

Towards new applied research and innovations



2015th was the year of essential changes and exciting time for our Center. In autumn we began the movement to new buildings equipped with modern technological and scientific infrastructure. We believe that not only a New Period begins in our history – it will be a New Beginning of Quality in Technological and Scientific Development enabling us to open modern trails to innovations, to extend applied scientific research in the development of high-tech business and creation of knowledge-based economy in Lithuania.

Of course, we will rely on research topics where we have substantial experience and comprehensive know-how such as Optoelectronics and Laser Technologies, Environment-friendly Technologies, Nuclear Physics and Radioecology, Organic Chemistry and Bionanotechnologies, Electrochemical Materials and Functional Materials, Electronics and Sensors, Fundamental Research, and Metrology.

Our approach is interdisciplinary problem-solving, since we believe that this way provides a unique opportunity to create synergies and mutual benefits from scientific expertise.

In 2015 the Center for Physical Sciences and Technology – the largest scientific institution in Lithuania – has celebrated the 5-year Anniversary. The international Conference entitled Center for Physical Sciences and Technology 2015: 5 Year Anniversary and New Beginning was dedicated and organized in Sunrise Valley, Vilnius, Lithuania, in November 2015.

To catalyze activities into international level and embrace comprehensive know-how in bridging applied research and high-tech business, we have formed International Advisory Board consisting of scientists of highest academic reputation and highly-ranked representatives from internationally leading high-tech companies.

We pride ourselves on supporting each other as an international team aiming to enrich culture of collaboration and enhance discovery impetus to go towards excellence.

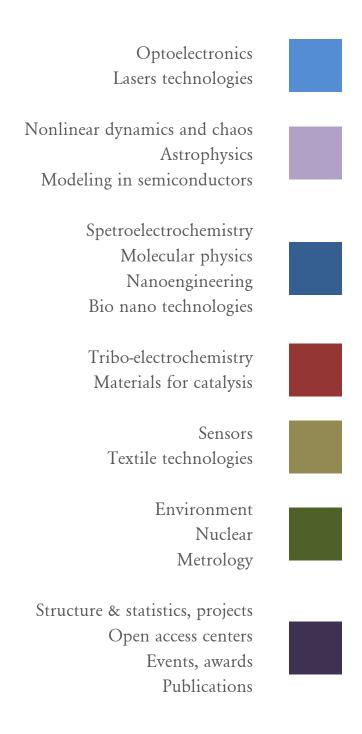
We believe that trailblazing should be our inherent feature.

Research achievements overview and modern trails of innovation are described in pages that begin here.

Gintaras Valušis Director of the Center

Fizinių ir technologijos mokslų centras (FTMC) Center for Physical Sciences and Technology

Contents



Optoelectronics



Semiconductors for the light technologies

Optoelectronics is widely recognized as one of the Key Enabling Technologies of the future. At Optoelectronics Department this field of research is developed in two main directions: i) epitaxial growth technology of semiconductor structures and devices for mid- and far-infrared spectral ranges and ii) terahertz frequency range components, systems, and applications. Moreover, the Department operates a most comprehensive set of standard optical characterization techniques that is intensely exploited also by other Lithuanian research groups and companies.

There are many paths you can follow when striving to improve device performance. One option is to keep it simple and try to improve the quality of the production processes, such as optimising the growth process of the epiwafer. This can pay dividends, particularly if the class of device is not well established. But by far the most radical route is to dispense with a mature material system, and adopt one that is yet to be tried and tested. That's what a team of FTMC researchers is doing, developing optoelectronic semiconductor components based on bismuth alloys rather than standard A_3B_5 compounds. This effort has had to start from scratch, developing models to understand device behaviour and establishing appropriate growth conditions before it is even possible to try and fabricate the first devices. An attractive attribute of bismide alloys is the behaviour of their energy gap: It decreases very rapidly with bismuth composition, allowing growth of telecom lasers on a GaAs substrate. Our research group is one of the world leaders in developing bismide based lasers, photodetectors, and terahertz components.

Terahertz (THz) radiation, which lies in the frequency gap between the infrared and microwaves, typically referred to as the frequencies from 100 GHz to 30 THz, has long been studied in fields such as astronomy and analytical science. However, recent technological innovation in photonics and nanotechnology is now enabling THz research to be applied to many more sectors. THz imaging holds promise for a multitude of applications from biomedical imaging to the inspection of semiconductor devices. We investigate different THz spectroscopy and imaging applications and develop novel optoelectronic THz frequency range components and systems. These are commercialized by two companies that have been started by the researchers of Optoelectronics Department.

When the size (atomic) matters

Dilute bismide layers are not just promising for the fabrication of telecom lasers and modulators - they also offer significant opportunities for the development of low-cost, efficient terahertz technologies. We have exploited very short photoexcited electron trapping times, which were typical in the first GaBiAs epitaxial layers grown with large bismuth content. The subpicosecond trapping times in GaBiAs, together with the narrow bandgap and relatively high electron mobility, make this material very attractive for manufacturing photo-conductive antennas for terahertz emission and detection. Such devices are in demand for spectroscopic, imaging, and security applications. Until recently, terahertz emitters and detectors were mainly manufactured from epitaxial layers of GaAs grown by MBE at low substrate temperatures. This approach is not ideal, because GaAs is transparent to wavelengths beyond 850 nm, so bulky and expensive femtosecond Ti:sapphire lasers are required for carrier excitation in this class of optoelectronic THz radiation system. In contrast, compact fibre or diode lasers emitting in the 1.0-1.5 μm range can activate optoelectronic THz emitters and detectors developed in Bismide-based systems have already commercialized. They are available from TERAVIL, a spin-off company of the FTMC.

Ga

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Fig. 1. Fibre-coupled photoconductive terahertz detector featuring a GaBiAs layer.

Looking into invisible

Terahertz (THz) imaging and spectroscopy could become cheaper and simpler with a chip integrated optics and detectors. Terahertz Photonics Laboratory develops sensitive compact detectors and systems for many practical applications such as security systems, materials testing, identification and medical diagnostics. A miniaturisation of spectroscopic THz imaging systems by integrating a room temperature InGaAs-based bowtie THz diode that has broadband operation up to 2.5 THz, with the secondary diffractive optics in a single chip is also pursued. The free-standing zone plates and cross shape filter arrays from thin metal film were developed and used for focusing and frequency selection purposes. Integrating them with the terahertz sensor makes the detector much more compact and reliable. The use of flat optics enables an order of magnitude increase in the detection capability, making such system very attractive for terahertz imaging applications.

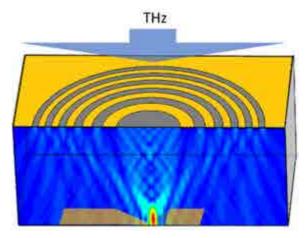
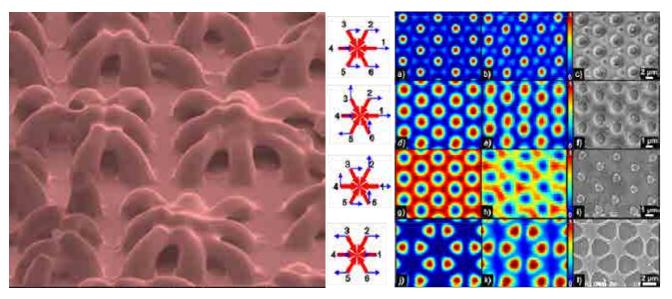


Fig. 2. The focusing features of the compact diffractive optics placed on the same chip with the THz sensor.

Laser technologies



Optical coatings, solid-state and fiber lasers, laser material processing and nanophotonics

Nowadays the lasers and laser technologies became the main building blocks in light application in diverse fields, from the heavy industry to toys for children. The Department of Laser Technologies with its five laboratories covers significant part of the optically related activity, ranging from new discovered effects to laser machines, and stepping through all technology readiness levels. The smart optical coatings developed in the Laboratory of Optical Coatings convert the pieces of glass into valuable products able to control spectral and temporal properties of the light. New laser sources, under development in the Fiber Laser and Solid-State Laser Laboratories that are based on tiny but smart fibres or active bulk crystals provide not only a new wavelengths of coherent radiation, but high peak power, ultra-short pulses and controlled wave front as well. Combining and merging of the coherent beams makes the lasers even more powerful.

The scope in material processing using ultrashort pulse lasers includes the investigations of the underlying processes in new devices as well as inventive and hard work on the practical problems in laser technologies. Thin film scribing for photovoltaics, efficient surface texturing utilizing laser beam interference, glass processing with lasers, nano-textures decorated by nanoparticles, dual-wavelength induced metal surface self-organisation, electroless plating of laser modified polymers, laser-induced transformations in graphene-like materials make up the main working topics of the Laboratory of Laser Microfabrication Technologies in 2015.

When the structure dimensions are smaller than light wavelength, new effects arise. The Laboratory of Nanophotonics deals with sub-wavelength structures, in this way enhancing interaction of photon propagating in micro-ring resonators with environment. This allows to construct sensitive tools for sensing applications.

Large group of scientist, PhD students and engineers work together in laser-related fields. Their tight collaboration with colleagues from other departments of FTMC (Optoelectronics, Physical Technologies, Nanoengineering, Organic Chemistry, Catalysis, Electrochemical Material Science, Characterization of Material Structure) facilitates progress in laser physics and applications.

Sculptured optical thin films

A technological method to form advanced optical coatings by evaporating material on a geometrically controlled substrate was mastered in FTMC. Anisotropic coatings named Sculptured Thin Films can be formed by manipulating the substrate and exploiting self-shadowing effect as shown in Fig.1a. Oxides, fluorides, and metals can be used as vapour source to form various nano-structured coatings (Fig.1c). By depositing material at glancing angles, the columnar thin films may be produced. Such structures are used for formation of waveplates or other phase control elements. By rotating the substrate around its normal, the chiral structure is established. Such a metamaterial exhibits Bragg reflection phenomena for circularly polarised light (Fig.1b). Due to the inherent porosity of Sculptured Thin Films, the applications for organic or gas phase material detection are also considered.

Ultrashort optical pulse generator based on nonlinear spectral re-shaping

A new design for an ultrashort fiber generator using spectral broadening, induced by the phase self-modulation during pulse propagation in a fiber, and double-alternating spectral filtering was demonstrated. The key components of the ultrashort fiber generator are: amplifiers (Gain 1, 2), optical Kerr media $(\chi^{(3)}),$ and filters, which transmit shorter (1) and longer (2) wavelengths. Optical cavity of the pulse generator is normally spectrally closed, and no longitudinal modes can oscillate inside the cavity. After entering the initial pulse, a stable self-sustainable generation of the pulse train can be obtained.

High-power NIR laser with composite Nd:YVO₄ rod

The ultrafast Nd:YVO₄ laser operating at 1342 nm wavelength demonstrates the highest average output power achieved from NIR DPSS laser in ps mode of operation. Picked from the oscillator train, seed pulses were injected into the cavity of the regenerative amplifier based on composite Nd:YVO₄ crystal with diffusion-bonded segments of multiple Nd doping concentration pumped at 880 nm. Optimised laser layout emits ~13 ps output pulses of 11 W average power at 300 kHz repetition rate with unsurpassed beam quality of M^2 < 1.1 despite the larger quantum defect. Output power is further converted to the 2nd, 3rd, 6th and 7th harmonics at 671, 447, 224, 192 nm wavelength, respectively.

Nanophotonic SOI ring sensor decorated by Au nanodiscs

A refractive index sensor based on an optical silicon-on-insulator (SOI) micro-ring resonator with a periodically arranged set of gold nanodisks is designed. Periodic arrangement of nanodisks selects a single resonance from a wide set of ring resonator modes and removes the mode splitting. Extraction of the electromagnetic energy into evanescent plasmonic modes enhances the light-analyte interaction and increases device sensitivity to variation of refractive index up to 176 nm/RIU.

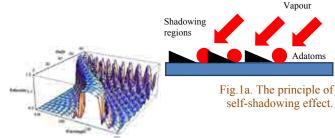


Fig.1b. Bragg phenomena for circularly polarised light.

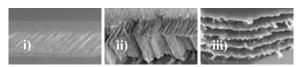


Fig.1c. SEM images of (i) Cu, (ii) TiO₂ columnar thin films and (iii) MgF₂ chiral thin film.

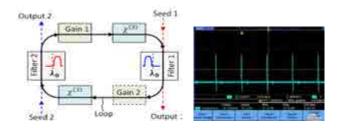


Fig. 2. Schematic diagram of the ultrashort pulse fiber generator and oscilloscope snapshot of the experimentally generated pulse train.

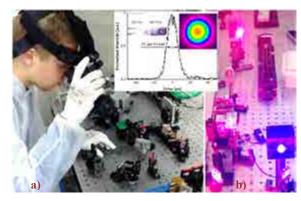


Fig. 3. (a) NIR regenerative amplifier set-up; (b) the 2nd and 3rd harmonics generation at 671 nm and 447 nm wavelength.

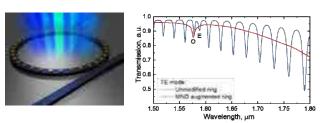


Fig. 4. The SOI optical ring resonator with implemented gold nanodisks and transmission spectra of unmodified (blue) and Au metal nanodisks augmented (red) SOI optical ring resonators.

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Laser patterning for CIGS devices

Solar cells based on Cu-chalcopyrite, Cu(In,Ga)Se₂ (CIGS), have been established to be the most efficient thin-film technology that converts sunlight into electricity. In order to maintain high efficiency over the large area, a laser scribing is needed to divide large scale device into smaller cells interconnected in series. Usually, three laser scribing processes, called P1, P2 and P3, are used for the module processing. Layer selectivity, low thermal damage, and high throughput are the main requirements for the industrial scribing processes. To realize these goals, we are carrying out the research on the CIGS processing using modern high power ultra-short pulsed lasers. Substantial part of the investigation is concentrated on P2 and P3 high-speed scribing.

Optical manipulations in polymeric structures

The four-beam interference lithography was shown to be easy, fast and flexible method to fabricate microaxicon-like elements over a large area. Optically transparent body with spherical surface is able to form a Bessel-like beam. The propagation of this beam behind the spherical structure with significant aberration, when $\beta_1 > \beta_2 > \beta_3$, is schematically shown in Fig. 6. Periodically arranged polymeric microaxicon-like arrays produced by the four-beam interference lithography technique paves the way for the development of tilt-tolerant wavefront sensors, optical tweezers, new optical imaging systems or novel materials processing tools.

Nano-structuring by combined laser irradiation

The periodic nano-surface-structures have found many applications during the last decade. That includes the control of surface wetting, light extraction and harvesting, chemical and mechanical alteration of materials, coloring of the surfaces, nano-textured surfaces for bio-sensors, micro-optical elements, and the light absorption enhancement.

A flexible method of nano-surface-structuring by temporally and spectrally combined laser irradiation was developed (Fig. 7a). The periodical structures with a controllable period varying from 200 nm to 600 nm were successfully fabricated on the stainless steel surface (Fig. 7b). The period was controlled by the delay between the beams.

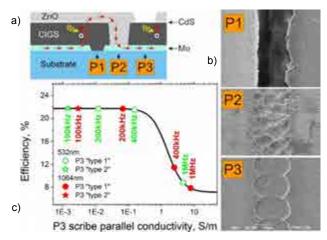


Fig. 5. a) Schematic view of the CIGS module series interconnect formed with three-step laser scribing, (b) SEM images of the laser patterns, (c) solar panel efficiency dependence on the P3 laser pattern parameters.

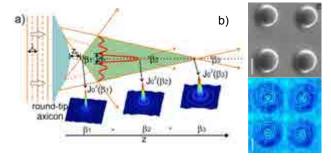


Fig. 6. (a) Bessel beam formation by spherically-shaped refractive axicon, (b) microaxicon-like structures fabricated by interference lithography, (c) beam intensity distributions exiting from the microaxicon-like structures (b) in the transverse plane, at distance 200 µm from the apex of the microaxicon-like elements.

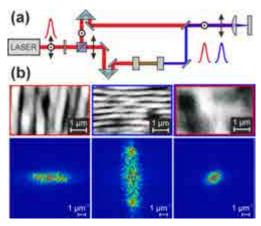
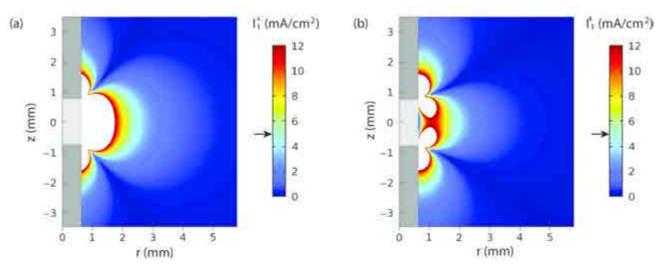


Fig. 7. (a) Set-up for the temporally and spectrally combined laser irradiation, (b) SEM images (top) and fast Fourier transforms (bottom) of the nano-surface-structures formed on the stainless steel surface by the combined laser irradiation



Nonlinear dynamics and chaos



Distribution of the amplitude of injected current density for subtalamic nucleus axons orientated perpendicular (a) and parallel (b) to the deep brain stimulation electrode in the (z, r) plane of the cylindrical coordinate system.

The development of chaos control and synchronization algorithms and their application to complex neural networks

Systems of many interacting oscillatory elements are of great interest in a wide variety of scientific fields including physics, chemistry, and biology. The synchronization of oscillations is a mechanism for neural communication, which endows individual brain areas with the ability to perform specific tasks. Conversely, extremely strong synchronization may cause various neurological disorders like Parkinson's disease or epilepsy. Using the methods of nonlinear dynamics and chaos theory we aim to develop efficient noninvasive (or weakly invasive) algorithms for desynchronization of neural networks, which could be applied to the new generation of neurostimulators meant for treatment of various neurological diseases.

Neurological diseases like epilepsy are characterized by a bistable neural network. The stable coherent and incoherent states of the network correspond to the disease and healthy states of a patient, respectively. We have developed two control algorithms to switch a network from a stable coherent (disease) state to the stable incoherent (healthy) state. One of them is based on an act and wait control, while another uses a multisite coordinate reset stimulation (MCRS). The idea and performance of the second algorithm are demonstrated in the figure. The network is stimulated at N different sites with periodic signals shifted in phase by $2\pi/N$. When the stimulation is switched on, the electrodes entrain subpopulations of neurons, so that N synchronous clusters are formed. After switching off the stimulation the network approaches a stable incoherent state with the uniform phase distribution. The MCRS algorithm works well for both all-toall coupled neurons and networks with the complex scale-free coupling topology.

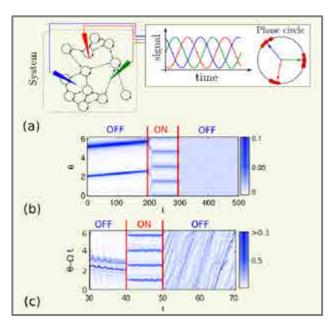


Fig. 1. (a) Demonstration of the MCRS idea with N=3 electrodes. Dynamics of phase distribution under MCRS with N=4 electrodes for the Kuramoto phase oscillators with (b) all-to-all coupling topology and (c) scale-free topology.

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Astrophysics



Stochasticity of stellar systems

We study dynamics and evolution of complex systems, from star clusters to galaxies, where stochastic effects play an important role on stellar populations. We employ ground- and space-based observations as well as parallel computer simulations of resolved & semi-resolved stellar systems, and active galactic nuclei (AGN).

Stochastic life of star clusters

The stochastic nature of mass distribution of stars upon their birth limits the applicability of simple stellar population (SSP) models to deriving star cluster parameters. We have developed a method based on full stochastic simulation of star clusters. For the first time a homogeneous study of the complete M33 galaxy star cluster system was performed using ground-based data, providing insight on the cluster formation and destruction processes in disk galaxies.

Central black holes shape galaxies

It has been known for a decade that AGN have a significant influence on their host galaxies, but the precise nature of this influence has been difficult to determine due to the range of spatial and temporal scales involved in the problem. We have modified the smoothed particle hydrodynamics (SPH) code GADGET-3 and have discovered that in galactic outflows caused by AGN winds a large fraction of the input energy is carried away by the lowest-density gas, while the densest gas behaves as if it was merely pushed by the ram pressure of the wind. This explains the observed velocities of AGN outflows and the simultaneous presence of gas flowing in toward the black hole.

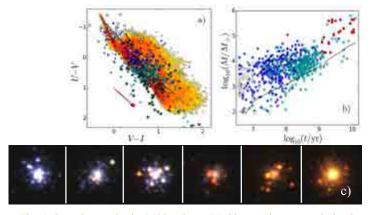


Fig. 1. Star clusters in the M33 galaxy. (a) Observations – symbols; the model grid is shown as a density map; solid line – SSP models.
(b) Derived parameters of 747 clusters. (c) Simulated star clusters in M33.

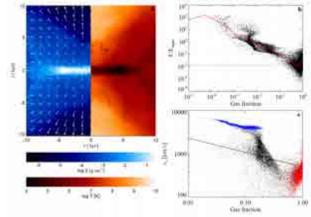


Fig. 2. AGN outflow. (a) Gas density and temperature distributions.
(b) Ratio of gas particle energy to the fraction of AGN input energy.
(c) Radial velocities of gas particles in the vertical direction – blue points, in the disk – red points; solid line – analytical prediction.



Modeling in semiconductors

Electronic structure calculations of processes at the defects in semiconductors

We develop and apply first-principles electronic structure techniques to address the properties of point defects in semiconductors. Most of the activity is focused in two core areas.

- 1. *Ab initio* theory of radiative and nonradiative processes related with the energy losses in opto-electronic devices. Recently, our focus was on group-III nitride materials used to manufacture green, blue, and UV light-emitting diodes. Our work has helped identifying the culprit defects that substantially diminish the performance of these devices.
- 2. Theoretical studies of defect spins in view of their application in quantum information processing and nanometrology. The materials we are currently most interested in are diamond, silicon carbide, and two-dimensional wide band-gap semiconductors. We are trying to understand phenomena such as electron-phonon coupling, optical spin initialization as well as charge dynamics at defects. This work will help finding or designing the best spin qubits.

Fig. 1. (a) Calculated band structure of 2D hexagonal boron nitride (image courtesy of M. Mackoit), (b) spin density associated with the gallium vacancy complex in gallium nitride, (c) luminescence lineshape at nitrogen-vacancy centers in diamond.

Boltzmann-Langevin approach for fluctuations in nitrides

A fluctuation-dissipation approach has been proposed for theoretic investigation of experimental results on heat dissipation in nitride semiconductors where electrons are under intense interaction with polar-optical phonons (Fig. 1a). The expansion in spherical harmonics (Fig. 1b) is used for numerical solution of the coupled Boltzmann-Langevin equations for non-equilibrium ("hot") electrons and phonons. The modeling of electron transport confirms the buildup of the hot-phonon distribution (Fig. 1c) and the increased population of the high energy electrons (Fig. 1c, inset). Boltzmann-Langevin approach allows calculation of electron noise temperature spectra directly in frequency domain (Fig. 1d). The ultrafast dissipation of heat is a prerequisite for efficient conversion of electric power into microwave and terahertz radiation. The developed model can be used to simulate heat flow in novel nitride-based devices, and propose new designs with the most efficient heat dissipation.

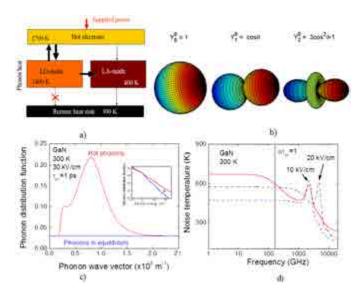
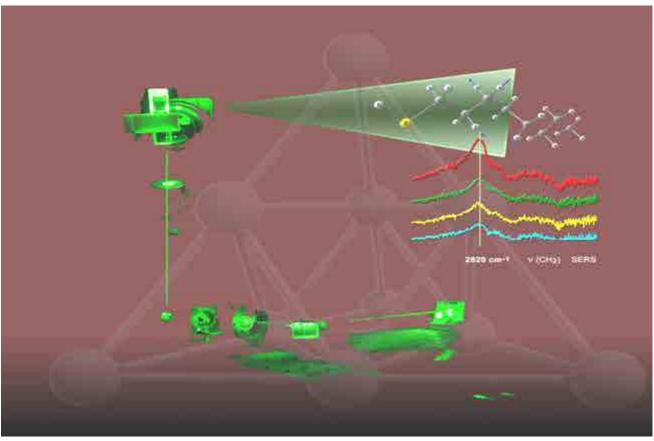


Fig. 2. (a) Heat-flow diagram, (b) spherical harmonics, (c) hot-phonon distribution (inset: the impact of hot phonons on electron distribution), and (d) calculated spectra of the electron noise temperature.

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Spectroscopy of adsorption and electrochemical processes at a metal-solution interface

Electron transfer reactions, electrocatalysis, function of biomolecules, and corrosion processes critically depend on adsorption of organic molecules at metal surfaces. Bifunctional self-assembled monolayers (SAMs) are widely used for construction of surfaces with desirable properties. Modification of model molecular systems with cholesterol moiety may be of interest, because cholesterol is essential component of mammalian membranes. We synthetically design several new structures, where cholesterol side was spaced from anchor, fluorophore and redox groups with a oligo(ethylene oxide) spacer arm via ether linkage to save the nature of cholesterol during embedding into a lipid bilayer. The electrochemically active derivative was reconstituted into tethered bilayer membrane (tBLMs). Upon reconstitution, it exhibited electrochemical activity. To predict and control the function of SAMs, molecular level understanding of monolayer architecture is required. We have used one of the most sensitive vibrational spectroscopic tools, surface-enhanced Raman spectroscopy (SERS) for in-situ probing the bonding, structure, and orientation of adsorbed molecules at Au, Ag, and Cu surfaces. In addition, reflection absorption infrared spectroscopy and sum frequency generation spectroscopy were used for analysis of electrochemical interface. The spectroscopic methods were coupled with first principle calculations and isotopic substitution approach. Spectroscopic experiments were conducted in-situ at controlled electrode potential. We have identified SERS marker bands which provide novel spectra-structure correlations applicable to molecular level control of structure, bonding, and stability of adsorbed molecules at electrochemical interface.

Establishing of spectra-structure correlations for adsorbed molecules

Spectra-structure correlations were established for adsorbed bifunctional monolayers and imidazole ring bearing molecules at metal surfaces. Structure and bonding of positive charge bearing self-assembled monolayer (Fig. 1) on Au and Ag electrodes was probed by SERS, first-principles calculations, isotopic substitution, and reductive desorption voltammetry. Based on analysis of immersion time-, and temperature-dependent SERS spectra as well as DFT calculations, the marker bands for monolayer structure, bonding and orientation have been established. In particular, the markers of alkyl chain all-trans conformation (1083 cm⁻¹ band, previously unrecognized in the case of relatively short bifunctional molecules), interaction of methylene groups with the surface (soft C-H mode), pyridinium ring environment marker band, and bonding with surface Au-S and Ag-S marker bands were proposed. Direct bonding of imidazole ring with metal surface was probed by metal isotopeedited (63Cu / 65Cu) SERS coupled with theoretical modeling of surface complex (Fig. 2).

Investigation of cholesterol-based tethers and markers for model membranes on electrode surface

A series of new bifunctional cholesterol compounds for tBLM systems were synthesized and tested spectroelectrochemically. Anchoring occurs through the insertion of the cholesterol moiety into the hydrophobic slab of the phospholipid layer, while the surface density of anchor molecules may be adjusted using disulfides terminated spacers. Another group of cholesterol derivatives contains either fluorescence probe or electroactive functional groups (Fig. 3). We demonstrated that electroactive group containing cholesterol derivatives can be reconstituted either into vesicles or tBLMs. In both cases an electrochemical signal can be generated on electrodes from these probes. In general, the newly synthesized compound may be utilized in a variety of applications involving tethered bilayer systems and vesicles.

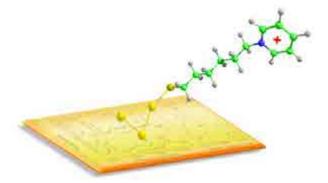


Fig. 1. SERS marker bands for structure, bonding, and orientation of positive charge-bearing pyridinium ring-terminated monolayer were evaluated.

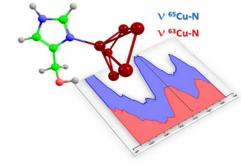


Fig. 2. The formation of a covalent bond between the metal and adsorbate was experimentally evidenced by metal isotopic (⁶³Cu / ⁶⁵Cu) frequency shift of v(Cu–N) mode at 222 cm⁻¹.

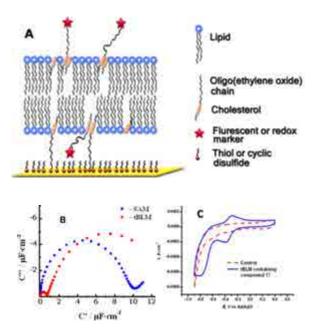
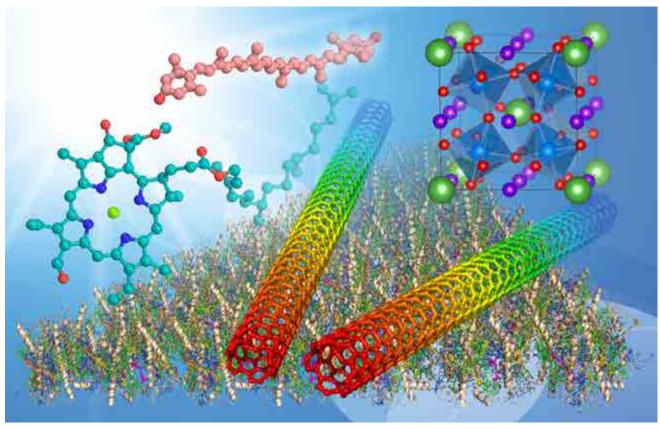


Fig. 3. (a) Cholesterol cyclic disulfide tether and markers for tBLM design and investigation. (b) Cole-Cole plots of electrochemical impedance spectra of mixed SAM and tBLM. (c) Cyclic voltammetry curves of the reduction of redox active marker embedded into tBLM.





Excitation dynamics and dissipation in natural and artificial molecular systems

Solar energy is a renewable source with a strong potential to increase its share in the global energy mix, partly filling the gap caused by the dwindling crude oil resources. "Classical" silicon solar cells are efficient and stable, but very energy-demanding during production. Large molecules and their assemblies are considered as novel constituents of light-accumulating systems. They absorb photons in the spectral region covering most of the solar irradiation spectrum. Usually it is achieved by encapsulation of such pigments inside proteins or by creating relevant artificial scaffolds. Close packing enables the cooperativity of the electronic excitations, which inhibits their non-radiative decay. The long lifetime becomes sufficient to utilize electron acceptance/donation ability of the pigments, which leads to conversion of the excitons into mobile charge carriers. All these processes determine the efficiency of various molecular networks playing the dominant role in various organic optoelectronic devices, like solar cells.

Molecular systems necessarily involve high degree of nuclear dynamics ranging from coherent nuclear vibrations at high frequencies to Brownian fluctuations (low frequency thermal vibrations as well as rotations) and up to proton transfer reactions in molecular complexes. In addition to that, the molecular aggregates have multiple closely lying electronic excited states (excitonic states), which are spectrally positioned in the same region. All this complexity of the energetic arrangement has to be taken into consideration in order to enhace the efficiency of the light-harvesting. The possibility of achieving this aim is well-exhibited in natural molecular complexes. For instance, in photosynthesis the flexibility of protein structure is a fundamental feature that probably has been utilized by Nature to select and optimize biologically relevant structural configurations. Comparative studies of natural and artificial molecular systems disclose additional possibilities of understanding the processes playing the dominant role in excitation dynamics and relaxation. We employ different time-resolved experimental approaches (pump-probe, fluorescence and single-molecule spectrosciopies, TREFISH, etc.) and theoretical techniques (open quantum system theory) for this purpose.

Carrier generation and motion in organic and hybrid solar cells

We investigate charge carrier generation, motion, and recombination in bulk heterojunction organic solar cells with different electron accepting materials. Fullerene-based materials at their high concentrations ensure high electron mobility and play a dominant role in carrier generation. Coupling between fullerene molecules was found to facilitate electron delocalization, which is important for efficient charge carrier separation. Electron motion and charge separation in solar cells with polymer- and semiconductor-based electron acceptors is much slower. Therefore the competition between carrier separation and recombination remains the main challenge in development of more efficient organic and hybrid solar cells.

Light harvesting in natural photosynthesis: from quantum coherence to photoprotection

In photosynthesis, distinct dynamic processes run on various time scales, keeping the whole apparatus efficient and robust. We study separate fast and slow photosynthetic processes, related to light harvesting, energy transfer, charge separation, and photoprotection. We have found that due to resonant conditions the electronic-vibrational nature of quantum coherence might significantly speed-up charge separation in the photosystem II reaction center of green plants. Regarding the plant's adaptation to different lighting conditions in photosynthesis, we investigate, how dynamic regulation of slow energy traps leads to economic photoprotection in photosystem II.

Endonuclease-induced DNA loop formation and disruption

We study the dynamics of interaction between DNA and site-specific restriction endonucleases, requiring two DNA targets. Investigation of a model system, restriction endonuclease Ecl18kI (Fig. 3), yielded kinetic rate constants of endonuclease-induced DNA loop formation and disruption. The rate of loop formation was found to be orders of magnitude slower than that which would results from the Brownian dynamics of DNA target juxtaposition. At the same time, DNA loop disrupts in about 1 s. In the ensuing study of a less well characterized enzyme, NgoMIV, its dynamic response proved to be highly heterogeneous. This was rationalized to be due to the heterogeneity of NgoMIV protein.

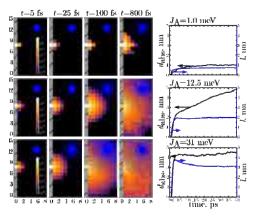


Fig. 1. Evolution of electron probability density at the donor (grey area) and acceptor interface at different times following photoexcitation for different inter-acceptor couplings J_A .

Filled blue circles illustrate the extent of electron coherence at a given time. In the rightmost column, the absolute charge separation distance (black lines) and delocalization radius (blue lines) are shown.

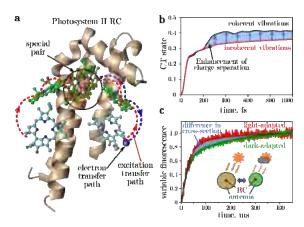


Fig. 2. (a) Photosystem II reaction center (RC), responsible for charge transfer (CT) in photosynthetic membrane of plants, (b) effect of coherent vs. incoherent molecular vibrations on charge transfer speed, (c) expansion of photosynthetic antenna and emergence of slow quenching traps in enlarged antenna in dark vs. light conditions.

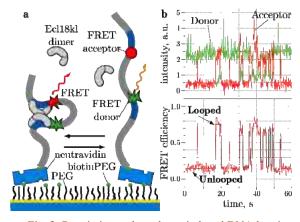
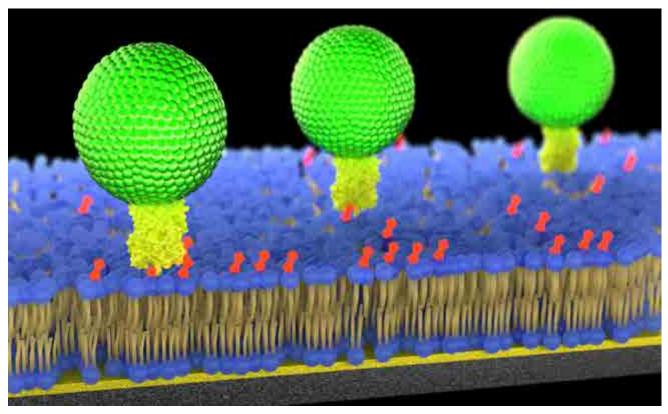


Fig. 3. Restriction endonuclease-induced DNA looping dynamics by the single-molecule FRET. (a) A scheme of surface immobilization of DNA fragments illustrating transition between looped and unlooped DNA due to the interaction with protein, (b) time traces of fluorescence intensity in single DNA donor and acceptor dye and the resulting FRET efficiency demonstrating dynamics between the looped and unlooped states.





Nanoengineering for biological applications

Mission – new tools and processes for fabrication of functional nanoarchitectures for broad applications in life sciences and medicine.

Aims – establishment of reliable experimental platforms for biophysical studies at different levels: proteins, single cells and tissues.

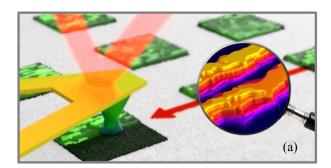
Tasks – high speed nanolithography of functional patterning of soft (molecular) and solid surfaces, cell membrane-mimetic assemblies, nanobiochips for single cell analysis, micro/nanofabrication of hydrogel interfaces for tissue engineering, electrochemical and optical sensing of biomolecules.

Nanoengineering and nanotechnology activities of the Department of Nanoengineering comprise surface nanopatterning using soft nanolithography, investigation of cellular life cycle by using nanoprobes and nanobiochips, electrochemical (bio)sensing and chemical synthesis. A variety of alternative nanofabrication techniques is available for fabrication of functional nanopatterns on different substrates: piezoelectric inkjet printing, colloidal nanolithography, microcontact printing (µCP), dip pen nanolithography (DPN). Spectroscopic and microscopic methods are used for surface characterisation and also for analysis of (bio)molecular interactions at the fabricated interphases: scanning probe microscopy (SPM), scanning electron microscopy (SEM), imaging ellipsometry and surface plasmon resonance. In the development of biosensor technologies, electrochemical methods are employed to study active protein monolayers, noble metal and graphene nanoparticles in multilayered analytical structures.

Nanofabrication of biochips

requires not only high precision in surface patterning but also maintenance of proteins and cells in their native environment. We have been developing a powerful array of alternative techniques that are based on self-assembly and surface chemistry and we are exploring applications in high throughput screening and cell technologies.

- 1. We have established a nanolithographic process for printing of lipid micro- and nanophases. Such cell membrane-mimetic architectures can be employed in biosensors, as well as vehicles for screening and controlled release of pharmaceuticals.
- 2. We are developing single-cell arrays that may be an attractive platform for biophysical studies of the cell lifecycle and also for medical applications such as detection of the circulating tumour cells.



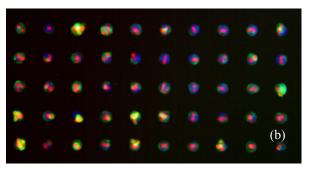
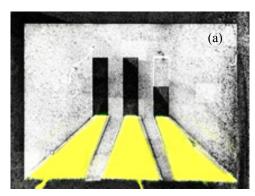


Fig. 1. (a) Formation of 1,2-dioleoyl-sn-glycero-3-phosphocholine lipid nanostructures with DPN. (b) Image of cells deposited on the protein nanopatterns on polyethylene glycol based hydrogel.

Electrochemical (bio)sensors

are fabricated by combining molecular nanolithography with various comodity tools and laser techniques.

- 1. Widely investigated nanomaterial graphene is also employed in sensor chip fabrication (Fig. 2a). Such chips are applied in miniaturised bioelectroanalysis, including sensitive determination of vitamin C.
- 2. Novel functional materials such as conducting polymers comprising vitamins are explored as nanostructured mediators. Such vitamin-based electrodes are used in the development of biosensors for detection of glutamate (Fig. 2b), cholesterol, hypoxantine, glucose, etc.



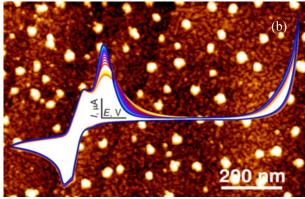
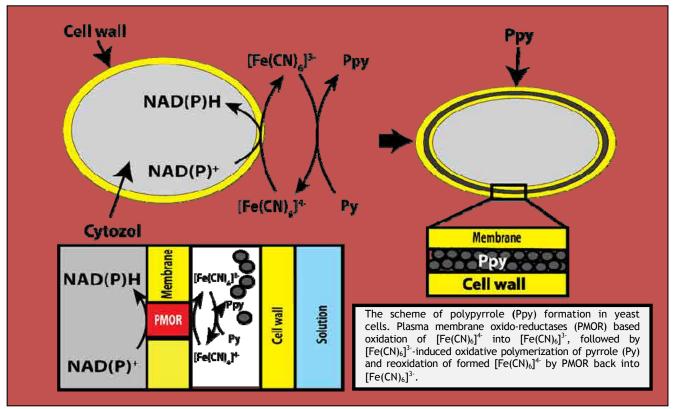


Fig. 2. (a) Microchip as a base for electrochemical biosensor (dimensions 7x5 mm). (b) Polymerised vitamin B_2 as conductive polymer with the polymerisation voltammogram.



Bio-nano technologies



Bio-sensor and living cell based technologies

The majority of electrochemical sensors and biosensors are based on chemical or biochemical structures selectively interacting with analyte. Depending on a type of a sensor, the role of such structures can be played by self-assembled organic and inorganic molecules, molecularly imprinted polymers, enzymes, antibodies, receptors, etc. Density functional theory and Monte Carlo simulations, both are powerful tools to model and predict the assemblies of organic molecules on selected substrates. However, the incorporation of sensing and biosensing structures in analytical systems is still a challenging task that could be solved by proper application of π - π conjugated polymers. Many different methods of their synthesis are used, ranging from the basic chemical or electrochemical, up to the enzymatic or microorganism-based (Fig. above). Various monomers could be polymerized by electrochemical and other methods. Nano-scaled molecular imprints could be created within conjugated polymers and very efficiently applied in sensor design.

An important issue for the development of nano-dimensional sensors is the electrochemical formation of nanometer thick layers of conjugated polymers and incorporation of biological objects within formed polymer layers, the problems which are studied at the Laboratory of Bio-nanotechnologies in the Department of Material Science and Electrical Engineering. Very important advantage of some conducting polymers in the design of amperometric enzymatic biosensors is related to facilitation of charge transfer from enzymes towards electrode. Possibility to graft some conjugated polymers to carbon based and some other surfaces opens a new avenue in the development of conjugated polymer based sensors. Electropermeabilization of living cells increases their applicability in the design of sensors and other bioelectronics devices. Tuning optical properties of ZnO based nanostructures and Al₂O₃/ZnO based nanolaminates by the number and thickness of Al₂O₃/ZnO layers allows to use them as substrates in the design of optical sensors and biosensors.

Optical properties of nanolaminates

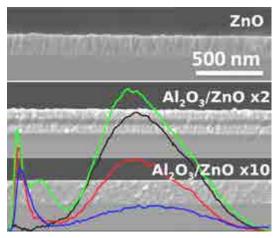
The advanced features of nanolaminates such as biocompatibility, easy surface modification, and enhanced photoluminescence (PL) at room temperature could provide good capacity for the development of nanolaminate based optical sensors and biosensors. Optical properties of Al₂O₃/ZnO nanolaminates designed by atomic layer deposition are studied by transmittance, PL and ellipsometric spectroscopy. The structure of the nanolaminates is characterized by SEM, GIXRD, and AFM. It was found that the optical response may be tuned by changing the sequence and structure of the nanolaminates. The band gap of ZnO single layers and the excitonic PL peak position are shifted to the UV region due to quantum confinement effects.

Electro-permeabilization of biological cell

The electrical field induced changes of yeast *Saccharomyces cerevisiae* cells permeabilization to the tetraphenylphosphonium (TTP⁺) ions is studied using nanosecond duration high power electrical pulses. The pulses generating electric field strength up to 190 kV/cm significantly (up to 65 times) increases the absorption rate of TTP⁺ ions without detectible influence on yeast cell viability. The pulse induced permeabilization increases the operation speed of whole cell biosensors, induces the programmed cell death (apoptosis), controls the promotors of valuable recombinant genes and electro-pasterization of liquid food to prolong the shelf life of products without damaging heat sensitive bioactive components of food.

Numerical engineering of molecular self-assemblies

Self-assembling of simple organic molecules with interacting vertices (H-bonds) into planar ordered structures is modeled using phase transition models. The molecules on a lattice are represented by simple geometrical forms with a minimal number of molecular orientations and governed by defined interaction rules. The assemblies of symmetric organic triangular molecules (TMA, BTB and their mixtures) as well as of reduced symmetry molecules (BHTC) are studied by density functional theory and Monte Carlo simulations. The phase diagrams are calculated, the growth dynamics of emerging structures is determined and the structures, which have not been previously seen in experiments, are predicted.



 $Fig.~1.~SEM~image~of~100~nm~ZnO~thin~film~and~two~Al_2O_3/ZnO~nanolaminates~of~different~sequence~and~their~PL~spectra.$

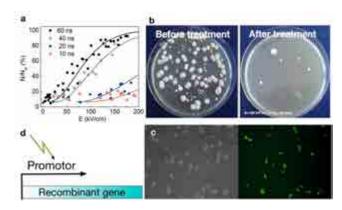


Fig. 2. Application of electro-permeabilization:
(a) enhancement of ion absorption rate after pulsed electric field treatment, (b) electro-pasterization of whey concentrate,
(c) induction of apoptosis in yeast cells,
(d) constructing a reporter system for electrically controlled gene expression.

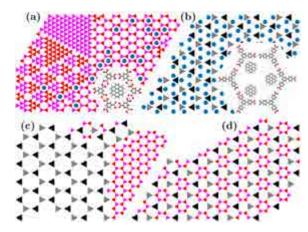
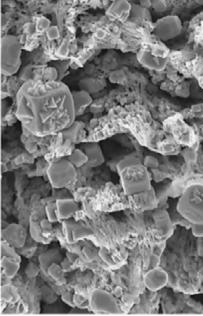


Fig. 3. Snapshots of ordered structures in (a) TMA - coronene, (b) BTB - coronene, (c) TMA - BTB (A and F phase-coexistence) and (d) TMA - BTB (mixed phase C) systems. Notations: TMA (red, pink), BTB (black, grey) and coronene (blue).









Electrochemical materials science

The R&D activities in this area are focused on the development of new functional materials, such as alloys of light and refractory metals (Mg, Al and Cr, Nb, Zr, Ta, respectively), nanomaterials and their arrays, including semiconductor nanowires loaded inside the alumina pores and nanostructured titanium or iron oxides, transparent conductive oxide layers and their heterostructures, corrosion resistant nanostructured electrodeposits of Cr and Zn alloys, etc. Much effort is also devoted to the search of

- new methods for the synthesis of superparamagnetic and luminescent nanoparticles, and investigation of their application possibilities in nanomedicine;
- new effective materials for photovoltaic and nanoelectronic technologies;
- technologies of deposition of smart coatings with active corrosion protection ability for metals in aggressive environments.

Electrochemical and chemical (electroless) as well as physical (magnetron sputtering, atomic layer deposition) methods are applied for the surface modification and production of new functional materials with exceptional anticorrosive, electrocatalytic, magnetic, mechanical and other properties. The integral part of the process of new materials development is thorough characterization of their structure, morphology, chemical composition as well as investigation of their corrosion behavior in solutions (including simulated biological ones) and atmosphere. Environmental friendliness is an imperative for all newly developed technologies.

Another trend of scientific research is related to tribology and formation of compositions of biofuels, lubricants and plasticizers, using biodegradable components. These activities include search for tribologically efficient materials for new type anodic aluminum coatings with exceptional resistance to friction and attrition. The results are tested directly in the Anodization pilot plant of the Department of Chemical Technologies. Corrosion, tribological, physical and electrochemical studies of the biofuels (ethanol, biodiesel, biolubricants) interaction with metal surfaces are carried out as well.

Corrosion Testing Laboratory, accredited in 2007, performs testing and evaluation of the corrosion-caused changes of metals, alloys, composite coatings, paints and lacquers in natural and artificial atmosphere as well as testing of microbially induced corrosion of materials in atmosphere and model medium.

The reliable method for coating of magnetic nanoparticles with gold

To obtain magnetic, luminescent or profitable drug delivering systems, functionalization of nanoparticles is usually required. These nm-scaled systems are fabricated by means of coating the magnetic nanoparticles with gold shell and subsequently attaching the required functional tags via sulfur link. New method for reliable covering of magnetic nanoparticles with gold shell using methionine amino acid as reducing agent for gold ions is developed for the first time. We also report the formation of methionine sulfoxide shell as stabilizing biocompatible hem for CoFe₂O₄@Au nanoparticles (Fig. 1).

Researching the mechanism of energy conversion

We are engaged in the basic research of processes related with the (photo)electrochemical energy conversion, with the primary aim of understanding the interfacial phenomena at molecular level. Novel mechanism of reversible hydrogen evolution and oxidation reactions (HER and HOR) on Pt, involving participation of molecular hydrogen ion, H₂⁺, has been proposed based on the analysis of charge and mass changes accompanying the processes. Thermodynamic analysis, experimental data and steric arguments show that H_2^+ is the nature's choice for an intermediate, which resolves the energy deficiency required for H₂ formation from H⁺ ions. The proposed mechanism explains consistently the dependence of mechanical properties of metals on the amount of absorbed hydrogen, the mechanism of hydrogenation and hydrogen transport through the metals. Based on these findings we provide further insights for the efficient solar hydrogen generation and storage.

Tribologically effective anodized aluminum coatings

Anodization is widely used to improve hardness, paintability and corrosion resistance of aluminum parts in robotics, lasers or aerospace. However, anodized surfaces are not resistant to friction and wear due to their brittleness and porosity. At Instutute of Chemistry / FTMC an innovative method is developed by S. Jankauskas, G. Bikulčius and S. Asadauskas to produce organo-metallic fillers within the nano-pores of anodized alumina. These fillers generate effective tribofilms in the friction zone, as confirmed by ball-on-plate tribometer data. Field testing by Lithuanian Speed Model Car Federation shows that mini-engine piston prototypes, treated with organometallic fillers, will last 6-8 times longer than pistons without fillers. These results demonstrate high commercialization potential of tribologically effective anodization technology.

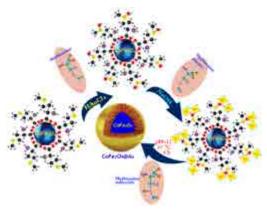


Fig. 1. Illustration of methionine-induced chlorauric acid reduction at the surface of cobalt ferrite nanoparticle.

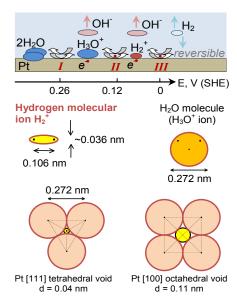


Fig. 2. Schematic sequence of HER and HOR processes on Pt electrode together with relative dimensions of participating species.

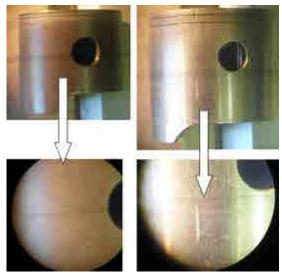
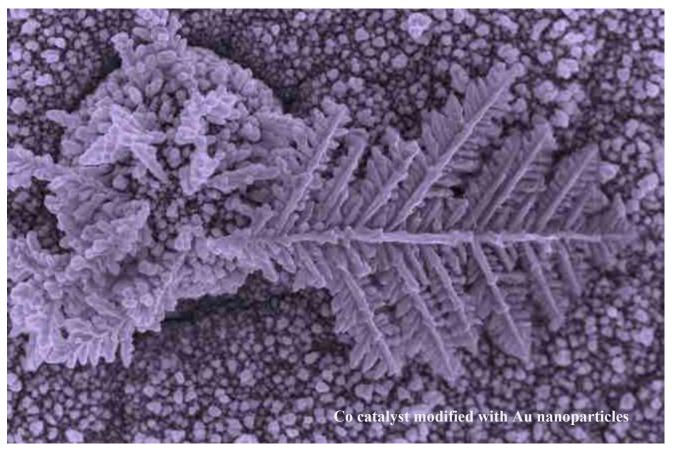


Fig. 3. Prototype piston with tribologically effective fillers (left) and piston without fillers (right) after the field test by Lithuanian Speed Model Car Federation.



Materials for catalysis

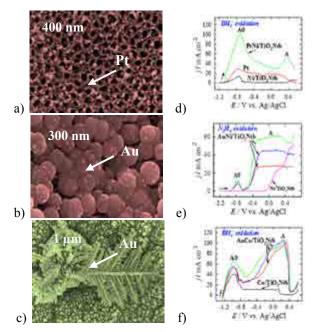


Electroless metal deposition: from fundamental research to application in microelectronics and fuel cells

Electroless metal plating is the well-known method for deposition of metal coatings by a controlled chemical reduction and formation of small (nano-scale) metal particles. The R&D activities of the Department of Catalysis in this area are focused on the development of new electroless metal plating processes as well as fundamental studies of reactions occurring in autocatalytic metal ions reduction by means of electrochemical quartz crystal microgravimetry. For LAM Research corporation (USA, California, Silicon Valley) we have developed the electroless deposition technologies of (i) continuous Pt and Pd layer using complexed Co²⁺ metal ion as reducing agent, (ii) continuous Co and Ni layers using complexed Ti³⁺ metal ions as reducing agent, (iii) continuous Pd layer using complexed Co²⁺ metal ions or Ti³⁺ metal ions as reducing agents. The technologies for deposition of high surface roughness copper coatings by electroless plating and thick (> 20μm) electroless Cu coatings used as contacts in solar cells were created. The latter has been put into use in industrial solar cell laboratory in UAB "Precizika-MET SC". The electroless metal plating method is also succesively used for fabrication of new catalytic materials for fuel cells. The non-noble metal and noble metal catalysts with low amount of noble metal supported titanium or titania nanotube arrayed surfaces, carbon, graphene powder or other supports with enhanced activity towards the oxidation of various fuels has been developed. Electroless metal plating is also used to deposit a conductive surface on a non-conductive object to allow it to be electroplated. Much effort is devoted to the development of palladium-free and environmentally friendly surface activation processes for activation of non-conductive surface prior its metallization.

Development of catalysts for fuel cells

The following technologies for fabrication of various catalysts for fuel cells were developed: (i) decoration of titanium and titania nanotubes with Pt, Au, Ni, Co, etc., particles by means of electroless metal plating and galvanic displacement, (ii) preparation of various metal and metal alloy/graphene catalysts by means of microwave synthesis. The catalysts were prepared by immobilization of metal (Cu, Co, Au, Pt, Ni) particles on the surfaces of Ti and laboratory grown titania nanotubes (TiO₂Ntb) via electrochemical or chemical methods. The decoration of Niplated TiO₂Ntb by Pt or Au nanoparticles enables to create catalysts with enhanced activity towards borohydride or hydrazine oxidation in an alkaline medium (Fig. 1). The catalysts obtained with low amounts of noble metal are promising anode materials and can be used in the fuel cells.



 $\label{eq:Fig.1.2} Fig.\ 1.\ SEM\ views\ of\ (a)\ Pt/TiO_2Ntb,\\ (b)\ AuNi/TiO_2Ntb\ and\ (c)\ AuCo/TiO_2Ntb.\\ The\ BH_4^-\ oxidation\ at\ (d)\ Pt/TiO_2Ntb,\ (f)\ AuCo/TiO_2Ntb\\ and\ (e)\ N_2H_4\ oxidation\ at\ AuNi/TiO_2Ntb.\\ \end{cases}$

Development of palladium-free activation technologies for metallization of dielectrics

A new palladium-free activation technology to activate the surface of dielectrics prior to electroless Cu deposition has been developed. The compounds of Co and other metals of Fe group have been used for activation of dielectrics surface instead of expensive palladium compounds, which are used in practice. The process is based on the following technological stages: (i) deposition of an ultra-thin film of metal (M_{ads}) on the surface of dielectric by its immersion in the Pd-free activation solution, (ii) formation of M(0) seeds on the surface of dielectrics after the reduction of the adsorbed metal particles to a metallic state, (iii) deposition of Cu film. A continuous Cu film has been deposited on a glass sheet after its activation in a solution of Ni and Cu compounds followed by reduction of adsorbed Ni and Cu layer to Ni(0) and Cu(0) in NaBH₄ solution (Fig. 2a).

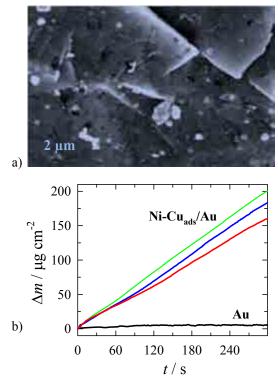
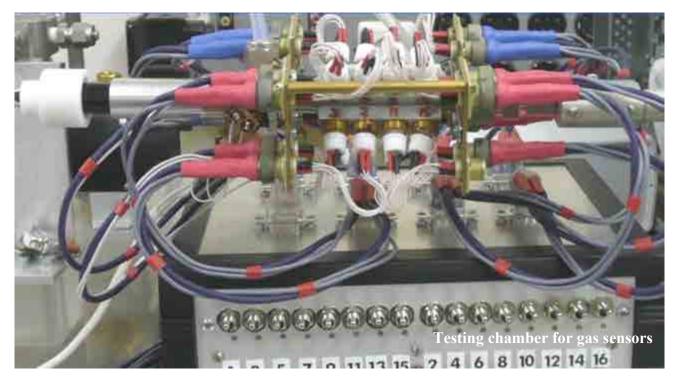


Fig. 2. (a) SEM view of Cu/glass after activation of glass with the Pd-free solution. (b) Mass gain during electroless Cu deposition on Au and that seeded with Ni(0) and Cu(0) particles.

Sensors



From bulk to nano sensors

We study and develop diverse types of sensors suitable for detection of physical and chemical characteristics of the environment: the power of pulsed microwave radiation, magnitude of pulsed magnetic field, amount of gases in air, etc. We investigate and use various materials for the development of the sensors starting with classical bulk semiconductors like silicon, thin films of pure materials and compounds, and finishing with specific nanoscale structures.

A resistive sensor (RS) is our basic development in a field of sensors devoted to high power microwave (HPM) pulse measurement. Its performance is based on electron heating effect in semiconductors. The RS is applied to the measurement of HPM in waveguides and free space. In comparison to the microwave diode, the RS measures HPM pulses directly, is overload resistant, and demonstrates a perfect long-term stability. Our main efforts are focused on the broadening of frequency range of a single RS and its application to systems detecting HPM threats.

Nanostructured manganite films are employed for the measurement of magnetic induction magnitude. CMR-B-scalar sensors with readings independent of the magnetic field direction are designed using colossal magnetoresistance (CMR) effect found in these films. Developed MOCVD film growth technology allows to obtain the films with predefined properties. The designed magnetic field measurement systems based on CMR-B-scalar sensors (stationary and handheld) are intended for various applications such as magnetic field distribution measurements in railguns, non-destructive pulsed-field magnets, and high power linear motors, used for industrial applications.

A few original types of prototype sensors for detecting of gases are developed. The sensors are successively used in several versions of electronic smell detection systems called electronic nose, applied for non-invasive detection of wound infection and the state of health of dairy cows. However, the main drawback of these sensors is related to their layered metal-oxide structure. The working temperatures of these sensors are above 550 K and this requires relatively high power consumption, too high for compact and autonomous systems. Therefore, we have started the project where we intend to apply the unique properties of nanosystems aiming to find very fast, sensitive and power saving methods as well as structures that can detect surrounding volatile compounds.

The developed sensors can be integrated in security systems, process control, human and animal health diagnostics, and product quality evaluation systems.

Development of high power microwave pulse sensors

We are developing resistive sensors (RSs) for high power microwave (HPM) pulse measurement. The performance of the RS is based on electron heating effect in semiconductors. The sensing element of the RS is embedded into a double ridged waveguide providing more than twofold increase in the frequency range in comparison with the standard rectangular waveguide used as a housing of the sensing element. The parameters of the sensing element are tuned to get a flat frequency response of the RS. The RS connected to a horn antenna comprises a single unit for HPM pulse power measurement in free space. Such a unit is used in a developed seeker for HPM pulse threats.

Development of high pulsed magnetic field sensors

We are developing colossal magnetoresistance (CMR) sensors insensitive to direction of magnetic induction **B** for measuring the magnitude of high pulsed magnetic fields up to the megagauss limit in a very small volumes $\approx \! 10^{-2}$ mm³. The sensors were fabricated from La-Sr(Ca)-Mn-O-based manganite nanofilms exhibiting CMR phenomenon. In constructing the sensors the attention was paid to the long-term stability of electrical and magnetic parameters of the nanostructured films and magnetic memory effects. The 4-channel system of CMR-B-scalar sensors is used in measurements of the diffusion processes in railguns and distribution of the transient magnetic fields in non-destructive pulsed-field magnets.

Development of hybrid technology for chemo & photo-sensitive systems

We are developing ultra-thin film (UTF) and hybrid technologies for novel type of combined micro- and nano-structures. The sensitivity of film characteristics to chemical environment and light makes these structures attractive to the practical applications and provides the basis for specific detectors and controllable detecting modules that can be integrated within smart systems. As a representative example, we demonstrate an original multi-layered construction with UTF-TiO₂ that responds to gas. A graphene sheet may be integrated in this construction and the surface properties can be modified by catalytic metals, nanoparticles and biomolecules. The light controlled response to gas was found in these hybrid structures.

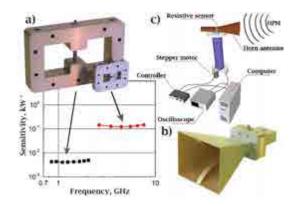


Fig. 1. (a) RSs in a double ridged waveguide and their sensitivity dependence on frequency, (b) the unit comprised of horn antenna, RS and matched load for microwave pulse power measurement in free space, (c) the seeker for HPM pulse threats with rotating unit for HPM pulse measurement.

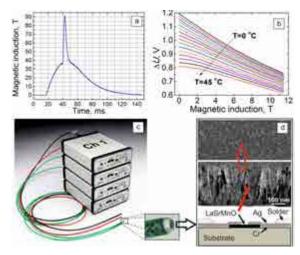


Fig. 2. (a) Sensor-registered record pulse magnetic field (HLD, Dresden), (b) output voltage versus magnetic field induction, (c) the 4-channel measuring system, (d) SEM and TEM images of nanostructured manganite film and schematic cross section of the sensor.

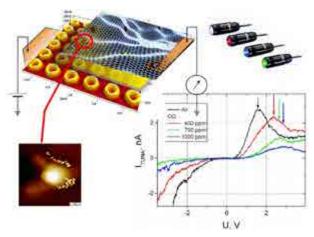


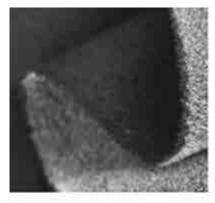
Fig. 3. Current voltage response to CO gas detected in an original hybrid multicomponent construction with ultra-thin film of TiO₂.

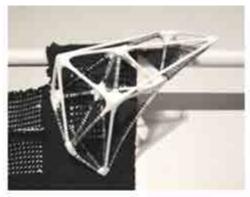
The properties of the layer are modified by graphene sheets and biomolecules bonded to Au-nanoparticles.

The response of the layer depends on light.



Textile technologies











Advanced textile materials

There is a great scope for textile to ensure and support human well-being for leisure, active lifestyle and safety, at the same time making the textile more friendly for the surrounding environment. This can be reached by a wide range of technological achievements in such areas as information technologies, mechatronics, robotics, advanced materials, bio- and nanotechnologies. Multidisciplinary research opens new opportunities for the development of technologies, tailor-made solutions and products for high value applications. The research in Textile Institute is focused on textile materials with functional and multifunctional properties processed by plasmochemical surface treatment; coating technologies and microand nanofinishing; smart textile garments with active thermoregulation using bio-ceramics, PCM and wearable electronics; protective clothing technologies based on numerical modeling of the heat exchange in textile garments and ballistic impact in protective vests; electro conductive and EMR shielding materials for protective clothing. Using recycled and bio-based fibers we develop new sustainable nonwoven materials and natural fiber composites for orthopedic garments and design prototypes of different kind of protective clothing.

Textile institute is offering a wide range of services: testing and certification, examination of quality of textile materials, prototyping of woven and knitted fabrics and garments, and applied research for industry.

Development of materials with thermoregulatory properties

Bio-ceramic additives have heat-retaining function caused by its far-infrared radiation (FIR) emission. In order to improve thermal efficiency of fabrics, primarily worn next to the skin, different textile materials containing Ti, Ge, Al, Si submicron scale ceramics were used. These textile materials with heat-retaining function can be used for a cold weather workwear. Also the textiles with incorporated micro-scale phase change materials (PCMs) capable to control actively the temperature of the body were developed. The PCMs in the form of organic microcapsules were incorporated by coating and impregnation methods. Due to transition to different phases, PCMs have the capacity to absorb, store and then to release heat energy. The higher is the enthalpy, the better thermoregulation effect is achieved.

Development of electroconductive materials

Electrically conductive textile materials for safeguarding dissipation of high electrostatic charge, providing effective protection against non-ionizing electromagnetic radiation (EMR), were developed and investigated. Two groups of textiles with different types of conductive additives were studied (Fig. 2a and b) and excellent electrostatic properties of developed samples were found: the surface resistivity is sufficiently low and the decay of charge is very high. Moreover, the applied conductive coatings may provide the fabrics with electrical properties better than metalized yarns inwrought. The distribution of conductive additives on the fabrics surface has an important influence on their EMR shielding effectiveness at the higher frequency range. The highest attenuation of the electromagnetic energy was obtained for the fabrics fully coated with conductive polymeric compositions.

Numerical modeling of heat exchange in textile fabrics

A structural model has been developed which analyzes the air and water vapor mass and heat exchange in multilayer textile packages widely used in military and protective clothing. The model is unidimensional, each element of which describes a single layer of the package. Most parameters of the model can be obtained by performing standard measurements. The values of some parameters were adjusted by comparing experimental data with numerical calculations. The model allows to obtain the temperatures between each pair of textile layers as well as in the 3D textile forced ventilation layer. The time point of sweating could be calculated for any combination of textile materials in the package.

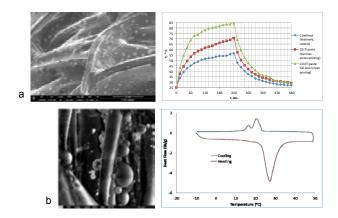


Fig. 1. (a) SEM micrographs of fabric with Ti bioceramic additives and heat accumulation/ release kinetic curves exposed to IR. (b) SEM micrographs and DSC thermograms of PET/cotton fabric with reactive PCM microcapsules.

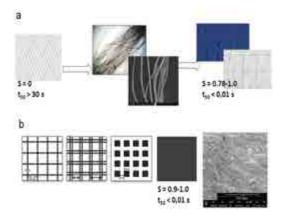


Fig. 2. (a) Fabrics with metalized conductive yarns, (b) fabrics coated with two different conductive polymeric compositions, containing conjugated polymer system PEDOT-PSS and conductive carbon filler as an absorber of EMR.

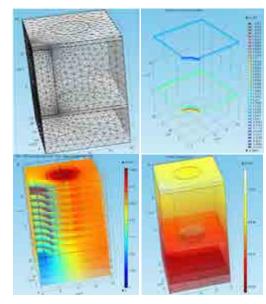
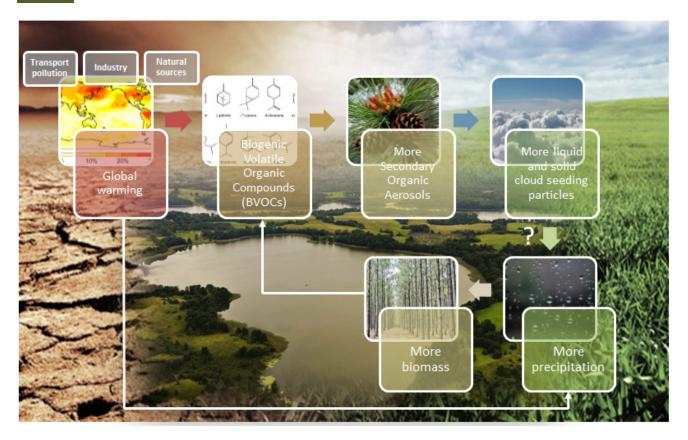


Fig.3. 3D textile structure model in microscale.

Environment



The environment-friendly technologies for observation, simulation, prevention and mitigation of atmospheric pollution, and relation to the climate change

A modern environmental research relies on solutions that bring together the recent achievements in technologies and sciences that underpin our understanding of the Nature to deliver a sustainable invironmental future and economic growth. In the Department of Environmental Research the main focus is directed towards investigations of chemical composition of non-refractory submicron aerosol particles using mass-spectrometry methods as well as to processes that control aerosol formation and evolution. We are also interested in the impact of changing atmospheric composition on air quality, human health, climate change and ecosystems. By conducting the fundamental and applied research, we are trying to find long-term solutions, expecially in experimental techniques devoted to aerosol studies, with the ultimate goal of promoting development towards modern environmentally-friendly technologies based on radionuclide methods which are suitable in the environmental science technologies in general and may be applied in the vicinity of facilities in particular.

Objectives: To develop and improve principles, means and technologies of the environment quality evaluation and to ensure the scientific competence in the field of the environment physics and chemistry, environment contamination and climate changes.

Tasks:

- i) Development of technologies and equipment for the environment protection quality control as well as methods and experimental basis in the environmental research, investigation of micro-admixture dynamics and balance in the environment components as well as the characterization of the impact of the environment contamination on the climate change.
- ii) Evaluation of efficient instrumentation and assessment of methods suitable for characterization of the impact of industry, transport and consumer sectors on the environment quality. The Department is especially interested in combining of spectrometric methods in evaluating the aerosol particle mass and sizes as well as in the investigations of physical-chemical aspects of the aerosol particle formation.

Innovative techniques for atmospheric organic aerosol composition measurement

A complete source apportionment of the offline-AMS water soluble organic (OA) and carbonaceous aerosol (OC/EC) spectra was performed over a set of filter samples collected simultaneously during a year period in the South-East Baltic region. In early spring this region is frequently affected by high pollution events due to biomass burning (BB). We investigated the impact of BB on the evolution and composition of aerosol in Preila, Lithuania. The results revealed that BB contributed the largest fraction to the total OA during winter, while biogenic secondary aerosol and sulfur secondary aerosol were the dominant OA sources during summer. The nitrogen output and traffic exhaust emissions were found to be only minor contributors to the total OA.

Development of innovative environment - friendly technologies

Development of New Biosorbent Filter. To preclude pollution by motorized vehicles, a commercial prototype of a vehicle exhaust gas biosorbent filter was developed. It makes use of chitosan, which is known by its high sorption capacity, filtration efficiency and selectivity for the purification of exhaust gas. Produced and anchored on the quartz glass fibers, the aerosol nanoparticles of the modified chitosan have larger sorption surface, high sorption capacity, mechanical stability, low pneumatic resistance of a biosorbent fiber material and very cheap production costs. The method and apparatus were successfully patented and commercialized.

Detection of Gaseous Oxidized Mercury (GOM). The species of GOM belong to the intermediate form of the most toxic and reactive gaseous atmospheric mercury (GAM). We developed the innovative technology and designed a model device for the detection of atmospheric GOM and its separation from predominant GAM in the atmospheric air. Two national and one European invention patents for innovations have been granted.

Sources and fate of organic carbon (OC) in the Baltic Sea

were studied to assess a possible leakage of chemical warfare agents (CWA) at the dumping site. Different origin and behaviour of lipids and total OC at the CWA dumpsite, as compared to the area affected by the terrestrial-freshwater OC input, were determined. Application of the end-member mixing-model-analysis allowed estimating the OC sources (continental, marine or fossil). The high contribution of fossil sources at the CWA dumpsite (~ 32 %) as compared to other stations (~13 %) in the Baltic Sea may indicate a leakage from the CWA.

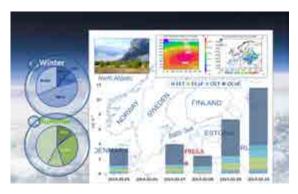


Fig. 1. Amount of OC/EC. OC_f and EC_f are attributed to primary and secondary fossil fuel combustion, OCn_f and ECn_f - to primary and secondary BB, biogenic emissions and non-fossil OC combustion.

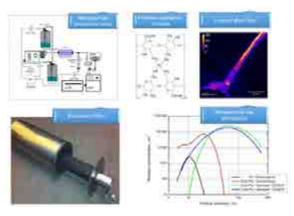


Fig. 2(a). Setup, outlook and results of the biosorbent filter.

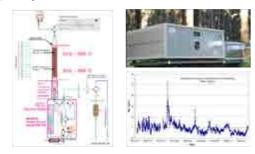


Fig. 2(b). Setup, outlook and results of the gaseous oxidized mercury analyzer, Gardis-7.

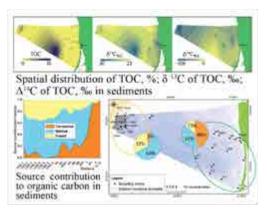


Fig. 3. Δ^{14} C and δ^{13} C as tracers of OC in Baltic Sea sediments.

Nuclear



Nuclear research: applications today and innovative technologies and methods in future

The Department of Nuclear Research develops and applies known and innovative technologies and methods in nuclear spectroscopy, nuclear energy safety, radiation protection, radiochemistry, radioecology, mass spectroscopy, Mössbauer spectroscopy, ion beam analysis and modification of materials. The keystones of the safety field are the safe operation assurance of nuclear facilities, the optimization of radioactive waste management, the assessment of shielding materials and the design and optimization of shielding for ionizing radiation. Special attention is paid to environmental impact assessment of energy generating facilities, elemental and isotopic analysis of groundwater, soil, lake silt, food fabrics and products, and also industrial stocks and medical samples with sensitivity up to 1 ppq (for non-interfered isotopes). Application of stable isotope ratio analysis (δ^{13} C, δ^{15} N, δ^{18} O and δ^{34} S) for environmental, biomedical and food samples stimulates new promising technologies. The ¹⁴C measurements open the potentially new field of activity related to carbon dating and analysis of triple carbon ratio of dedicated samples. Complimentary information on material properties (magnetic properties, oxidation and corrosion of iron compounds) is determined by Mössbauer spectroscopy. Development of ion beam methods for material analysis and modification is an important part of our activities having intersection both with the semiconductor materials and the applications to laser technology.

Advanced technologies for nuclear fuel cycle

are developed. By using nuclear spectroscopy, radiochemistry and computer modelling (MCNP, SCALE program packages), we perform the studies of nuclide content of radioactive waste produced by nuclear power plants (NPPs), analyze the processes of radionuclides transport through the engineering barriers, and enable nuclear facility safety and safety of technologies for management of the radioactive waste.

The experimentally validated nuclide vector technology for decommissioning of NPP's was created and implemented in Kozloduj and Ignalina NPP's. The results of radiological characterization are analyzed and recommendations are worked out for new technological solutions. Identification of the most significant radionuclides in the irradiated graphite and prediction of the radiation dose rate for a personnel handling the irradiated graphite waste in Ignalina NPP Unit 1 have been accomplished.

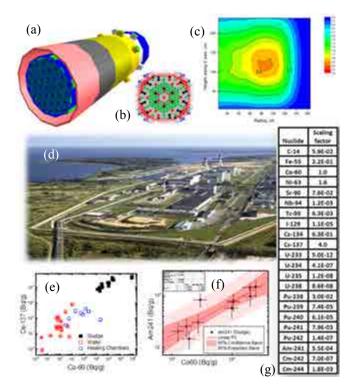


Fig. 1. (a) The 3D model of PWR reactor, (b) core fuel loading pattern, (c) relative neutron flux inside reactor core, (d) NPP site, (e) experimental data of nuclear spectrometry, (f) experimental/modeling data analysis and (g) scaling factors for radioactive waste.

Mössbauer spectroscopy

was used for the characterization of structural and ferromagnetic properties of advanced material for spintronic application. Layered MM'P2S6 materials are most promising as various ferroic phases found in these compounds. The main feature of multiferroics is coexistence of more than one type of ferroic ordering. In MM'P2S6 compounds ferroelectric, ferrimagnetic or antiferromagnetic phase transitions depend on the M and M' cations properties. In Mössbauer study of Cu_{0.15}Fe_{1.7}PS₃ crystal the temperature dependence of hyperfine parameters reflecting local iron environment and spin state in range 9-300 K were determined. The substitution of Fe atoms by Cu, changes the phase transition character, spin ordering of iron atoms and decreases the antiferromagnetic transition temperature from 120 K to 109 K.

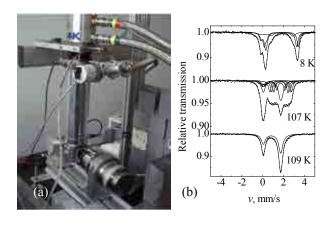


Fig. 2. (a) Mössbauer spectrometer and (b) spectra of Cu_{0.15}Fe_{1.7}PS₃.

Mass spectrometry for new applications

Accelerator Mass Spectrometry (AMS) is an ultra-sensitive technique for measuring ¹⁴C isotopic ratio in carbon. Stable isotope (¹³C, ¹⁵N, ¹⁸O and ³⁴S) analysis is performed using modern isotope ratio mass spectrometers (IRMS) with input devices. We study size-segregated atmospheric and combustion aerosols; neutron irradiation reconstruction in the reactor graphite using the ¹³C/¹²C ratio and ¹⁴C analysis of carbon; carbon and nitrogen variations in the sediments of the Curonian Lagoon and the Baltic Sea; trophic position and food webs of the animals; stoichiometry of bionanocomposites, etc. We also use stable isotopes for food authentication studies.

The laboratory is accredited according to ISO 17025 method ENV 12140 "Fruit and vegetable juices – Determination of the stable carbon isotope ratio (¹³C/¹²C) of sugars from fruit juices – Method using the isotope ratio mass spectrometry".



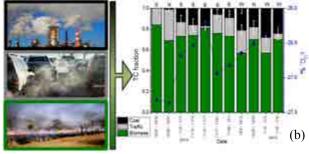


Fig. 3. (a) AMS equipment, (b) estimated fraction of coal combustion, traffic emissions and biomass burning (also - as stable carbon istotope ratio values (blue dots)) in the aerosol particles.

Structural characterization of advanced optical coatings

has been performed by the Tandetron 4110A ion accelerator. The influence of various production processes on the optical properties of the coating structure of thin layer was analyzed by Rutherford backscattering (RBS) experiments, and Nb₂O₅/SiO₂ film thicknesses and element concentrations of optical coatings were determined. Depth profile of AR₃₅₅+HT₅₃₂₊₁₀₆₄ optical coating was estimated from proton and Li ion backscattered spectra (Fig. 4). Obtained information is important to control various stages of sputtering process and understand the effects of additional elements or impact of the layer itself on final refractive index distribution of coatings as well as their resistance to laser radiation.

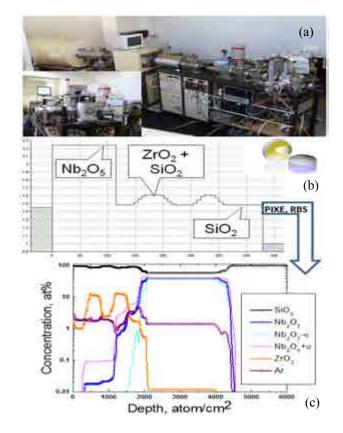


Fig. 4. (a) Tandetron 4110A ion accelerator, (b), (c) depth profile and concentrations of AR_{355} + $HT_{532+1064}$ optical coating estimated from RBS spectra.





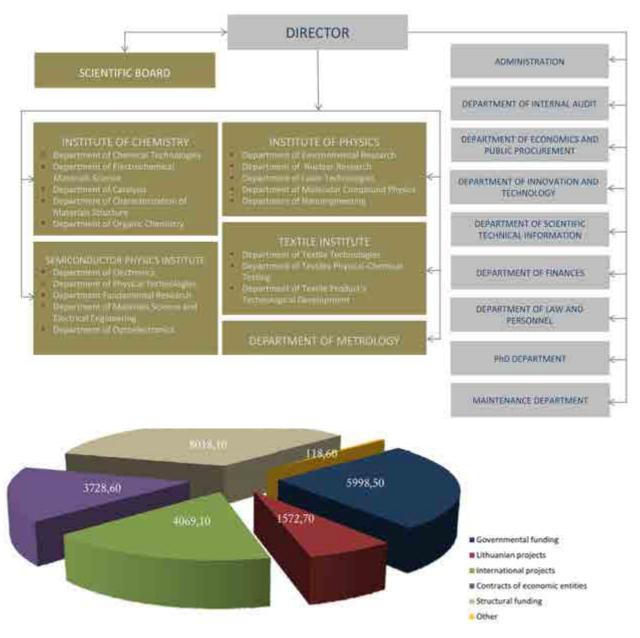
Research in national metrology institute of Lithuania

Man's knowledge of nature, the universe, and how to adapt nature to his purpose, advances in step with his ability to measure precisely.

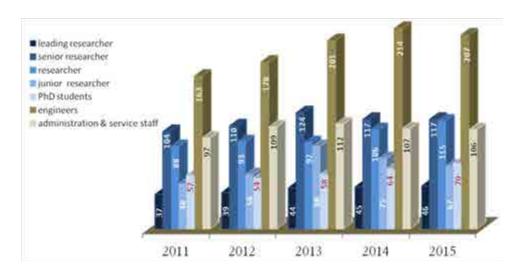
The metrology assures the correctness, accuracy and reliability of measurement results. The measurement as such is not the specificity of the metrology science. The core of metrology lies in validation of the result, particularly by specifying its actual limitations. Since July 1, 2014 the Metrology Department was authorized to perform and implement the functions of the National Metrology Institute.

The Metrology Department maintains national standards in five different metrology fields. The Time and Frequency Standard Laboratory is reproducing the value of a unit of time (the second) and the unit of frequency (the Hertz). Its mission is the representation of Lithuanian Coordinated Universal Time UTC(LT), in this way ensuring the traceability of the magnitudes reproduced to the International System of Units (SI), disseminating them to Lithuanian scientific establishments, personal and legal bodies by calibrating their working standards and measurement devices, disseminating Lithuanian time scale, and other relevant means. The mission of the Electrical Standards Laboratory is maintaining and developing the standards of unit of voltage (the Volt) and unit of resistance (the Ohm), thus ensuring their traceability to the SI system, calibrating working standards and measurement devices, pursuing research in the field of measurement of voltage, resistance and electrical current. The Temperature Unit Standard Laboratory is implementing the international temperature scale ITS-90 and the value of the unit of temperature (the Kelvin), and ensuring their traceability to the SI system. Lithuanian national standard of the temperature unit in the range from -195°C to +961,78 °C is of the primary level and +1084,62 °C freezing point of Cu is of the secondary level. In the Ionizing Radiation Metrology Laboratory radionuclides have been standardized by applying primary methods. The Triple-to-Double Coincidence Ratio method was used for standardization of tritium achieving the expanded uncertainty of the activity <1%. The response of dose calibrators was compared with the secondary standard of the National Metrology Institute in Prague for measuring activities of short-lived radionuclides used in nuclear medicine: F-18, Ga-67, Tc-99m, In-111, I-123, and I-131. The metrological activity is not restricted to standards of the physical units. Reliable and accurate chemical measurements in health care, food safety and environment protection fields are provided by the Laboratory for Metrology in Chemistry.

Structure and statistics



Budget of FTMC 2015, kEur



Staff dynamics



Lithuanian-Swiss cooperation programme R&D project "Aerosol in Lithuania: Investigation of primary–secondary and regional–local contributions to particulate matter in the south-eastern Baltic region" (AEROLIT)

V. Ulevičius

Lithuanian-Swiss cooperation programme R&D project "Single-Cell-on-a-Chip Platform for Metabolite Sensing and Integrated Analysis"

R. Valiokas

7th Framework programme project "Polymer-Carbon Nanotubes Active Systems for Photovoltaics"

L. Valkūnas

7th Framework programme project
"Hub of Application Laboratories for Equipment Assessment
in Laser Based Manufacturing" (APPOLO)

G. Račiukaitis

7th Framework programme project "Novel Type of Terahertz Devices"

A. Krotkus

Research Executive Agency (REA), delegated by the European Commission project "Camelina&crambe Oil Crops as Sources for Medium-chain Oils for Specialty Oleochemicals" (COSMOS)

S. Asadauskas

Research Executive Agency (REA), delegated by the European Commission project "Energy losses in nitride light-emitting diodes" (NITRIDE-SRH)

A. Alkauskas

European Commission European Atomic Energy Community (Euratom) project "Baltic Region Initiative for Long Lasting Innovative Nuclear Technologies" (BRILLIANT)

L. Juodis

European Space Agency (ESA) project
"Bismides for Infrared photodetector" (BIRD)

A. Krotkus

















Open access centers



OAC for Electron microscopy, X-ray diffractometry and spectrometry

has well developed infrastructure and experienced staff for the characterisation of solid materials using SEM, SEM-FIB, TEM, EDX, XRD, HRXRD, WDXRF, XPS techniques.

Available equipment:

- Scanning electron microscopes: Helios Nanolab 650, EVO-50;
- Transmission electron microscope Tecnai G2 F20 X-TWIN;
- X-ray diffractometers: SmartLab (Rigaku), D8 Advance (Bruker);
- X-ray fluorescence spectrometer (WDXRF) Axios mAX (Panalytical);
- X-ray photoelectron spectrometer ESCALAB-MKII;
- Carbon and sulphur analyser CS-2000.



OAC for Prototype formation and integration

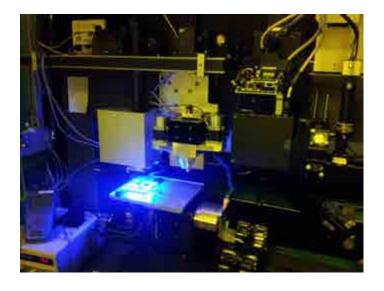
The activity is focused on the two objectives: (i) technology for the research and teaching and (ii) development, innovations and applications. Scientists and industrial partners are provided with a complete set of processes required for manufacturing of a prototype of a mico- and nano-device.

The OAC has a group of highly qualified, ambitious and young scientists. The Si-compatible and hybrid technologies is the primary interest of their research with main targets being the functioning models and prototypes of light emitting structures, photodetectors, elements of the optoelectronic devices and chemical sensors.

Available equipment:

- deposition of functional layers, namely molecular beam epitaxy, atomic layer deposition, chemical vapor deposition, magnetron sputtering;
- formation of the device structures including laser lithography and wet bench chemical tools;
- thermal processing;
- chip assembling;
- testing of electrical properties under controlled atmosphere, temperature and illumination.

The equipment is installed within the technology area with special laboratories and clean rooms. The clean rooms for the semiconductor processing include zones from the ISO class 5 to the ISO class 7. The total area of the clean rooms is about 300 m^2 .



OAC of Processing Technologies BALTFAB

is a joint open user facility between Laser technologies and Nano-engineering departments, offering a full range of nano/micro and macro fabrication as well as laser patterning, marking and cutting on any required material. State of the art Laser-fab is equipped with full variety of industrial ns, ps and fs lasers. The team is experts to set-up, test and develop laser micro-machining processes and systems. Soft nano-lithography tools for rapid creation of nano-structures are tested to be live cell compatible. The patterns are routinely applied to improve the bio-compatibility of medical devices. The team is developing tools for detection of

molecules on surfaces, to fasten the testing and evaluation of cells or drugs. More: see www.baltfab.com

Services:

- Laser processing: in-Glass marking; laser beam interference ablation; laser direct writing; ultrashort pulse laser ablation
- Molecular: dip pen nanolithography; microcontact printing; piezoelectric inkjet printing; colloidal nanolithography
- Analytical: bio AFM; electrochemical sensors; imaging surface plasmon ellipsometry

Available equipment:

- Ultra short pulse Laser stations for rent and user training services.
- Dip pen nanolithography and imaging ellipsometry for creating and imaging of molecular surfaces.



OAC for converse and chemical coatings

specializes in aluminum and its alloys anodation, galvanic precious metals plating and related fields. The services provided: electrodeposition of protective, decorative as well as technical converse (anodic) coatings, structural etching of decoration elements, adsorption coloring of anodized surfaces, modification of aluminum and its alloys surfaces with a passivation film that provides the required conductivity, protection and other properties, chemical deposition of passivation coatings onto alloy steels.

Available equipment:

- Experimental equipment for environment-friendly galvanic processes, anodizing line.
- Chemical passivation line for chromium-free passivation process of aluminium and its alloys, IRIDITE NCP.

ANNUAL REPORT 2015 35

Events



ANNUAL FTMC CONFERENCE

/25-26 02 2015/

Reports on development of Long-Term Programs of scientific research and experimental development have been presented by the program leaders. Invited talks were given on the most interesting results obtained in 2014. G. Valušis, the Director of FTMC, presented his annual report mentioning the achievements of the year and nominating best scientists.



OPENING OF SUNRISE VALLEY TECHNOLOGY AND INNOVATION CENTER

/10 06 2015/

Benefits of collaboration and synergy of science, business and the government were emphasized by the honored guests of the event. 'Our scientists have much to offer to the world in the field of high technologies. Investments in high-tech not only result in developing of progress but also

create new jobs and attract foreign investment to Lithuania' told D. Grybauskaitė, the President of Lithuania, participating in the opening ceremony. Director of FTMC G. Valušis noted the urgency of science and business cooperation and expressed ambition to transfer the good traditions of Lithuanian lasers into new areas – optoelectronics, nano-engineering, development of new functional materials and emphasized the mission of science to generate new technologies and innovations in the country.



LITHUANIAN NATIONAL CONFERENCE OF PHYSICS

/17-19 06 2005/

The Center has co-organized the the 41-st Lithuanian National Conference of Physics. This traditional biannual event is an important meeting of Lithuanian physicists working in Lithuania and abroad as well as the researchers from physics-related fields, physics teachers and all interested in new trends in physics. More than 360 works have been presented in the conference (see: http://lnfk.ftmc.lt/tezes/LNFK41.pdf).



VISIT OF THE ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

/10 09 2015/

Sunrise Valley Technology and Innovation Centre has been visited by the experts from the Organisation for Economic Co-operation and Development (OECD). This organization provides a forum for governments to work together sharing

experiences and seeking solutions to common problems. The OECD is considering issues related to macroeconomics, environmental protection, education, science, technology and innovation.



THE SWEDISH ROYAL COUPLE VISITED SUNRISE VALLEY TECHNOLOGY AND INNOVATION CENTRE

/08 10 2015/

The Swedish Royal Couple - King Carl XVI Gustaf and Queen Silvia have visited Sunrise Valley technology and Innovation Center accompanied by the Lithuanian Prime

Minister A. Butkevičius and his wife, Swedish businessmen and other honored guests. The focus of this visit was set on cooperation in education and science between Lithuania and Sweden.



CONFERENCE TO COMMEMORATE THE 5TH ANNIVERSARY OF FTMC

/19-20 11 2015/

The Center has organized the international conference "Center for Physical Sciences and Technology 2015: 5 Years and a New Start" with participation of world-known scientists and other honored guests. The emphasis has been on identifying new challenging directions of

scientific interest. The essential change is related to moving of the FTMC to a new building equipped with modern scientific and technological infrastructure. The International Advisory Board of the FTMC has been created.

Awards



Kęstutis Pyragas - For scientific achievements

Chaotic phenomena of complex systems are the area where K. Pyragas revealed himself as the world's outstanding scientist. For 20 years the scientific community of chaotic phenomena has known and is applying the chaos control method developed by K. Pyragas. New K.Pyragas ideas are under way: over a couple of years he is focusing on modeling and control of living neural systems. His knowledge has been recognized this year by the APS program "Outstanding Referees" granting him the highest rating since beginning of the program in 2008.



Vidmantas Remeikis - For innovations

The innovations form a space with a multitude of degrees of freedom. V. Remeikis has proved by his activity that he is well comfortable here. Since the student times when he started his scientific carrier by designing gadgets for the radioactive material research, many years have been devoted to developing the materials science and environmental research spectroscopy. Moreover, mainly due to his combined scientific competence, management and diplomatic abilities the FTMC has built the new Technology and Innovation Center in the area of Savanoriu avenue – the national flagman of synergy of science and business, the new member of Saulètekis valley.



Audrius Alkauskas - Debut of the year

Theoretical physicist Audrius Alkauskas is back after 12 years of very successful studies and research in Switzerland and USA. He is aware of the importance to him to practice and share his knowledge here in Lithuania. (It is great to keep again the Lithuanian affiliation.)



Algimantas Undzėnas - For the life merits

Algimantas Undzėnas – is our patriarch of organic chemistry of light and charge sensitive materials. He did a huge job by patiently indoctrinating culture of chemistry science among the omniscient physicists. Now we are ready for the future challenges indeed.

Publications



Publications with FTMC affilations in 2015 in top quartile (Q1) journals

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- Mikalauskaitė, A.; Kondrotas, R.; Niaura, G.; Jagminas, A. Gold-coated cobalt ferrite nanoparticles via methionineinduced reduction // Journal of Physical Chemistry. C, 119(30), 17398-17407 (2015).
- 12. Matulaitienė, I.; Kuodis, Z.; Matijoška, A.; Eicher-Lorka, O.; Niaura, G. SERS of the positive charge bearing pyridinium ring terminated self-assembled monolayers: structure and bonding spectral markers // Journal of Physical Chemistry. C, 119(47), 26481-26492 (2015).
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