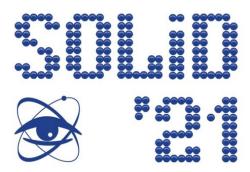




Solid State Physics for 21st century



EXECUTIVE REPORT FOR INTERNATIONAL SCIENTIFIC ADVISORY BOARD

Prague, May 2023





Project "Solid State Physics for 21st Century" (SOLID21) funded from Operational Program Research, Development and Education (abbreviated OP VVV) of EU with the budget exceeding 20 million Euro aims to strengthen the research excellence of the Institute of Physics of the Czech Academy of Sciences (FZU), public research institution, to become one of the leading European centres in the fields of nanoelectronics, photonics, magnetism, functional and bioactive materials and plasma technologies. The mission of the project is to address the most relevant scientific and technological challenges of the 21st century.

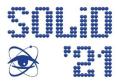
The project brings together the best teams of FZU with established research record in key disciplines of solid state physics into a joint focused research centre. The outcome of five cooperating Research Programmes (RP) achieved in 2021 year has been briefly summarized in this Report.

As a part of the project, we finished the construction of a new multifunctional building delivered in October 2021 that provides a versatile space for modern physical laboratories and new scientific facilities, the absence of which has limited further progress at FZU. New laboratories are equipped and fully functional.

The outcomes of the project include new knowledge about electronic, optical and structural processes and energy conversions and storage in nanostructured and modern materials. The gained knowledge will be applied in the development of new electronic, magnetoelectric, optoelectronic and photonic devices and sensors in physical and chemical sciences, engineering, biology and medicine, corresponding to the key enabling technologies defined by the Research and Innovation Strategy for Smart Specialization of the Czech Republic. Thus the project is specifically designed to reach out to industry within national and international research and innovation activities and few examples are provided below.

The researchers involved in the project also collaborate with universities to strongly engage students, providing the opportunity to expand and develop their professional skills. Furthermore, extended collaboration with many national and foreign institutions around the globe has already become well evidenced in so far published original papers the number of which far exceeded the original plan and related indicators. We succeeded also in the award of higher number of international projects with respect to original plan. In this way SOLID21 further promotes full integration of FZU into the European Research Area and world researcher's community.





Research programme Physics for Material Engineering (RP1) – head Oleg Heczko

Various ferroelastic and multi-ferroic materials are main research topic covering research of advanced functional materials with properties controled through the manipulation of specific microstructures formed by various phase transformation *from twinning to liquid crystals*. It consists of five Research Activities (RA) and technical support division: RA1- Functional ferroelastic materials and layers (P. Šittner), RA2 - NiTi shape memory alloys for technical applications (L. Heller), RA3 – Magnetic materials with martensitic transformation (O. Heczko), RA4 - Physical research of piezoelectric materials (J. Hlinka), RA5 - Multifunctional liquid crystals and composites (V. Novotná).

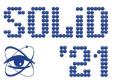
RA1 We developed a synchrotron diffraction method for analysis of texture evolution during tensile deformation of NiTi wire [1] and theoretical computational framework linking redistribution of preferred crystallographic orientations due to the activated deformation processes to the texture evolution (milestone 1.04). We applied it to monitor evolution of austenite and martensite textures in superelastic and shape memory NiTi wires (milestone 1.02). We performed additional series of synchrotron x-ray diffraction experiments focussing texture evolution during various thermomechanical loads on various NiTi wires. Finally, we investigated a possibility of thermal manipulation of NiTi surfaces deformed by nanoindentation (milestone 1.06). Ondřej Tyc who completed his PhD in 2021 spent 6 months on postdoc stay at EMAT Antwerps learning methods of transmission electron microscopy from experts.

RA2 Deformation processes activated within B19' martensite in nanocrystalline NiTi wires subjected to heating under constant applied stress were investigated by thermomechanical testing combined with post mortem analysis of martensite variant microstructures in deformed wires [2] and wrote invited review article on this topic for special issue of SMST Journal. These results fulfil the milestone 1.10. We designed and built NiTi polymer composite using PMMA coated NiTi and investigated its thermomechanical properties thus fulfilling milestone 1.13. Finally, we investigated origins of fatigue of SMAs experiencing stress concentrations due to elastic anisotropy and grain interactions in polycrystals. Effects of microstructure parameters on stress redistribution in polycrystals was studied statistically in collaboration with mathematicians from Charles University in Prague, Faculty of Mathematics and Physics.

RA3 We continued studying the magnetic shape memory or magnetoelastic multiferroic materials and its potential new derivatives. Thanks to our expertise we were asked to write summary of available effects for MRS Bulletin [3] connected with on-line worldwide webinar. We further compared obtained experimental results with theory to identify where theory is not still sufficient in invited extensive review for RRL physica status solidi. In cooperation with RP5 we evaluated thin films of new Heusler alloys based on Rh and Co (Co₂TiSn) which is gearing to completion. Concerning mobility, we hosted senior researcher O. Sozinov (one of the fathers of MSM research) from Finland and several PhD students from Spain, Slovakia and Finland. Now we host as. prof. M. Obata from Japan. The research work was done with the participation of PhD students of Faculty of Nuclear Sciences and Physical Engineering, CTU Prague from them two successfully finished their PhD degree in March 2023.

RA4 – The team of RA4 was lately concentrating on exploration of possibilities of engineering of suitable conductive or polarizable domain boundaries in perovskite materials. In particular, M. Pasciak and P. Márton participated in a systematic experimental and theoretical study of tunable piezoelectric domain boundaries in otherwise nonpolar lead zirconate perovskite within a large international collaboration involving recognized University partners from Xian, Chiba, Tokyo, Oxford, Warwick and Vancouver. In their recently completed work, it has been shown that the density, volume and polarity of the boundaries can be successfully controlled by a moderate mechanical stress or electric field. These outstanding results were published in





Advanced Materials [4]. In the meantime, the team has actively participated (J. Hlinka as a chairman of the program committee) in the 15th International Meeting on Ferroelectricity, 26-30 March 2023, Tel Aviv, Israel. It was decided that the next, 16th International Meeting on Ferroelectricity will be held in Prague under the auspices of the FZÚ.

RA5 We followed our research on hybrid systems based on ferroelectric liquid crystalline compounds admixed by magnetic nanoparticles. Most work was done in cooperation with our partners from MAGNELIQ consortium. The EU project H2020 FET Open MAGNELIQ 899285 is concentrated on preparation of magnetoelectric liquid. Magnetic nanoplatelets (MNPL) prepared from barium hexaferrite were successively hybridized by highly polar organic molecules synthesized by our group [5]. Additionally, such hybridized system was mixed with ferroelectric nematics, which has been recently prepared and studied by RA5 research group. PhD student Sergei Mironov with his supervisor Alexei Bubnov studied photosensitive properties of newly synthesized monomeric compounds, that are intended for preparation of various polymeric structures. The first photosensitive studies are focused on photoizomerization dynamics and possibility to apply proposed molecular structures in various applications.

Instrumentation

We successfully installed new magnetometer Microsense in new SOLID21 pavilion and demonstrated its sensitivity in measuring the nanometer thin films. The X-ray tomograph (X-ray microscope) has more than one year of operation and is regularly used to characterize samples mostly from RP1, as well as texture goniometer. In December 2022, small angle X-ray scattering diffractometer (SAXS) was installed and first experiments had been carried out since then. This instumentation was financed from multiple resources.

Problems and Risks

During SOLID21 project we established new top line of research and also kept abreast in the development of the fields in established lines of research as also demonstrated in awarding main conference of the field to FZU,Prague with O. Heczko as a chairman. The main risk for future is a sustainability of broad research established from SOLID21 in the unclear finance situation. To alleviate the situation, we pursued new proposal, based on the SOLID21 acquisitions and achieved results, in the frame of new funding program OP JAK (Top notch research call). Our RP participated and formed substantial part of the five years proposal Ferrmion (Ferroic Multifunctionalities) supposed to start in January 2024 and new research grants from Czech Scientific Foundation.

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Research Programme Nanoelectronics (RP 2) – head Stanislav Kamba RP 2 consists of five Research Activities (RA):

The programme is focused on research of various semiconducting, magnetic and multiferroic nanostructures. A total of 12 PhD students from Charles University and Czech Technical University were involved in this RP, four them have already defended their dissertations.

The selected major achievements, milestones, projects and collaborations in 2022-2023.

RA1 - Nonlinear optoelectronic and local transport phenomena in semiconductors and semiconductor nanostructures (P. Kužel):

We published as co-authors (within a large international consortium) a general methodical paper on the behaviour of charge carriers in perovskite materials for solar cells [1]. Implications for mobilities and lifetimes of photogenerated charge carriers obtained by contactless terahertz or microwave measurements are discussed.

We measured and interpreted local conductivity of GaAs and Si nanowires (defended thesis of V. Pushkarev); we also studied local anisotropic conductivity of defects in antiferromagnetic layers of CuMnAs (prospective metallic layers for antiferromagnetic memories): publication was sent to Advanced Physics Research (now on ArXive: https://arxiv.org/abs/2303.15268). Milestones M2.05 and M2.07 were fulfilled.

RA2 - Control of single-electron charged states in molecules (P. Jelínek):

We have been analyzing light-driven spin switching of 1D coordination in π -d conjugated polymers and preparing a publication describing this phenomenon. We have achieved control of multi-electron-spin charge state switching in molecular chains on surfaces. This achievement fulfilled milestone M2.12. We also investigated the enhancement of charge transport across dimeric molecular junctions that self-assemble between two gold electrodes in π - π stabilized binding configurations of molecular junctions. In collaboration with Japanese colleagues, we have published a study of the thermoelectric properties of molecular circuits. [2]

RA3 - *Graphene and 2D materials* (J. Červenka):

We have investigated electron transport and physical properties of various 3D porous structures of graphene and 2D materials. In a very close collaboration with RA1 we studied the interaction of graphene aerogels with THz radiation. We revealed the mechanisms of charge carrier transport and ultrafast (picosecond) photoconductivity in these materials [3]. We discovered high-temperature fire resistance and self-extinguishing behaviour of cellular graphene aerogels which can resist temperatures up to 1500 °C [4]. We also investigated charge-transfer and ion intercalation processes in graphene-based electrodes in highly concentrated aqueous electrolytes [5]. Milestones M2.16 and M2.17 were fulfilled.

RA4 - Magnetoelectric coupling and spin interactions in multiferroic materials (S. Kamba): Using free-electron lasers generating strong terahertz pulses, we pumped electromagnons in multiferroics with Y- and Z-hexaferrite crystal structures at the TeraFermi lab (Trieste) and the Helmholz Center in Rossendorf near Dresden. We observed shifts of the electromagnon frequencies depending on the intensity of the THz pulses, which were explained by a change of the conical ferrimagnetic structure. [6]

We have characterized in detail the new high-temperature multiferroic BiMn₃Cr₄O₁₂ and found that the phase transition to the antiferromagnetic phase is induced by a displacive ferroelectric (i.e., structural) phase transition. Thus, this is a completely new mechanism for the formation of multiferroic ordering. [7] We further studied the effect of Fe impurity on the magnetic ordering and dynamic magnetoelectric coupling in multiferroic TbMnO₃.[8] The last two papers were published in collaboration with the University of Porto.

With this, we have met the last milestones M2.20, M2.23, M2.24 and M2.27.





RA5 - Magnetic anisotropy and magnetization dynamics in nanostructured strongly correlated magnetic materials (A. Shick):

We studied the doping of a Bi₂Te₃ single crystal using ARPES and ab initio electronic structure calculations. The Fe, Ru, and Os dopants give rise to the shift of the Dirac cone at the surface in the direction towards the conductivity band minimum.[9]

We report DFT plus exact diagonalization of the multiorbital Anderson impurity model calculations for the Co adatom on the top of a Cu(001) surface. A singlet many-body ground state and Kondo resonance are found when the spin-orbit coupling is included in the calculations. The differential conductance is evaluated in good agreement with the scanning tunneling microscopy data. The results illustrate the essential role which the spin-orbit coupling is playing in the formation of a Kondo singlet for the multiorbital impurity in low dimensions.[10]

The electronic structure, spin and orbital magnetic moments, and the magnetic anisotropy energy in selected U-based compounds are investigated using of the correlated band theory [11]. Our studies suggest a viable route for further development of the rare-earth-lean permanent magnets by replacing a part of U atoms by some rare-earth like Sm in UFeSi₂. With this, we have met milestones M2.30 and M2.31.

Summary

The most of milestones planned for the project have been accomplished. Only the milestone M2.29 has been postponed to the second quarter of 2023 and is expected to be achieved in June 2023.

Thanks to the Solid21 project, we have made two major investments (THz SNOM and ALD), which has significantly improved the quality of our work. We can now prepare thin films that we could not previously grow and we can measure local THz conductivity in semiconducting nanostructures. This has enabled us to publish our results in higher quality journals than before. In addition, the collaboration with other research teams not only within the Institute of Physics but also with scientists abroad has been significantly strengthened.

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Research Program Photonics and Energy Conversion (RP 3) – head Martin Nikl

RP 3 is composed of five Research Activities: RA1 - Phosphors for solid state light sources (V. Jarý); RA2 - New material concepts and technologies of scintillation materials (J. Pejchal); RA3 - Luminescence of nanostructures of silicon and other semiconductors (K. Kůsová); RA4 - Nanostructures for photovoltaic solar energy conversion (A. Fejfar) and RA5 - Thermoelectric materials, heat transfer and thermoelectric applications (J. Hejtmánek).

The selected major achievements, milestones, projects and collaborations in 2021:

All planned milestones were fulfilled, all devices installed and fully operational. We have installed new cathodoluminescence set-up enabling both the spectra and decays measurements in UV/VIS spectra range and ns-ms time domain. It will be valuable tool especially in our industrial collaborations (RA1,RA2). We were awarded by two new European projects, Pilatus and Unicorn in RA4 and RA2, respectively, which will further intensify our extensive international collaborations with both the academic and industrial partners. Domestic industrial collaboration with CRYTUR and Georadis companies has been intensified by newly awarded project from Technological Agency CR. M. Nikl is Chief Editor of special issue of IEEE Trans, Nucl. Science publishing collection of papers from SCINT2022 conference.

RA1: We published in Physical Review Applied (IF 4.931) the study devoted to ultrafast KLuS₂:Pr³⁺ phosphor [1] which has significant application potential. V. Jarý and J. Pejchal published a monography dealing with scintillation materials [2], the first of its kind in Czech language intended especially for students. After technological modifications at the halide mPD setup we successfully grew Lu₂S₃:Pr sulfide single crystals, *first time in the world* by this technology. After adaptation of plasma deposition technology of sulfides (RA5) the very first samples of polycrystalline Lu_{32.11} S_{48.00} have been obtained which opens the way to dope them further and obtain large area X-ray imaging elements. In the frame of ongoing applied research TA CR project with CRYTUR we tested several compositions of doubly doped garnets for persistent luminescence. V. Jary participates further in the "Open Science" project of CzAS focused on education of high school students.

RA2: In collaboration with about ten domestic and foreign institutions we have published nearly 30 papers in last 12 months, some of them in top Q1 international journals, focused on the bulk, thin film and nanocomposite scintillators. We mention the Cs-Cu-I bulk halides in collaboration with prof. Wu group from SICCAS, China, e.g. [3], CsPbBr₃ nanocrystals embedded in polystyrene matrix in collaboration with prof. Cuba group at CTU [4], crucible-free method for crystal growth in collaboration with prof. Yoshikawa group in Tohoku university [5] and energy partitioning in multicomponent nanoscintillators in collaboration with prof. Monguzzi group, Universita di Milano-Bicocca [6]. New Horizon Europe project UNICORN start on June 1, 2023 with 7 partners from 5 EU countries, focused on breakthrough technologies for nanocomposite scintillators and their broadscale production and application. New applied research field was opened and TACR project awarded with CRYTUR and Georadis companies focused on heavy perovskite scintillators for environmental applications. Technology transfer of InGaN-GaN multiple quantum wells manufacturing continues to OSRAM company. V. Vaněček won the 1st place in M. Odehnal Prize with collection of papers, e.g. [7], published during his PhD studies.

RA3: We finished and published the study focused on surface modifications of semiconductor nanoparticles with the help of plasma activated water with high content of nitrogen which paves the way for much more efficient nanoparticle surface treatment compared to traditional methods [8]. We are engaged in the organisation of Symposium EL07-Group IV Nanostructures for Emerging Optoelectronic Applications within a MRS Spring Meeting 2023, San Francisco which is a top international event.

RA4: On November 1, 2022 we started the Horizon Europe project Pilatus "Digitalised pilot lines for silicon heterojunction tunnel interdigitated back contact solar cells and modules" in





consortium of 19 partners from 8 European countries, https://pilatus-project.eu/. Its output will be three pilot production lines for highly efficient photovoltaic cells and modules fully located at EU territory. In FZU we focus on photoluminescence experiments for fast characterization of backside contacts dedicated for online control during production process.

RA5: We studied ferromagnetic insulator CdCr₂Se₄, in which essential influence of magnetic field onto low temperature magnetic excitation can be observed, namely due to the advantage of absence of spin-wave masking by free charge carriers or nuclear effects [9]. In collaboration with IJL Nancy we focused on InTe which appear promising candidate for thermoelectric applications due to its very low lattice thermal conductivity. We continue in the organization of the 19th European thermoelectric conference, https://thermoelectric-conference.eu/, RA5 members are in the organizing Committee and will prepare special issue of Solid State Science (Elsevier) with topics "Advances in thermoelectrics" as Guest Editors.

Common experimental base: Apart from routine help to other RA's with material structure determinations, the Dept. of Structures team organized several workshops focused on using the program Jana (solution of crystal and magnetic structures, [10]). We succeeded in calculating (3d+2) modulated structure of the new structural phase of ferrocene and described how its modulated structure influences the molecule dipole moment [11].

Problems and risk management for the following period: The covid-19 induced uncertainties and limitations are hopefully over. Instead, we are facing uncertainties related to the available financial sources with the dip in 2023 and unclear situation in following years due to the state budget deficiencies. In FZU we prepared three big institutional project proposals in OP JAK, "Top notch research" call, the result of which will be known around the end of year. We have put an extensive effort for proposal preparation in another grant schemes (apart from common Czech Science Foundation) especially those related to Horizon Europe to secure maximum project-based funds for our future research need.

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Research Program Physics for bio (RP4) - head Oleg Lunov

RP4 consists of five Research activities (RA): RA1 - Biophysics of high-gradient magnetic fields (O. Lunov); RA2 - Plasma and irradiation for bioapplications (A. Dejneka); RA3 - Bioelectronics and biosensors (A. Kromka); RA4 - Nanoparticles for theranostics (I. Kratochvílová) and RA5 - Biomaterials and biointerfaces (Š. Potocký). RP4 aims to create unique *interdisciplinary platform* that would merge complex research across physics, chemistry, biology, and medicine. Our goal is to gain deep insights in *fundamental mechanistic understanding* of how selected physical factors (e.g., magnetic fields, non-thermal plasma, various nanoparticles, diamond, or diamond-like carbon biomaterials) affect biological systems. RP4 closely cooperates with other research programs.

The selected major achievements in 2022 are summarized below.

Overall, RP4, in collaboration with other RP's, published 19 papers during the reported period from 01/01/2022 to 31/12/2022. RA1: We continued with research on biological effects of magnetic fields. We theoretically demonstrated that a high magnetic field might accelerate diffusion of diamagnetic species while slowing the diffusion of paramagnetic molecules in cell cytoplasm. [1]. RA2: We conducted a critical analysis of the non-thermal plasma-triggered modulation of immune cells. Importantly, we analyze pitfalls in the field and identify persisting challenges. We show that the identification of misconceptions opens a door to the development of a research strategy to overcome these limitations. RA3: We made a technological breakthrough in the fabrication of boron-doped diamond using only a liquid precursor (trimethylborate) and hydrogen gas without the need for additional hydrocarbons. Such a new concept allows to achieve high deposition rates, high doping levels and low resistance values of the diamond layer grown at low pressure over large areas. At the same time, by changing the process parameters, it is possible to control the doping level and layer morphology by changing the B/C and B/O ratios. This work shows that liquid organic precursors are promising to accelerate diamond growth and to incorporate not only boron but also various impurities such as phosphorus, silicon and others. [2]. **RA4:** We continued with studying novel nanomaterials. Multi-walled carbon nanotubes (MWCNTs) and two different types of graphene platelets (GPs) were tested if their intracellular presence modulates a proinflammatory response from human primary monocytes towards common pathogens. We confirmed that all tested carbon-based nanomaterials (C-BNMs) caused neither direct cytotoxicity nor the release of tumor necrosis factor α, interleukin (IL)-6 or IL-10. All the tested C-BNMs enhanced monocyte phagocytosis and accelerated their differentiation towards macrophages. This study confirms the immunomodulatory potential of C-BNMs [3]. RA5: The successfully prepared threedimensional (laser irradiation) NCD-coated reservoirs dedicated to human endothelial and mesenchymal stem cell proliferation and colonization experiments are under evaluation for a base of a highly vascularized bone tissue. The newly opened collaboration with the Biomedical Center of the Slovak Academy of Sciences is supporting this goal. The F, H, and O diamond surface terminations were tested against monocultures as well as their co-culture. The cell numbers and viabilities show that O termination of a diamond surface is the best option for cell growth with respect to other terminations. On the first day of cultivation, the number of hMSC significantly exceeded the number on the control with the viability of almost 100 %. Similar results were also achieved for hMSCs where the co-culture significantly exceeded the cell number on the control. On the third day, the number of hMSCs remained significantly the highest, even against the control. On the seventh day of cultivation, both cell types formed a confluent layer. It is expected to reach the M4.20 milestone within the end of the project along with a cell culture protocol. In collaboration with the Faculty of Science of Charles University, we experimentally demonstrated that exposure of solutions with E. coli to the electrochemical process leads to a significant elimination of bacteria in NaCl and phosphate buffer saline solutions, which was explained by the synergistic effect of the chloride components. The results





obtained confirm the highly promising potential of boron-doped diamond electrodes (see result of RA3) for electrochemistry and wastewater treatment since the presence of chloride salts in wastewater is common [4].

Summary of goals for 2023

RA1: In 2023, we aim to reveal a role of magnetic fields on endogenous biological processes. Our work shows that new methods are needed to elucidate the effects of magnetic fields at the cellular level. As part of the presentation of these results, we expect to reach a *milestone M4.04* (June 2023). **RA2:** Previously we revealed how plasma affects wound healing processes in vivo. During this period, we are going to address the idea that addressing the issues highlighted in this review will accelerate the clinical translation of low-temperature plasma treatments. As part of the presentation of these results, we assume the achievement of the *M4.08 milestone* (June 2023). **RA3:** The successful implementation of new approach for boron-doped diamond deposition sets the *milestone M4.12*. The validation of this concept for silicon or phosphorus doping is a subject to the investment of a bubbler in the existing depositing system and tests. **RA4:** We will continue study of interactions of nanoparticles with cells and subcellular compartments. We will analyse the effect of various sizes, shapes, and surface properties including organic and biomolecular functionalization (*milestone M4.16*). **RA5:** The culture protocols utilising nonstructured and structured functionalized diamond surfaces is subject of approaching *milestone M4.20* (June 2023) according to the plan.

Progress in external links of RP (universities, industry) and international standing

We continue with the large European cooperation network in the frame of **COST** Action n CA17112 PRO-EURO DILI Network (https://proeurodilinet.eu/). We organized sucessful closing meeting of this COST Action (https://proeurodilinet.eu/ca-17112-closing-meeting-9-10-march-2023-prague-czechia). In the next phase of research, the PRO-EURO DILI Network will expand its scope from medicines to herbs and herbal dietary supplements. Even these can damage the liver, either when used incorrectly or in combination with certain medications. We have extended collaboration Friedrich-Schiller-Universität and Leibniz Institute of Photonic Technology, Jena, Germany. We have initiated new collaboration within the joint project application with Dr. Katarina Kozics from Biomedical Center of the Slovak Academy of Sciences and Dr. Gabriel Vanko from Institute of Electrical Engineering of the Slovak academy of sciences, both from Slovakia. Research of RP4 shows great potential for clinically oriented biotechnologies. Thus, we established and propelled fruitful cooperation with national and international hospitals, namely Institute for Clinical & Experimental Medicine (IKEM), Prague; Department of Pediatric Research, Oslo University Hospital; General University Hospital of the First Faculty of Medicine, Charles University, Faculty of Electrical Engineering, Czech Technical University. Translation of plasma technology into real-life applications continues with industrial partners FOTON, s.r.o L.E.T. Optomechanika Praha s.r.o. and SINDAT spol. s.r.o. RP4 as well actively cooperates with other RPs of SOLID21 project. For examples with RP5 in the field of plasma technologies.

Potential problems and risk management in 2023

RAs within RP4 are being implemented on time and with a high-quality level. It is plausible to expect in 2023 risks associated with some ineffective collaboration among different RAs. The required collaboration will be ensured through a strong internal communication structure fostered and aided by RP leader, ensuring effective information flow.

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Research program Plasmatic Technologies (RP 5) – head Zdeněk Hubička

RP5 is composed of six Research activities (RA): RA1- R&D of advanced low temperature plasma systems for thin film polycrystalline materials (Z. Hubička); RA2 - Plasma diagnostics, optimization of plasma deposition systems, and monitoring of deposition processes (M. Čada); RA3 - Plasma methods of preparation of thin metallic and intermetallic layers (J. Lančok); RA4 - Thin-film chemical sensors (M. Novotný); RA5 - Optical materials-plasmon structures (J. Bulíř) and RA6 - Structures exhibiting a combination of ferromagnetic properties (M. Tjunina).

The selected major achievements in 2022 are summarized below.

RA1: The new configuration of dual reactive HiPIMS plasma was applied for the deposition of semiconducting polycrystalline CuWO₄ ternary oxides [1]. The new plasma system for the deposition of sulphides and selenides was fully finished and polycrystalline lutetium sulphide thin films were deposited and investigated (collaboration with RP3).

RA2: The reactive pulsed hollow cathode discharge [2] and HiPIMS pulsed magnetron system in various magnetic field configurations [3] were investigated. Ion distribution function and ionization fraction of sputtered particles were determined and physical models of processes in plasma were created.

RA3: Ab initio calculation of band structure and characteristics of ARPES of Bi₂Se₃ and Bi₂Te₃ were studied [4]. In cooperation with RP1 we finished magnetic and magnetooptics analyses of full and half Heuslers, RhMnSb and CoTiSn compounds. By means of plasmon resonance (with RA5) we performed targeted modification of 2D MXenes to create biocompatible materials (with RP4) [5].

RA4: Chemical gas sensors based on metal oxides (eg. CuO) were fabricated by PLD [6]. Advanced sensors utilizing QCM approach based on black metals were fabricated by evaporation and magnetron sputtering [7]. We have started the research of black metal ZnO:Eu thin film sensors with RP3.

RA5: The research in the field of plasmonic metamaterials was extended by another class of materials ScN [8] and CrN. The main motivation is the research of metamaterials with extreme anisotropy of optical properties, where individual components of permittivity reach opposite signs in different directions.

RA6: Thin films of LaAlO₃ and BaTiO₃ (BTO) on SrRuO₃/SrTiO₃ (STO) were epitaxially grown by PLD. Optical and ferroelectric properties were studied considering strong effects caused by oxygen vacancies. [9,10].

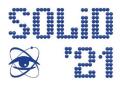
Links to RPs: We enlarged the cooperation within all RPs: RP1 - characterisation of magnetic and magnetoptics properties of Heusler alloys; RP2 - ultrathin HfO₂ films as a novel material for ferroelectric memories, fabrication of MnO/NiO multilayers.; RP3 - we continued collaborative research focused on optical properties of metal oxides and iodines [11]. RP4 - in cooperation with diamond group we participated on the preparation and characterisation of multi-layered diamond thin films.[12].

Milestones and new instrumentation:

We successfully fabricated Heusler alloy thin films of extraordinary magnetic and magnetooptics properties M5.14. Currently we are finishing calculation and comparison of experimental data on Heusler alloy thin of nonstoichiometric and defects M5.15. Milestones 5.19 and 5.20 were achieved by successful fabrication of nanostructured sensing layers. Plasmonic nitrides properties were optimized utilizing in-situ spectral ellipsometry M5.23. Thin ferroelectric and magnetic oxides thin films have been successfully fabricated by PLD. M5.26. The milestone M5.27, M5.23, M5.08, M5.09, M5.04, M5.05 will be fulfilled before the end of the project.

Domestic and international cooperation:





The collaboration with UCT (Dr.A.Lyutakov) has been focused on the research of MXene. We have initiated collaboration with prof.M.Kawamura (Kitami Institute of Technology, Japan) related to black metals films research. In frame of 2D MXene thin films we established cooperation with prof. V. Kruglyak form University of Exeter and received grant from Royal Chemical Society. L. Patrone of CNRS in Toulon participated in characterization of sensing layer surfaces by STM and AFM.

Problems and risk management: We had to solve the problem with delay in the construction of new building affecting the completion of the instrumental infrastructure there.

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