in efficiency and functionality. These include: i) developing a PIC compatible light source, ii) increasing the functionality of the integrated waveguides in the active components of PIC and iii) demonstrating monolithic integration of various optical components on a single optical chip.

The first issue is related to a CMOS process compatible light source on chip. Several candidates, such as Ge lasers, Erbium doped lasers, plasmon laser sources and hybrid lasers (GaAs, InAs/GaAs quantum dots) have been considered for this application in the literature, however, none have yet demonstrated sufficient emission efficiency.

Another important field of research concerns the development of functional waveguide in PIC components. Functional waveguides could be employed in various devices such as sensors, low-drive voltage modulators and other.

Until very recently much effort had been devoted towards maximizing the performance of single optical components and building complex PICs implementing the “module integration”. This causes the built optical devices to be less efficient and reliable. Thus a great challenge in the field of PIC development is to achieve “true integration” - monolithic integration of different optical components on a single chip. The device with complex functionality made on a single chip is more reliable, has smaller footprint, it consumes less power and possesses other benefits. The “true integration” is yet in its infancy if compared to the electronic industry and it will be one of the main research topics in the next decades.

Developing the prototyping capabilities will open further collaboration with Latvian SME like RD Alfa microelectronics, ALFA RPAR, Baltic Scientific Instruments, EuroLCDS.

The research activities at ISSP UL were supported by ERDF project “Development of research infrastructure National Research Centre for Nanostructured and Multifunctional Materials, Constructions and Related Technologies”.

Current experience and advantages

In the ISSP UL much effort is directed towards solving the light source and waveguide functionalization issues mentioned above.

The ISSP UL has demonstrated the competence in developing efficient and cheap light sources [38, 39]. We have presented Er doped systems for lasing, materials for organic lasers, research results on quantum dots, all of which are potential candidates for application as light sources in PICs. The above results are frequently published and transmitted to local and international patents.

Also, various materials that would allow functionalization of waveguides in PICs have been developed at the ISSP. These materials exhibit change in the material property depending on electric field strength (electro-optic materials), incident light intensity (opto-optic materials with Kerr nonlinearity), on mechanical pressure (piezo- and electro-striction effect), on atmospheric gas concentration, etc. During the recent years the ISSP UL has made important steps in actual design of PIC comprising the mentioned materials. As an example, we have described a hybrid SOI/polymer EO waveguide Mach-Zehnder interferometric (MZI) modulator capable of operating in the visible and NIR part of the spectrum. The preparation steps as well as numerical simulations of the design were published in a recent paper [35] and currently an EU patents are pending an [40, 41]. High optical nonlinearity, low power consumption and cost of the electro-optic device are predicted by the researchers.

The development of the mentioned materials and technology require sophisticated equipment and adequate clean rooms. By the support of ERDF project “Development of research infrastructure National Research Centre for Nanostructured and Multifunctional Materials, Constructions and Related Technologies” setting up of open access laboratory “LATNANO-C” at ISSP UL was performed. During the period of 2012-2015, 3.0 million EUR were invested for establishing 800 m² of 5-8 ISO clean room facility as well as for purchasing equipment, e.g., TEM, SEM-FIB, used for material characterization. For prototyping at present we have installed a thin film vacuum deposition cluster tool (SAF 25-50, Sidrabe) and a micro pattern generator (μ PG 101, Heidelberg Instruments) for direct writing applications and low volume mask making.

Future R&D&I prospect

The researchers at ISSP UL are pursuing the course of photonics component development, integration and packaging. As mentioned above, the ISSP UL has made all the necessary preparations for this purpose. We have established a basis for material development and characterization, optical component designing, etc. The logical next step would be to apply the know-how for device development and prototyping.

The prototyping activities at ISSP UL are planned in relation with R&D activities within the topics of research direction “Functional materials for electronics and photonics”. The current trends in the scientific community, experience and available tools at ISSP UL suggest that the prototyping should be done on polymer and Silicon Photonics (SP) made on SOI platforms.

On the polymer platform we aim to build waveguide components by employing direct micro-patterning. Using such approach waveguides with the resolution of a couple of micrometers can be prepared, which is sufficient for attaining low refractive index waveguide components. Employing the direct writing approach waveguides in materials such as SU-8 and PMMA will be formed. The functionality of the waveguides will be obtained for example by integrating sensing materials such as EO, luminescent and others.

The SP waveguide devices on SOI platform are prepared with resolution which is couple of orders of magnitude higher than that of direct laser micro-patterning. With the high resolution lithography tools various optical components can be fabricated. As mentioned, SP is one of the most popular scientific and industrial topics and is currently saturated by research done on only SOI platforms. The novel approach realized by the ISSP UL would include creating hybrid devices on SP. The hybrid devices will employ organic, perovskite and other materials on the developed SP. We aim to demonstrate photonic hybrid devices for ICT, such as high-speed optical modulators, tunable multiplexers and other. The high resolution lithography will also allow preparing grating structures suited used for prototyping distributed feedback organic lasers, grating couplers and other optical elements.

Enabling resources, technology, infrastructure

The realization of the mentioned and similar ideas here at the ISSP UL requires access to the advanced fabrication technology that is currently unavailable in Latvia.

For prototyping of photonic and microelectronic devices the following technology and tools are necessary. Some of tools and technology (sputtering/evaporation tools, film characterization tools, optical microscopes, surface optical and/or mechanical profilometers, wet benches, spin-coaters, ovens and hotplates) are available ISSP UL. At the same time some essential tools and technologies like large area electron beam lithography (EBL) system, wet and dry etching systems, ion implantation system and post processing tools should be implemented to advance prototyping facilities at ISSP UL to internationally recognized level.

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Selected highlights - 2018

E. Butanovs, S. Vlassov, A. Kuzmin, S. Piskunov, J. Butikova, B. Polyakov
Fast-Response Single-Nanowire Photodetector Based on ZnO/WS₂ Core/Shell Heterostructures

ACS Applied Materials and Interfaces, 2018, 10(16) (pp. 13869-13876)

[DOI: 10.1021/acami.8b02241](https://doi.org/10.1021/acami.8b02241)

SNIP(2017)= 1.543, IF(2017)= 8.097

L. Skuja, N. Ollier, K. Kajihara, K. Smits, Creation of glass-characteristic point defects in crystalline SiO₂ by 2.5 MeV electrons and by fast neutrons, *J. Non-Cryst. Solids*. 505 (2019) 252-259
[doi:10.1016/j.jnoncrysol.2018.11.014](https://doi.org/10.1016/j.jnoncrysol.2018.11.014)
SNIP=1.19, IF=2.34,

V. Karitans, E. Nitiss, A. Tokmakovs, and K. Pudzs
Optical phase retrieval using four rotated versions of a single binary mask - simulation results.
Proc. SPIE, 2018, **10694**, 106940C (pp. 1-7).
DOI: [10.1117/12.2311861](https://doi.org/10.1117/12.2311861)
SNIP: 0.335

IV. Energy

Domain: Energy

The increasing energy demand due to growing global population and the critical relationship between energy, environment and sustainability lead to novel discoveries and advancement in the field of energy materials in search of alternative resources. Advanced energy materials covers major subjects such as fuel cells, organic and inorganic photovoltaic, flexible, printed and thin film batteries, lithium ion and Lithium coating batteries, supercapacitors, piezoelectric energy harvesters, hydrogen generation and storage, thermoelectric, photo catalysis solar fuels and thermosolor power, thermonuclear fusion. Thermoelectric and pyroelectric materials help in capturing heat and are transformed into electrical power. The vibration, movement and sound are captured by piezoelectric materials that are transformed into electric power. Initially, thermoelectric materials are limited due to small conversion efficiency, but the occurrence of nanostructural thermoelectric materials led to significant development in enhancing thermoelectric properties. The pyroelectric effect is being used in sensors.

The description of selected issues, its current state of the art, future prospects, needs and expected results are given below.

- I. Materials for batteries
- II. Materials for hydrogen production and storage
- III. Materials for application in fusion facilities

Materials for batteries

Lithium ion batteries (LIBs) are the energy storage devices that provide the highest voltage and charge capacity compared to other rechargeable batteries. The wide applications of LIBs in portable electronics have changed our daily life significantly. Recently LIBs entered into the commercial electric vehicle market. Using commercially available LIB with the organic-based electrolyte safety issue is always a major concern, especially for high-rate or high power applications. To improve the safety features as well as the miniaturization capability of LIBs, a new cell design using solid electrolyte instead of liquid electrolytes has recently received a great deal of attention. In the solid state Li ion batteries, the cathode and anode will be separated by a dense inorganic solid electrolyte.

Solid state lithium batteries have several advantages over lithium batteries with liquid or polymer electrolyte: a wide operating temperature range, high safety and energy density.

The main drawback that limits the implementation of solid state batteries are relatively low ionic conductivity of the solid electrolyte and high charge transfer resistance of the interfaces anode/solid electrolyte and solid electrolyte/cathode. The other disadvantage is lithium losses at high temperature thermal treatment during the preparation of batteries. The race is on around the world to develop a new generation of batteries that can perform beyond the limits of the current lithium ion based battery. There has been a certain degree of success with the sodium ion battery development which has a single positive charge - the same as lithium. In the future replacement of single charge ions with plus-two charge ions, for example, magnesium will open a credible design path for a new class of high voltage and energy batteries. Having established that magnesium can be reversibly inserted into the electrode material brings researchers one step closer to a prototype.

Current experience and advantages

Cathode materials studied at ISSP UL include LiFePO_4 in the form of powder material and thin films, LiFePO_4 composite with graphene, reduced graphene oxide and other carbon additives. Large capacity and high rate capability $\text{LiFePO}_4/\text{C}/\text{graphene}$ cathodes and LiFePO_4 thin films which can possibly be up-scaled to develop large area thin films have been prepared at ISSP UL.

Anode materials: Graphene, reduced graphene oxide, high surface area carbon, MeO ($\text{Me}=\text{Fe}, \text{Co}, \text{Ti}\dots$) composites with carbon containing additives have been studied at ISSP UL. The high charge capacity of graphene composites indicates that they are promising anode materials for future rechargeable batteries.

Future R&D&I prospect

- Development of thick film lithium ion batteries with high performance, which will be achieved by increasing the ionic conductivity of the solid electrolyte and the planar deposition of anode and cathode as counter micro-strips on solid electrolyte films. This will reduce the electrical resistance of interfaces between the solid electrolyte and the anode/cathode electrodes.
- Design of new sodium ion batteries as an alternative to lithium ion batteries because the feedstock raw materials used in the manufacture of lithium batteries is limited.
- Configuration of magnesium ion batteries as a two plus charged ion battery with enhanced energy and power density.

Enabling resources, technology, infrastructure

Advanced electrochemical impedance spectroscopy equipment possessing low current electrochemical detection and frequency response analyzer modules are required. Equipment for zeta potential determination including electrophoretic mobility is necessary. Synthesis of the samples requires controlled atmosphere glovebox, ultrasonic reactor and vacuum furnace.

Materials for hydrogen production and storage

Currently, world energy (transport, stationary applications) is based on burning of fossil energy sources, leading to environmental pollution and irreversible depletion of Earth resources. Renewable energy resources such as sun and wind, are not always available when energy is needed, therefore, energy storage is actual, and hydrogen can be used as an efficient energy carrier to store the electricity from renewables. Hydrogen produced in such a way can be stored in compressed gas containers or in metal hydrides, nano-porous composites, and converted back into electricity when needed with fuel cell without open burning and CO_2 emissions.

Current experience and advantages

Different thin film technologies (electrochemical deposition, spray pyrolysis, electrophoretic deposition, anodic oxidation, magnetron sputtering) are used to obtain

electrodes for hydrogen production in electrolysis and photo-electrochemical splitting methods. Metal alloys and their composites, ion exchanged natural and synthetic zeolites, few layer graphene sheet stacks are synthesized and studied; sulphonated PEEK and Nafion membranes are modified with nano-crystalline oxides for hydrogen separation and ion conduction research.

Future R&D&I prospect

- Development, synthesis and research of new materials, thin coatings and innovative technologies for hydrogen production (water electrolysis, photocatalysis, bio-hydrogen production from waste), storage and usage;
- Applications in energy storage and environmental monitoring applications (air pollution reduction, odour removal);
- Elaboration and research of new membrane and catalyst materials for application in fuel cells and for hydrogen sensing.

Enabling resources, technology, infrastructure

Spray pyrolysis systems to obtain thin film electrodes for hydrogen production and sensor applications are required. Glovebox, microwave hydrothermal reactor and vacuum drying furnace is needed for sample preparation. Advanced electrochemical impedance spectroscopy equipment is necessary.

Materials for application in fusion facilities

EUROfusion is a consortium coordinating fusion research in 28 European countries, involving 30 national research institutes and about 150 university groups; in terms of number of involved member states it is the largest European Research organization. The main objective of EUROfusion is to achieve electricity generation from fusion reactions in a process that mimics the source of energy of the sun and the stars. The work programme of EUROfusion is based on the fusion roadmap which describes the research plan to achieve as early as possible electricity from fusion.

The fusion roadmap is organised around three main devices:

1. The international ITER (International thermonuclear experimental reactor) project - a collaboration of 34 countries - with the aim to achieve conditions in which the fusion reactions in the plasma yield a power of 500 MW versus an input power of 50 MW.
2. A demonstration reactor DEMO which will for the first time demonstrate electricity generation from fusion.
3. A dedicated neutron source DONES (DEMO Oriented Neutron Source) that mimics the neutron spectrum of a fusion reactor and that is needed to test and validate new materials.

The EUROfusion work programme is set up in a way that each country gives contributions that are aligned according to their specific strengths. Latvia has a deep expertise in the field of materials and in plasma-facing components and is giving valuable contributions to the European fusion endeavour.

Institute of Solid State Physics, University of Latvia actively participates in the materials research on fusion. A number of more elaborated issues and projects are itemized as follows:

- Multiscale theory and large scale modelling of functional materials for diagnostics;
- Combination of different experimental studies (optical, EPR, Raman, EXAFS etc.) and multiscale computer modelling, e.g., by validation of computer modelling by advanced

materials (including understanding the mechanism for nucleation of Y2O3 precipitate in the ferritic steel lattice (ODS));

- XANES spectra measured at absorption edges (revealing valence state of the absorbing atom and the local symmetry around it);

- Local atomic structure (interatomic distances) and dynamics (MSRDs) around absorbing atoms, including radial distribution functions for all samples for all measured absorbing atoms;

- Radiation stability of MgO, Al2O3, MgAl2O4 spinels is controlled by radiation defect mobility and secondary reactions (recombination and aggregation, colloids);

- Defect annealing parameters (e.g. migration energies) for electron- and neutron/heavy ion- irradiated materials, due to uniform- and track distributions, respectively;

- Access to Large Scale Facilities (Synchrotron, Neutron, tokamaks, heavy ion radiation research) as a great opportunities for small countries.

Apart from research activities in traditional EUROfusion Work packages, two highly ranged Enabling Research projects are elaborated in ISSP UL:

(1) When and how ODS particles are formed? X-ray Absorption Spectroscopy and atomic-scale modelling of ODS steels - AWP15-ENR-01/UL-01; 2015-2017;

(2) Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion applications (AETA) - AWP19 ENR - 01 ISSP-UL-02; 2019-20120.

Selected highlights - 2018

Yu.A. Mastrikov, R. Merkle, E.A. Kotomin, M.M. Kuklja, and J. Maier.
Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes.

J. Mater. Chem. A, 2018, **6**, pp. 11929-11940.

DOI: [10.1039/c8ta02058b](https://doi.org/10.1039/c8ta02058b)

SNIP(2017)=1.550, IF(2017)=9.931

G.S. Nusinovich and O. Dumbrajs.

Possible gyrotron operation in the "no start current" zone caused by the axial dependence of the phase of the resonator field.

Phys. Plasmas, 2018, **25**, 093108 (pp. 1-7).

DOI: [10.1063/1.5045317](https://doi.org/10.1063/1.5045317)

SNIP(2017)=0.682, IF(2017)=1.941

V.N. Kuzovkov, E.A. Kotomin, and A.I. Popov.

Kinetics of the electronic center annealing in Al₂O₃ crystals.

J. Nucl. Mater., 2018, **502**, pp. 295-300.

DOI: [10.1016/j.jnucmat.2018.02.022](https://doi.org/10.1016/j.jnucmat.2018.02.022)

SNIP(2017)=1.380, IF(2017)=2.447

E. Kotomin, V. Kuzovkov, A.I. Popov, J. Maier, and R. Vila.

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