DEPARTMENT FOR ADVANCED MATERIALS

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At the Advanced Materials Department, novel materials are developed by an understanding of the mutual dependence of their structural and functional characteristics. Contemporary technologies, which enable the synthesis of materials with atomic- and microstructural-scale precision, are applied to prepare beforehand-designed structured ceramics, thin films, and nanoparticles with the desired crystal structure, chemical composition, and microstructure. Among our important objectives is the development of: i) new oxide materials for efficient high-temperature thermoelectric energy conversion, ii) new materials with improved antibacterial and photocatalytic effects, and iii) novel functional oxide materials for various electronic applications.

Thermoelectric materials

In the scope of the research on oxide materials as possible candidates for p-type thermoelements in hightemperature thermoelectric modules we continued our investigations of coherently intergrown layered cobaltates Ca, Na, Co, Oa, which we found to be promising in terms of environmental and high-temperature stability. Atomically resolved transmission electron microscopy, performed with Cs-probe corrected scanning transmission electron Prof. Danilo Suvorov microscopy, revealed a diversity between the octahedral CoO₂ layers within the individual grains. The prismatic sites between the layers can be occupied by sodium and calcium ions or the interlayer space can be occupied with the three-layer CaO-CoO-CaO rock-salt type stacking. Parts of the individual grains exhibit a structural ordering



of the interlayer ions in a zig-zag manner, which was confirmed to be the most stable variant by density functional theory (DFT) calculations. Using electron-energy-loss spectroscopy (EELS) we probed individual CoO₂ layers neighbouring different interlayer structural arrangements and found

that the oxidation state of cobalt ions and, consequently, the electrical charge within the octahedral layers is not significantly affected by the apparent interlayer structure. These observations imply that the observed differences in the structure between the octahedral CoO₂ layers could also be a consequence of an out-of-zone rotation of the interlayer stacking. The spontaneous interlayer diversity in intergrown cobaltates appears promising for the design of new thermoelectric heterostructures.

As an n-type candidate we investigated the donor-doped perovskite CaMnO₂, which exhibits temperature-stable electrical properties. By inducing the formation of Ruddlesden-Popper polytypic faults with excess CaO we were able to control the microstructural development and transport properties of the ceramics. With the appropriate amount of excess CaO, a grid-like morphology was obtained, which resulted in a threefold decrease of the thermal conductivity. Furthermore, with the introduction of planar faults within the perovskite grains, the electrical transport properties change, resulting in a transition from semiconducting to metallic behaviour and an increase in the Seebeck coefficient. These observations suggest that electrically insulating polytypic faults induce a low-dimensional character within the conductive perovskite matrix.

In addition to previous investigations we also focused on the synthesis of novel functional materials based on layered titanium disulfide (Figure 2), with optimized electrical and thermal transport properties. The titanium disulfide forms thermodynamically stable natural superstructures on (self) intercalation and consequently possesses the properties of a highly mobile semiconductor with a low thermal conductivity. Apart from that, it is nontoxic, has a low mass density, and consists of abundant and low-cost elements. Dihalcogenides of this type would be a good replacement for toxic, scarce and expensive materials based on bismuth telluride, which currently have no suitable alternatives as thermoelectric materials in the range of low and medium temperatures. Intercalated TiS2 crystals of various morphologies were prepared with solid-state and solvothermal synthesis. In order to pre- along the [010] and [001] directions.

Gallium nanoparticles on hydroxyapatite are a new biomaterial with an antibacterial action.

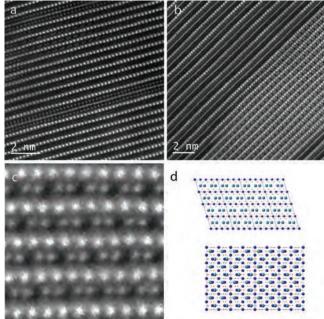


Figure 1. Structural diversity between CoO, layers of intergrown cobaltates: a) rock-salt stacking of CaO-CoO-CaO, b) rock-salt stacking and ordering of calcium ions, c) close-up of ordered calcium ions and d) calculated structural model with ordered calcium ions between the CoO layers viewed

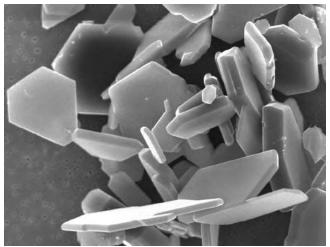


Figure 2. SEM image of layered TiS, crystals.

serve the desired structure, as-prepared starting materials were densified to the bulk by PECS (pulsed electric current sintering). It is shown that the structuring could have a significant impact on the electrical and thermal transport properties of these materials.

Photocatalytic and antibacterial materials

The photocatalytic efficiency of a wide-band-gap semiconductor TiO_2 was enhanced in the ultraviolet range and also shifted to the visible region, by the coupling of TiO_2 anatase nanoparticles with noble-metal (Au) nanoparticles. The TiO_2/Au nanocomposites were formed using a bifunctional bridging linker that contained both the carboxylic group and the thiol group to enable binding to the TiO_2 and the Au nanoparticle surfaces, respectively. Additionally, the bifunctional bridging linker served as a capping agent for the noble-metal particles, thus preventing their growth and agglomeration. The homogeneously distributed Au particles (4-10 nm) were attached to the TiO_2 particles (~ 10 nm) to form an effective contact between the two phases. In this way the life-time of the TiO₂ photo-induced charge carriers

was prolonged and the UV photocatalytic activity was enhanced. The plasmonic properties of the Au induced a visible-light response of the material. The prepared composite effectively degrades the organic dye methylene blue and inhibits the growth of the bacteria *Escherichia coli*.

For photocatalytic applications we also synthesized doped (Ce, Zr, Si) anatase with spherical particles ranging from 2 to 7 μ m. The particles exhibit a mesoporous microstructure and consisted of nanosized primary crystallites with a size up to 20 nm, depending on the synthesis parameters. The obtained doped anatase exhibits interesting photocatalytic properties, even being calcined at 1050 °C.

In 2014 we continued our research on antibacterial materials that include gallium components. We developed new nanocomposite materials that combine bioactive (hydroxyapatite) and antibacterial (metallic nanoparticles) components.

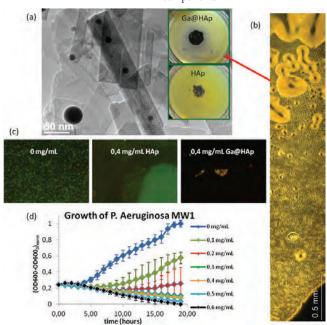


Figure 3. Ga nanoparticles on hydroxyapatite and their antibacterial action against P. Aeruginosa MW1: (a) diffusion antibiogram; (b) inhibition zone under phase-contrast microscope with the material at the bottom (black) and the edge of the inhibition zone at the top; (c) merged images of green (live+dead) and red (dead bacteria) fluorescence for P. Aeruginosa under fluorescence microscope after incubation without any material, with HAp and with Ga@HAp, respectively; (d) microdillution antibiogram assay of suspension with different concentrations of Ga@ HAp; bacause of the material's absorption at 600 nm and its sedimentation during shaking and incubation the starting absorbances (optical densities, OD600) were subtracted and all the values are normalized to [0,1].

1. Amino-acid-functionalized Au nanoparticles on a hydroxyapatite containing Ga3+ ions (Au/amino acid@HAp(Ga))

The loading of hydroxyapatite with Ga³⁺ ions approaches saturation in about 24 hours and yields approximately 15 wt % of Ga(III) in hydroxyapatite, which is slowly released from the material during aging in PBS. We found that Au/amino acid@HAp(Ga) (Au/Arg@HAp(Ga), Au/Gly@HAp(Ga) and Au/His@HAp(Ga)) inhibit the growth of *Escherichia coli* MG1655.

2. Ga nanoparticles on hydroxyapatite (Ga@HAp, Figure 3)

Gallium nanoparticles on hydroxyapatite are a new biomaterial withan antibacterial action. We found that it markedly inhibits the growth of *Pseudomonas aeruginosa* MW1 in PA01 (Figure 3). The diffusion antibiogram assay showed an inhibition zone around Ga@HAp, which contained no bacteria according to phase-contrast microscopy images (Figure 3, a and b). In a microdillution antibiogram of the suspension of the material we obtained minimal inhibition concentration (MIC) at 0.3 mg/mL, which in 24 h completely inhibited the growth of *P. aeruginosa* (Figure 3, d), while 0.4 mg/mL was the lowest concentration that effectively prevented the growth in 48 h. So far we have achieved such coverage of hydroxyapatite with Ga nanoparticles that approximately 15 wt % of Ga was in Ga@HAp. Although no major bactericidal effect was noticed, the live/dead fluorescence microscopy assay showed more agglomerates of dead bacteria for MIC of Ga@HAp than for the control (0 mg/mL or hydroxyapatite, Figure 3, c).

The application of vanadium pentoxide (V_2O_5) as antibacterial material is limited by its reasonably high solubility in aqueous solutions. Because of that we developed a method to control the solubility of V_2O_5 by the formation of 1D structures and their incorporation within a biocompatible polymeric matrix. Experimental results confirmed that by embedding vanadium pentoxide into the polymer matrix an efficient solubility control can be achieved. The elution of materials designed in such way provides vanadate within a concentration range known from the literature as bioactive. Moreover, test-

ing the interactions of the 1D nanostructured vanadium pentoxide with bacterial cells confirmed the inhibition of bacterial growth in a medium containing hydrogen peroxide. The main goal for future research in this field is to optimize the composite properties in order to combine both bioactive and antibacterial properties.

Functionalized oxides for electronic applications

With a solid-state synthesis we prepared ceramic components based on nonstehiometric sillenites, which contained M^{2*} (Co^{2*}, Fe^{2*}), M^{3*} (Ga^{3*}, In^{3*}) and M^{5*} (V^{5*}) cations. We investigated their dielectric properties in the radio (<1 MHz) and microwave (46 GHz) frequency ranges. The results of the dielectric measurements in the radio-frequency range have shown that the dielectric constant decreases with the increasing valence of the

 M^{n*} cation in the sillenite ceramic, with values between 51 (Co²⁺) and 34 (V⁵⁺). The temperature coefficient of the dielectric constant changes from a pronounced negative -198 ppm/K (Co²⁺) to a highly positive 187 ppm/K (V⁵⁺). The microwave dielectric measurements also show a decrease in the dielectric constant from 57 (Co²⁺) to 35 (V⁵⁺) with an increase of the Mⁿ⁺ cation's valence, whereas the quality factor increases from 742 GHz (Co²⁺) to 1736 GHz (V⁵⁺). Suitable dielectric properties for further use in the electronics industry were obtained for a sillenite ceramic with Ga³⁺, as its values are $\varepsilon \approx$

The results of the study revealed, for the first time, an effective pathway for the preparation of a SrO-induced buffer layer on a silicon substrate using PLD, which can be subsequently utilized for the epitaxial growth of functional oxides.

40, $\tan \delta = 0.001$, $\tau_k = 0$ ppm/K in the radio-frequency range (1MHz) and $\epsilon \approx 47$, Qxf= 1615 GHz, and $\tau_f = -11.65$ ppm/K in the microwave range (5 GHz).

In the scope of the MNT-ERA.NET project "Nanostructured ferroelectric films for biosensors" (Naferbio), which was coordinated by Prof. Spartak Gevorgian from Chalmers University of Technology, Sweden, we developed intrinsically tunable bulk acoustic wave resonators, based on sol-gel $0.70Pb(Mg_{1/3}Nb_{2/3}O_3-0.30PbTiO_3 (PMN-PT))$ thin films with a record high effective electromechanical coupling coefficient of 13% and a tunability of the series resonance frequency up to 4.0%. The enhanced electro-acoustic properties of the PMN-PT resonators were attributed to the mechanism of polarization rotation occurring in the region of the morphotropic phase boundary. In the study we analysed the electroacoustic performance of the PMN-PT resonators using the theory of dc field-induced piezoelectric effect in ferroelectrics, while the extrinsic acoustic losses in the PMN-PT resonators were analysed using a model of the wave scattering at reflections from rough interfaces. The mechanical *Q*-factor of the resonators totals up to 70 at 4.1 GHz and is limited mainly by losses in the PMN-PT film.

For the investigations of electroceramics with improved dielectric properties we focused on BaTiO.. In order to prepare a densely sintered dielectric ceramic with submicron-sized grains, we investigated a sintering process for nanosized BaTiO,. The research on BaTiO, ferroelectric particles also included the (i) sintering of defined BaTiO, particles and a determination of the dielectric properties of sintered ceramics and (ii) tailoring the shape, polarization and crystal orientation of plate-like ferroelectric particles. In the first part we studied the sintering of BaTiO, particles, which according to a transmission electron microscope (TEM) examination, showed a square-like shape. The actual three-dimensional shape was neither an ideal cube nor an octahedron. The formed particles were not spherical and also not fully faceted. The development of the microstructure during sintering of these particles could be very interesting in terms of the mechanisms that control the grain growth. Depending on the driving force of the different mechanisms, the sintered ceramics consisted of normal growing grains, stagnant grains (growth rate is very low) or abnormal grains (liquid-phase sintering). Our investigations revealed that the relative contribution of a particular type of grains depended on the Ba: Ti ratio and sintering regime: two-step or isothermal sintering. The Ba:Ti ratio was controlled by the intensity of the acetic acid washing after the hydrothermal synthesis of the BaTiO, powders. In the ceramics with Ba:Ti=1.01:1 and two-step sintering, stagnant grains prevailed, while normal grains in addition to stagnant and abnormal grains were present in the ceramics after the isothermal sintering. The former ceramics consisted of grains with an average grain size of 2 µm and exhibited a higher dielectric constant (ε) and lower dielectric losses (tan δ) at room temperature, compared to the isothermally sintered ceramics with an average grain size of 15 µm. These ceramics exhibited a high dielectric constant of 11000 at the Curie temperature (121 °C). In the barium-deficient ceramics (Ba/Ti=0.98:1) a small amount of secondary Ba_cTi₁₀O₄₀ phase formed and the abnormal and stagnant grains dominated over the normal grains, which resulted in a low relative density (84-89%) and a deterioration of the dielectric properties.

In the scope of the study of ferroelectric crystals with a defined shape, polarization and crystal orientation we dealt with the synthesis of $Bi_{4x}Nd_xTi_3O_{12}$ and $BaTiO_3$ plates. The research was focused on the study of synthesis conditions, which enabled tailoring the size of the ferroelectric $Bi_{4x}Nd_xTi_3O_{12}$ ($0 \le x \le 0.85$) plates and their topo-chemical transformation into $BaTiO_3$ plates. Varying the synthesis conditions provides us with dimensional control of the $Bi_{4x}Nd_xTi_3O_{12}$ plates, from 100 nm to several microns in width, and from 20 nm to 100 nm in thickness. The influence of bismuth substitution with neodymium on the morphology of the $Bi_{4x}Nd_xTi_3O_{12}$ plates and their ferroelectric characteristics and domain structure was studied by means of electron microscopy, differential scanning calorimetry

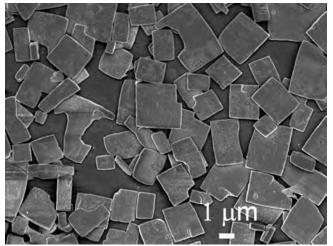


Figure 4: Ferroelectric tetragonal $BaTiO_3$ plates with a preferential (002) orientation.

(DSC) and piezo-force microscopy (PFM). DSC analyses revealed the decrease of the Curie temperature by 40°C when x changed from x=0 to x=0.2. The PFM investigations showed the presence of irregularly shaped ferroelectric domains and polarization in the plane of the $Bi_{38}Nd_{0.2}Ti_{2}O_{12}$ plate.

The dimensions, crystal structure and orientation of the singlecrystalline BaTiO₃ plates, which were topo-chemically converted from the Bi_{4x}Nd_xTi₃O₁₂ plates, were controlled by the template size, the composition and by the conversion conditions. Bi₄Ti₃O₁₂-based plates mainly led to (002)-oriented tetragonal BaTiO₃ plates (Figure 4), whereas Bi_{4x}Nd_xTi₃O₁₂ (0.2≤x≤0.85) favoured (200)-oriented cubic BaTiO₃ plates. In this study we faced the challenge of preparing highly tetragonal (002)-oriented BaTiO₃ plates that are considerably less than 1 µm in width and less than 100 nm in thickness. The development of such ferroelectric plates is of great interest in the study of ferroelectric behaviour on the nanoscale and for the realization of miniaturized ferroelectric devices by assembling their plates.

The investigations of the ferroelectric particles with a defined shape were performed in the scope of INNOINKS (MATERA-ERA-NET) project in cooperation with the Microelectronics and Materials Physics Laboratories

(University of Oulu, Finland), the Institute of Electronic Materials Technology (Poland), Sachtleben Pigments Oy, Pulse Finland Oy and the NOF Corporation (Japan). The continuation of the research, which is focused on the tailoring of the polarization and crystal orientation of ferroelectric plates, is now going on in the framework of the ARRS projekt: Engineering of structural and microstructural characteristics in contemporary dielectrics and

Funding was approved for the SCOPES project entitled "Intelligent Scaffolds as a Tool for Advanced Tissue Regeneration". The project is funded by the Swiss government, coordinated by a partner from ETH and includes two participants from Slovenia (IJS) and Serbia (TMF). For a period of three years we are going to investigate the formation of innovative bioactive and antibacterial nanomaterials, which will be incorporated within a porous polymeric matrix to form stable scaffolds and will be later on tested for interactions with human stem cells. ferroelectrics with perovskite and perovskite-like crystal structures.

The perovskite structure of piezoelectrics has been extensively studied due to the intrinsic (structural) contribution to enhanced piezoelectric effects. For defined compositions of the piezoelectric solid solutions the morphotropic phase boundaries (MPBs) form, where the electromechanical properties reach the highest values. Our research was based on determining the crystal structure at the MPB in the $(Na_{1,x}K_x)_{0,5}Bi_{0,5}TiO_3$ solid solution system (at x =0.2). From a detailed structural analyses of the MPB material by XRD and *in-situ* TEM it was concluded that the crystal structure in its virgin state is pseudocubic, with no preferential lattice orientations. It actually becomes morphotropic (i.e., with two or more structures coexisting) after the material is subjected to external forces (e.g., grinding, polishing, poling, etc.). Depending on the type of sample treatment the structure of the crystal lattice evolves with a tetragonal symmetry, with a rhombohedral one, or with the

coexistence of both symmetries. A large benefit of such behaviour is that the lattice of the as-prepared material has almost no restrictions with respect to the direction of the lattice deformation upon the application of external fields. Thus, large piezoelectric effects are observed at MPBs.

The work was also directed to the synthesis of cobalt ferrite nanoparticles (CFO). We investigated the effect of oleic acid concentration on the physicochemical properties of solvothermally derived cobalt ferrite nanoparticles (CFO). Without the oleic acid, agglomerated nanoplatelets with a crystallite size of about 19 nm were obtained, according to the X-ray diffraction and transmission electron microscopy. However, the addition of oleic acid decreases the size of the CFO nanoparticles and at critical concentration, which was determined to be 0.25 M, well-dispersed, non-agglomerated spherical particles of about 6 nm were obtained. A further increase in the oleic acid concentration affected the particle size only slightly, with a relatively constant surface coverage of the oleic acid ligand.

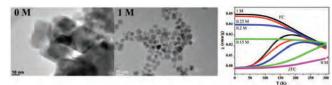


Figure 5: TEM images of CFO nanoparticles synthesized with 0- and 1-M oleic acid concentration. Low-temperature measurements of the particles' susceptibility versus the oleic acid concentration.

The results of our study indicate that particle-size control was achieved by bridging bidentate interactions between the oleic acid molecules and the metal atoms on the surface of the nanoparticles, as determined by Fourier transform infrared spectra. These interactions affected the surface strain of the nanoparticles considerably, but kept the initial cation redistribution according to the Raman spectra. The room-temperature magnetic measurements revealed that oleic acid enables us to effectively control the magnetic behaviour of the CFO, which changes from ferrimagnetic to superparamagnetic at a critical concentration. Interparticle interactions are further

interpreted using low-temperature magnetic measurements, which also showed a decreased surface anisotropy for the samples prepared with an oleic acid concentration above the critical value. An investigation of the treatment

time showed that the capping with oleic acid is already achieved after 1 h of synthesis, but in order to improve the crystallization and consequently achieve the desired magnetic response a synthesis time of at least 4 h is required.

With our research on thin-film synthesis using pulsed-laser deposition (PLD) we focused on the epitaxial integration of strontium titanate (SrTiO₂) with silicon (Si). Epitaxial SrTiO₂ (STO) on Si serves as an excellent template layer and thus enables various functional oxide thin films to be integrated in the epitaxial form with silicon substrates. We started with an investigation of both thermal and strontium-induced deoxidation processes for the elimination of the native SiO₂ from the Si surface. The aim was to prepare a surface, appropriate for the further deposition of the strontium (Sr) buffer layer, which is based on 1/2 ML of Sr coverage. High-temperature annealing (T>1100°C) proved to be the most efficient deoxidation process, since the β-SiC islands that form on the Si surface either during thermal or Sr-assisted deoxidation, can easily be dissociated at such a high temperature. Additionally, we showed the ability to prepare highly-ordered sub-monolayer structures of Sr on a Si surface with the PLD method. Using the reflection high-energy electron diffraction (RHEED) technique we observed characteristic two-domain $(2\times3)+(3\times2)$ pattern at 1/6 ML Sr coverage and $(1\times2)+(2\times1)$ pattern at $\frac{1}{2}$ ML Sr coverage. The $\frac{1}{2}$ ML of Sr on Si acts as an effective passivation layer, which is a prerequisite for the successful epitaxial growth of the STO layer. By means of X-ray photoelectron spectroscopy (XPS) and X-ray reflectivity (XRR) we determined very critical initial parameters for the STO deposition by the method of kinetically controlled sequential deposition (KCSD). Based on the RHEED and X-ray diffraction results (XRD), it is concluded that STO is epitaxially grown on Si with an out-of plane relationship of STO(001) Si(001) and an in-plane relationship of STO[110] Si[100]. Because of the recent commercialization of large-area PLD systems we believe the results of our work are very relevant for implementation of oxide electronics integrated with Si platform and bring

in an alternative manufacturing route. The epitaxial growth of functional oxides on silicon substrates requires atomically defined surfaces, which are most effectively prepared using Srinduced deoxidation. The manipulation of metallic Sr is nevertheless very delicate and requires alternative buffer materials. In our study the applicability of the chemically much more stable SrO in the process of native-oxide removal and silicon-surface stabilization was investigated using the PLD technique, while the as-derived surfaces were analysed in-situ using RHEED and ex-situ using XPS, XRR and atomic force microscopy. After the deposition of the SrO over Si/SiO₂, in a vacuum, different annealing conditions, with the temperature ranging up to 850°C, were applied. Due to the deposition taking place in a vacuum a multilayer composed of SrO, SrSiO₃, modified Si, and Si as a substrate was initially formed. During the subsequent annealing the topmost layer epitaxially orders in the form of islands, while a further increase in the annealing temperature induced rapid desorption and surface

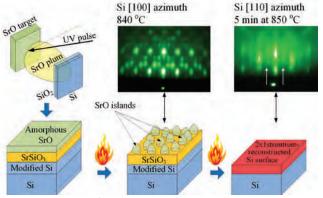


Figure 6: Schematics of SrO-induced surface deoxidation and reconstruction of Si surface using a PLD technique.

deoxidation, leading to a 2×1 Sr-reconstructed silicon surface. The results of the study revealed, for the first time, an effective pathway for the preparation of a SrO-induced buffer layer on a silicon substrate using PLD, which can be subsequently utilized for the epitaxial growth of functional oxides.

The project "Thin-Film-Energy-Storage Devices on the basis of PLZT and Cu-electrodes" with industrial partner EPCOS OHG, Deutschlandsberg, Austria, focuses on the solid-state chemistry of zirconium-rich $Pb_{(1,x)}La_x(Zr_yTi_{(1,y)})$ O₃ (PLZT), as well as the growth of PLZT thin films using pulsed-laser deposition. The purpose of the project is to develop new materials and technologies for advanced energy-storage applications. With the cooperation of the industrial partner Knauf Insulation d.o., the research work on the joint project was focused on mineral fibres and their composites. We have worked on research subjects such as the composition and melting behaviour of raw materials, the influence of the aging process on the morphology and composition of mineral fibres, the specific heat and enthalpy change determination of glass melts, the thermal stability of mineral wools, binders and gypsum boards and the synthesis of new composites materials based on mineral fibres with improved insulation properties.

Some outstanding publications in the past year

- Vukomanović, M., Logar, M., Škapin, S. D., Suvorov, D.: Hydroxyapatite/gold/arginine : designing the structure to create antibacterial activity. *Journal of materials chemistry. B, Materials for biology and medicine*, 2014, vol. 2014, issue 11, 1557-1564, doi: 10.1039/C3TB21612H
- Žunič, V., Vukomanović, M., Škapin, S. D., Suvorov, D., Kovač, J.: Photocatalytic properties of TiO₂ and TiO₂/Pt : a sol-precipitation, sonochemical and hydrothermal approach. *Ultrasonics Sonochemistry*, 2014, vol. 21, issue 1, 367-375, doi: 10.1016/j.ultsonch.2013.05.018

- 3. Jovanović, Z., Spreitzer, M., Kovač, J., Klement, D., Suvorov, D.: Silicon surface deoxidation using strontium oxide deposited with the pulsed laser deposition technique. ACS applied materials & interfaces, ISSN 1944-8244. [Print ed.], 2014, vol. 6, issue 20, str. 18205-18214, doi: 10.1021/am505202p.
- Li, L., Spreitzer, M., Suvorov, D.: Unique dielectric tunability of $Ag(Nb_{(1,v)}Ta_v)O_3(x=0.0.5)$ ceramics with fer-4 rielectric polar order. Applied physics letters, ISSN 0003-6951. [Print ed.], 2014, vol. 104, no. 18, str. 182902-1-182902-5, doi: 10.1063/1.4875581.
- 5. Jovanović, S., Spreitzer, M., Tramšek, M., Trontelj, Z., Suvorov, D.: Effect of oleic acid concentration on the physicochemical properties of cobalt ferrite nanoparticles. The journal of physical chemistry. C, Nanomaterials and interfaces, ISSN 1932-7447, 2014, vol. 118, issue 25, str. 13844-13856, doi: 10.1021/jp500578f.

INTERNATIONAL PROJECTS

- Thin-Film-Energy-Storage Device on the basis of PLZT and Cu-Electrodes 1. Prof. Danilo Suvorov
- EPCOS OHG Technological Characterisation Test of OGK-5 (RGRES) Ashes for Verification of 2 Usability in the Process of Rock Wool Production Prof Danilo Suvorov
- Enel Ingegneria e Ricerca S.p.A 3.
- Microwave Tunable Materials, Composites and Devices Asst. Prof. Boštjan Jančar
- NATO North Atlantic Treaty Organisation 4 Multifunctional Ferroelectric Materials based on Ag(Nb,Ta)O3
- Prof. Danilo Suvorov Slovenian Research Agency
- Biomineralization at the Nanoscale: From the Natural Systems to the Laboratory 5. Asst. Prof. Srečo Davor Škapin Slovenian Research Agency
- 6 3D Composite Plasmonic Metal/Semiconductor Photo-catalyst for Efficient Solar to Fuel Energy Conversion
 - Dr. Manca Logar Slovenian Research Agency

RESEARCH PROGRAM

Contemporary Inorganic Materials and Nanotechnologies Prof. Danilo Suvorov

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BIBLIOGRAPHY

ORIGINAL ARTICLE

- 1. Jihwan An, Takane Usui, Manca Logar, Joonsuk Park, Dickson Thian, Sam Kim, Kihyun Kim, Fritz B. Prinz, "Plasma processing for crystallization and densification of ALD BaTiO₃ thin films", *ACS appl.* mater. interfaces, vol. 6, issue 13, pp. 10656-10660, 2014.
- 2. Ljudmila Benedik, G. Sibbens, Adrian Moens, Roger Eykens, Marijan Nečemer, Srečo D. Škapin, Peter Kump, "Preparation of thick uranium layers on aluminium and stainless steel backings", In: Proceedings of the 19th International Conference on Radionuclide Metrology and its

R & D GRANTS AND CONTRACTS Nanoengineering of Self-assembled Materials

- Prof. Danilo Suvorov
- Engineering of Structural and Microstructural Characteristics in Contemporary 2 Dielectrics and Ferroelectrics with Perovskite and Perovskite-like Crystal Structures Prof. Danilo Suvorov
- Growth of High Quality Piezoelectric Thin Films on Silicon using Pulsed Laser 3 Deposition Dr. Matjaž Spreitzer
- 4 New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics Prof. Danilo Suvorov
- 5 INNOINKS: Novel Inorganic Inks for Hybrid Printed Electronic Demonstrators Prof. Danilo Suvorov
- 6 NAFERBIO: Nanostructured Ferroelectric Films for Biosensor
- Prof. Danilo Suvorov 7. Enabling Technology for High-quality piezoMEMS Dr. Matjaž Spreitzer
- 8 SCOPES; Intelligent Scaffolds as a Tool for Advanced Tissue Regeneration Dr. Marija Vukomanović

NEW CONTRACT

Development and Characterisation of Mineral Wool Fibres Prof. Danilo Suvorov

Postgraduates

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- 13. Urška Gabor, B. Sc.
- 14. Dr. Sonja Jovanović, left 01. 11. 14
- 15. Dejan Klement, B. Sc.
- 16. Mario Kurtjak, B. Sc.
- Tilen Sever, B. Sc. 17 Technical officers
- 18. David Fabijan, B. Sc.
- 19. Damjan Vengust, B. Sc.
- Technical and administrative staff
- 20. Maja Šimaga, M. Sc.
- 21. Silvo Zupančič

Applications, 17-21 June 2013, Antwerp, Appl. radiat. isotopes, vol. 87, pp. 238-241, 2014.

- 3. Mario Bianchetti, Mojca Otoničar, Noemi E. Walsöe de Reca, "Caracterización de nanofilms de ceria dopada con itria o con samaria", In: 30a Congreso Argentino de Química, 22 al 24 de Octubre de 2014, J. Argent. Chem. Soc., vol. 101, no. 1/2, 5 pp., 2014.
- 4. Lili Cai, in Sun Cho Cho, Manca Logar, Apurva Mehta, Jiajun He, Chi Hwan Lee, Pratap Mahesh Rao, Yunzhe Feng, Jennifer Wilcox, Friedrich B. Prinz, Xiaolin Zheng, "Sol-flame synthesis of cobalt-doped TiO₂ nanowires with enhanced electrocatalytic activity for oxygen evolution reaction", PCCP. Phys. chem. chem. phys., vol. 16, issue 24, 16 pp.ustr. 12299-12306, 2014.

- 5. in Sun Cho Cho, Manca Logar, Chi Hwan Lee, Lili Cai, Fritz B. Prinz, Xiaolin Zheng, "Rapid and controllable flame reduction of TiO_2 nanowires for enhanced solar water splitting", *Nano lett.*, vol. 14, issue 1, pp. 24-31, 2014.
- 6. Anup Lal Dadlani, Peter Schindler, Manca Logar, Stephen P. Walch, Friedrich B. Prinz, "Energy states of ligand capped Ag nanoparticles: relating surface plasmon resonance to work function", *The journal of physical chemistry. C, Nanomaterials and interfaces*, vol. 118, issue 43, pp. 24827-24832, 2014.
- Cene Filipič, Asja Veber, Špela Kunej, Adrijan Levstik, "Polarons in Bi_{12.47}Al_{0.53}O_{19.5}", *J. phys. sci. appl.*, vol. 4, no. 7, pp. 430-435, 2014.
- Aleksandra Janošević Ležaić, Igor A. Pašti, Marija Vukomanović, Gordana Ćirić-Marjanović, "Polyaniline tannate - synthesis, characterization and electrochemical assessment of superoxide anion radical scavenging activity", *Electrochim. acta*, vol. 142, pp. 92-100, 2014.
- 9. Sonja Jovanović, Matjaž Spreitzer, Mojca Otoničar, Jae-Ho Jeon, Danilo Suvorov, "pH control of magnetic properties in precipitationhydrothermal-derived CoFe₂O₄", *J. alloys compd.*, vol. 589, pp. 271-277, 2014.
- 10. Sonja Jovanović, Matjaž Spreitzer, Melita Tramšek, Zvonko Trontelj, Danilo Suvorov, "Effect of oleic acid concentration on the physicochemical properties of cobalt ferrite nanoparticles", *The journal of physical chemistry. C, Nanomaterials and interfaces*, vol. 118, issue 25, pp. 13844-13856, 2014.
- 11. Zoran Jovanović, Matjaž Spreitzer, Janez Kovač, Dejan Klement, Danilo Suvorov, "Silicon surface deoxidation using strontium oxide deposited with the pulsed laser deposition technique", *ACS appl. mater. interfaces*, vol. 6, issue 20, pp. 18205-18214, 2014.
- Jozefina Katić, Mirjana Metikoš-Huković, Srečo D. Škapin, Mladen Petravić, M. Varašanec, "The potential-assisted deposition as valuable tool for producing functional apatite coatings on metallic materials", *Electrochim. acta*, vol. 127, pp. 173-179, 2014.
 Dejan Klement, Matjaž Spreitzer, Danilo Suvorov, "Suppressed
- 13. Dejan Klement, Matjaž Spreitzer, Danilo Suvorov, "Suppressed temperature dependence of the resonant frequency of a $AgNb_{0.5}Ta_{0.5}O_3$ composite vs. single-phase ceramics", *J. Eur. Ceram. Soc.*, vol. 34, issue 6, pp. 1537-1545, 2014.
- 14. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, "Influence of the glass-calcium carbonate mixture's characteristics on the foaming process and the properties of the foam glass", *J. Eur. Ceram. Soc.*, vol. 34, no. 6, pp. 1591-1598, 2014.
- 15. Jakob Koenig, Danilo Suvorov, "Uniaxial stress dependence of the permittivity and the hardening effect in the $Na_{0.5}Bi_{0.5}TiO_3 K_{0.5}Bi_{0.5}TiO_3$ system", *Ferroelectrics*, vol. 470, no. 1, pp. 201-211, 2014.
- Mario Kurtjak, Tomaž Urbič, "A simple water model in the presence of inert Lennard-Jones obstacles II: the hydrophobic effect", *Mol. Phys.*, pp. 1-12.
- Mario Kurtjak, Tomaž Urbič, "Water in the presence of inert Lennard-Jones obstacles", *Mol. Phys.*, vol. 112, no. 8, pp. 1132-1148, 2014.
 Lei Li, Matjaž Spreitzer, Danilo Suvorov, "Unique dielectric tunability
- 18. Lei Li, Matjaž Spreitzer, Danilo Suvorov, "Unique dielectric tunability of Ag(Nb_{1-x}Ta_x)O₃ (x=0-0.5) ceramics with ferrielectric polar order", *Appl. phys. lett.*, vol. 104, no. 18, pp. 182902-1-182902-5, 2014.
- Manca Logar, Ines Bračko, Anton Potočnik, Boštjan Jančar, "Cu and CuO/titanate nanobelt based network assemblies for enhanced visible light photocatalysis", *Langmuir*, vol. 30, issue 16, pp. 4852-4862, 2014.
- A. S. Nikolić, M. Bošković, Vojislav Spasojević, Boštjan Jančar, "Magnetite/Mn-ferrite nanocomposite with improved magnetic properties", *Mater. lett.*, vol. 120, pp. 86-89, 2014.
- Rasmus R. Petersen, Jakob Koenig, Morten M. Smedskjaer, Yuanzheng Yue, "Effect of Na₂CO₃ as foaming agent on dynamics and structure of foam glass melts", *J. non-cryst. solids*, vol. 400, pp. 1-5, sep. 2014.
- 22. Rasmus R. Petersen, Jakob Koenig, Morten M. Smedskjaer, Yuanzheng Yue, "Foaming of CRT panel glass powder using Na₂CO₃", *Eur. j. glass sci. technol., A Glass technol.*, vol. 55, no. 1, pp. 1-6, 2014.
- Aleksandra A. Rakić, Marija Vukomanović, Gordana Ćirić-Marjanović, "Formation of nanostructured polyaniline by dopant-free oxidation of aniline in a water/isopropanol mixture", *Chem. zvesti*, vol. 68, issue 3, pp. 372-383, 2014.

- 24. A. N. Suslov, Dmitrii Durilin, Oleg V. Ovchar, Anatolii Belous, Boštjan Jančar, Matjaž Spreitzer, "Synthesis and dielectric and nonlinear properties of BaTi_{1-x}ZrxO₃ ceramic", *Inorg. mater.*, vol. 50, no. 11, pp. 1125-1130, 2014.
- 25. Polona Umek, Carla Bittencourt, Peter Guttmann, Alexandre Gloter, Srečo D. Škapin, Denis Arčon, "Mn²⁺ substitutional doping of TiO₂ nanoribbon: a three-step approach", *The journal of physical chemistry. C, Nanomaterials and interfaces*, vol. 118, no. 36, pp. 21250-21257, 2014.
- 26. Ljiljana Veselinović, Miodrag Mitrić, Lidija T. Mančić, Marija Vukomanović, Branka Hadžić, Smilja Marković, Dragan Uskoković, "The effect of Sn for Ti substitution on the average and local crystal structure of $BaTi_{1-x}Sn_xO_3(0 \le x \le 0.20)$ ", *J. Appl. Crystallogr.*, vol. 47, no. 3, pp. 999-1007, 2014.
- M. M. Vopson, E. Zemaityte, Matjaž Spreitzer, E. Namvar, "Multiferroic composites for magnetic data storage beyond the super-paramagnetic limit", *J. appl. phys.*, vol. 116, no. 11, pp. 113910-1-113910-5, 2014.
- A. Vorobiev, Matjaž Spreitzer, Asja Veber, Danilo Suvorov, Spartak Gevorgian, "Intrinsically tunable bulk acoustic wave resonators based on sol-gel grown PMN-PT films", *J. appl. phys.*, vol. 116, no. 6, pp. 064101-1-064101-8, 2014.
- 29. Marija Vukomanović, Manca Logar, Srečo D. Škapin, Danilo Suvorov, "Hydroxyapatite/gold/arginine: designing the structure to create antibacterial activity", *J. mater. chem. B*, vol. 2014, issue 11, pp. 1557-1564, 2014.
- 30. Vojka Žunič, Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, Janez Kovač, "Photocatalytic properties of TiO_2 and TiO_2/Pt : a solprecipitation, sonochemical and hydrothermal approach", *Ultrason. sonochem.*, vol. 21, issue 1, pp. 367-375, 2014.

PUBLISHED CONFERENCE CONTRIBUTION

1. A. Suslov, Dmitrii Durilin, Oleg V. Ovchar, Anatolii Belous, Viktor Bovtun, Martin Kempa, Boštjan Jančar, Matjaž Spreitzer, "Synthesis and dielectric properties of BaTi_{1-x}Zr_xO₃ -based ceramic and film materials", In: *ELNANO 2014*, 34th International Conference on Electronics and Nanotechnology, 15 April - 18 April 2014, Kyiv, Ukraine, Kyiv, National Technical University of Ukraine Kyiv Polytechnic Institute Polytekhnichna, 2014, pp. 66-69.

PATENT APPLICATION

- 1. Boštjan Jančar, Damjan Vengust, Danilo Suvorov, *Thermoelectric ceramic materials and generators made thereof*, EP14177502.3, European Patent Attorneys, 2014.
- 2. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, *A method to produce foam glasses*, 53861DK01, Danish Patent and Trademark Office, 7.7.2014.

MENTORING

- 1. Sonja Jovanović, Synthesis of cobalt ferrite nanoparticles and their embedding into magnetoelectric composite film via block co-polymer self-assembly: doctoral dissertation, Ljubljana, 2014 (mentor Danilo Suvorov; co-mentor Matjaž Spreitzer).
- 2. Mojca Otoničar, *Intragranular nanostructure of the (Na1-xKx)o.5 Bio.5 TiO3 perovskite solid solutions:* doctoral dissertation, Ljubljana, 2014 (mentor Srečo D. Škapin; co-mentor Boštjan Jančar).
- Vojka Žunič, Synthesis and characterization of TiO₂ nano-powders and TiO₂/Pt nano-composites for photocatalytic applications: doctoral dissertation, Ljubljana, 2014 (mentor Danilo Suvorov; co-mentor Srečo D. Škapin).
- 4. Vladimira Petrovič, *High temperature application of nano TiO₂ on the ceramic substrate and determination of the photocatalytic efficiency:* master's thesis, Ljubljana, 2014 (mentor Srečo D. Škapin; co-mentor Vilma Ducman).