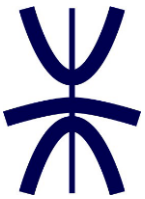
Bulgarian Academy of Sciences

GEORGI NADJAKOV INSTITUTE
OF SOLID STATE PHYSICS



SOFIA, BULGARIA

B O O K O F A B S T R A C T S

22nd INTERNATIONAL SCHOOL ON CONDENSED MATTER PHYSICS

State of the Art in Functional Materials & Technologies

August 29th - September 2nd, 2022
Varna, Bulgaria

Dedicated to 50th anniversary of
Georgi Nadjakov Institute of Solid State Physics
Bulgarian Academy of Sciences

Supported by:

Organising Committee

Chairman

Prof. Hassan Chamati, Director
Georgi Nadjakov Institute of Solid State Physics,
Bulgarian Academy of Sciences,
Sofia, Bulgaria

Local Organising Committee

Julia Genova (scientific secretary), Radka Gegova-Dzhurkova, Miroslav Georgiev, T. Hristova-Vasileva, Poornima Santhosh, Albert Varonov

International Programme Committee

Francis Balestra (INP-Minatec, Grenoble, France)
Sarbajit Banerjee (Texas A&M University, Texas, USA)
Oleg Batishchev (A. N. Frumkin IPCE RAS, Moscow, Russia)
Irina Bineva (ISSP-BAS, Sofia, Bulgaria)
Vladan Celebonovic (Institute of Physics, Belgrade, Serbia)
Hassan Chamati (ISSP-BAS, Sofia, Bulgaria)
Doriana Dimova-Malinovska (CLSENES-BAS, Sofia)
Julia Genova (ISSP-BAS, Sofia, Bulgaria)
Aleš Iglič (University of Ljubljana, Slovenia)
Samo Kralj (University of Maribor, Slovenia)
Paul Montgomery (Unistra-CNRS, Strasbourg, France)
Ekaterina Iordanova (ISSP-BAS, Sofia, Bulgaria)
Albena Paskaleva (ISSP-BAS, Sofia, Bulgaria)
Peter Petrik (MFA, EK Centre for Energy Research, Budapest, Hungary)
Bruno Rizzuti (University of Calabria, Italy)
Philippe Vanderbemden (Institut Montefiore, Liège, Belgium)

Local Scientific Council

Bulgarian Academy of Sciences:
J. Revalski (President of BAS), S. Dimitrova (Scientific Secretary of BAS)
Georgi Nadjakov Institute of Solid State Physics:
H. Chamati, J. Genova, E. Iordanova, A. Paskaleva
Central Laboratory of Solar Energy and New Energy Sources:
D. Dimova-Malinovska
Sofia University, Faculty of Physics:
V. Donchev (Head of Department)
Plovdiv University Paisii Hilendarski,
Faculty of Physics and Engineering Technologies: T. Yovcheva (Vice Rector)

TABLE OF CONTENTS

BULGARIAN ACADEMY OF SCIENCES
GEORGI NADJAKOV INSTITUTE OF SOLID STATE PHYSICS
22nd INTERNATIONAL SCHOOL ON CONDENSED MATTER PHYSICS
"State of the Art in Functional Materials & Technologies"
August 29th - September 2nd, 2022 – Varna, Bulgaria

P R O G R A M

August 28th (Sunday)

16:00-18:00	Registration
20:00	**Get Together Party**

August 29th (Monday)

09:10-09:30	Opening Ceremony
09:30-11:00	**Chair: H. Chamati**
09:30-10:15	I. MIHAILESCU, "Direct Energy Deposition of Functional Materials via Laser Additive Manufacturing: Process Modeling versus Experimental Verification" *Georgi Nadjakov Memorial Lecture*
10:15-11:00	S. REYNOLDS, "Carrier Transport and Dielectric Properties of Methylammonium Lead Halide Perovskite Single Crystals" *Milko Borisov Memorial Lecture*
11:00-11:30	Coffee break / Collective photo
11:30-12:30	**Chair: E. Iordanova**
11:30-12:10	I. BINEVA, "AFM and XRD - the Powerful Combination for Nanostructured Thin Films Characterization"
12:10-12:30	K. BUCHKOV, "Magneto-optical and multiferroic properties of transition-metal (Fe, Co or Ni)-doped ZnO layers deposited by ALD"
12:30-16:00	Lunch break
16:00-18:00	**Chair: A. Iglič**
16:00-16:40	S. KRALJ, "Domain-like Structures in Physical Fields"
16:40:17:00	D. GEORGIEVA, "An electrochemical impedance spectroscopy study of the influence of miltefosine on lung cancer cells and endothelial cells"
17:00-17:40	D. SOARES, "*ACS Omega:* A high-quality, open access, broad scope journal from the American Chemical Society"
17:40-18:20	Five minutes' presentations of posters of young participants

August 30th (Tuesday)

09:10-10:30	**Chair: S. Kralj**
09:10-09:50	N. POKLAR ULRIH, "Archaeolipids and their potential use as a coating material"
09:50-10:30	P. SANTHOSH, "Archaeosomes: Next-generation liposomes based on archaeal lipids for drug delivery and biomedical applications"

10:30-11:00	Coffee break
11:00-12:20	**Chair: N. Poklar Ulrih**
11:00-11:40	E. IORDANOVA, "The future is vast: Regenerative medicine perspectives and technology trends in advanced implantable biomaterial strategies"
11:40-12:20	A. IGLIČ, "Hydrothermally synthesized TiO_2 nanostructures"
12:20-16:00	Lunch break
16:00-17:40	**Chair: N. Nedyalkov**
16:00-16:40	F. BALESTRA, "Challenges and solutions for high performance green nanoelectronics devices and materials"
16:40-17:20	A. VASEASHTA, "Hierarchical integration of electrospinning and 3D/4D printing process for prototyping of smart structures"
17:20-17:40	K. LOVCHINOV, "Investigations of zirconium oxide layers obtained by electrochemical process at different temperatures"
17:40-19:00	**First poster session**

August 31st (Wednesday)

09:10-10:30	**Chair: I. Bineva**
09:10-09:50	P. MONTGOMERY, "Characterization of functional materials using coherence scanning interferometry and environmental chambers"
09:50-10:30	P. PETRIK, "Nanomaterials at interfaces for optical sensing"
10:30-11:00	Coffee break
11:00-12:20	**Chair: S. Baranovskii**
11:00-11:40	Ph.VANDERBEMDEN, "Joule resistive heating of a shape memory composite: some design rules to predict the temperature in samples with rectangular cross-section"
11:40-12:20	T. KOUTZAROVA, "Phase transitions in magneto-electric hexaferrites"
12:20-16:00	Lunch break
16:00-17:40	**Chair: Ph. Vanderbemden**
16:00-16:40	S. BARANOVSKII, "Effects of alloy disorder in organic and inorganic semiconductors"
16:40-17:00	N. IVANOV, "Mixed-spin kagome strips"
17:00-17:20	N. IVANOVA, "Physical properties of SOPC at low temperatures through the Slipid force field"
17:20-17:40	E. ANGELOVA, "Dynamic simulation of the quasiparticle excitations spectra"
17:40-19:00	**Second poster session**

September 1st (Thursday)

09:10-10:30	**Chair: E. Guziewicz**
09:10-09:50	D. MALKA, "Controlling high speed mach zehnder modulator quadrature bias point using Si PIN diode phase-Shifter"

09:50-10:30 T. HRISTOVA-VASILEVA, "Silver and gold containing compounds of p-block elements as perspective materials for plasmonics"

10:30-11:00 Coffee break

11:00-12:20 **Chair: A. Paskaleva**
11:00-11:40 E. GUZIEWICZ, "Acceptor doping of zinc oxide – defect complexes in nanoscale"
11:40-12:20 S. BANERJEE, "Designing electrode architectures across length scales: Some lessons learned from Li-ion and "Beyond Li" Chemistries"

12:20-16:00 Lunch break

16:00-17:20 **Chair: S. Banerjee**
16:00-16:40 M. FABIAN, "Investigation of the surface reactivity of a carbon steel container exposed to different types of environments and conditions"
16:40-17:20 M. GEORGIEV, "Single-molecule magnets: The huge zero-field splitting revisited"

17:20-17:40 Coffee break

17:40-18:20 **Chair: M. Fabian**
17:40-18:00 I. TOLNAI, "Stabilization and characterization of simulated liquid radioactive waste in a new type of cement mixture"
18:00-18:20 M. SHEHADI, "Measurement of nonlinear optical characteristics of GaN using femtosecond z-scan technique"

20:00 **Farewell Dinner**

September 2nd (Friday)

09:10-10:30 **Chair: N. Ivanov**
09:10-09:50 Z. DANEL, "Star polymer chains in confined geometries: theory and simulations"
09:50-10:30 V. ČELEBONOVIČ, "The Hubbard model and optics of 2D materials"

10:30-11:00 Coffee break

11:00-12:00 **Chair: H. Chamati**
11:00-11:20 G. YANKOV, "Ablation damage and threshold in transparent media - case study at ns, ps and fs laser pulses"
11:20-11:40 H. KODURU, "Optical properties of multi-layers structured PEO/PVP solid polymer membranes doped with sodium perchlorate"
11:40-12:00 A. REZNIK, "Lead Oxide X-ray photoconductive layers for application in direct conversion medical imaging detectors"

12:00 **Closing Ceremony**

POSTER PRESENTATIONS

1. FIRST POSTER SESSION, August 30th (Tuesday)

1.1. G. Exner, Y. Marinov, B. Veerabhadraswamy, C. Yelamaggad, P. Rafailov, V. Georgieva, "Effect of the nanofiller concentration on its dispersion in a system of liquid crystalline SB(3R)-11 and single wall carbon nanotubes"

1.2. J. Halun, Z. Danel, "Investigation of ideal star polymers in confined geometries"

1.3. Y. Marinov, H. Koduru, G. Exner, N. Scaramuzza, "PEO/Starch-nanocrystals based Solid Polymer Electrolyte Membranes for Magnesium – Ion Conducting Applications"

1.4. Y. Marinov, T. Vlakhov, G. Hadjichristov, "Volatile organic compound vapor sensing with nano-thin Langmuir-Blodgett phospholipide monolayer"

1.5. M. Marudova, S. Milenkova, N. Zahariev, B. Pilicheva, "Formulation and characterization of Benzydamine loaded casein/chitosan nanocomplexes"

1.6. P. Kuterba, Z. Danel, W. Janke, H. Christiansen, "Numerical calculations of the monomer density profiles of real ring polymer chains in a slit geometry of two parallel walls with mixed b.c."

1.7. A. Grigorov, A. Viraneva, M. Marudova, T. Yovcheva, "Benzydamine hydrochloride immobilization in multilayer structures based on lyophilized polylactic acid and poly(ε-caprolactone)"

1.8. B. Katranchev, M. Petrov, H. Naradikian, P. Rafailov, "Graphene oxide induced sub-structures of bi-tilted smectic CG in dimer liquid crystals"

1.9. D. Christova, M. Staneva, S. Ivanova, M. Alexandrova, P. Ublekov, M. Dencheva-Zarkova, J. Genova, I. Tsibranska, B. Tylkowski, "Surface Modification of Polyethersulfon Nanofiltration Membrane for Improving Water-Ethanol Separation"

1.10. E. Pisanova, "On the Critical Specific Heat Capacity of a Model of Structural Phase Transitions with Long-range Interaction"

1.11. G. Hadjichristov, Y. Marinov, T. Vlakhov, "Thin films of nanocomposites from glassy-state tris(keto-hydrozone) discotic liquid crystals and single-walled carbon nanotubes, for optoelectronics"

1.12. G. R. Ivanov, T. Vlakhov, E. Bogdanova, G. Hadjichristov, Y. Marinov, "Gas Sensing of Volatile Organic Compounds by Arachidic Acid Langmuir-Blodgett Sensing Layers and Electrical Impedance Spectroscopy"

1.13. G. Mihova, A. Andreeva, N. Zografov, "Comparative Study of Protective Coating Properties of CR-39 Based Ophthalmic Lenses"

1.14. B. Gechev, G. Zsivanovits, A. Iliev, M. Marudova, "Chitosan/grapeseed oil multicomponent edible films – design and properties"

1.15. M. Dencheva-Zarkova, J. Genova, I. Tsibranska, "Effect of pressure and cross-flow velocity on membrane behavior in red wine nanofiltration"

1.16. M. Lazarova, M. Dencheva-Zarkova, D. Yankov, J. Genova, "Effect of Driving Pressure and Flux Rate on Red Wine Nanofiltration"

1.17. R. Kamburova, M. Danev, M. Primatarowa, "Soliton dynamics in two ferromagnetic chains coupled through interactions between opposite and diagonal spins"

1.18. M. Milanova, S. Georgiev, V. Donchev, "Doping of dilute nitride compounds grown by liquid phase epitaxy"

1.19. S. Milenkova, M. Marudova, N. Zahariev, B. Pilicheva, "Chitosan-based particles by emulsion crosslinking"

1.20. S. Minkovska, G. Hadjichristov, A. Neacsu, V. Chihaia, Y. Fedorov, "Photoswitchable photochromic fluorescent spirooxazine derivative for metal ions sensing: Photopysical properties and quantum-chemical calculations"

1.21. T. Vlakhov, G. Hadjichristov, Y. Marinov, "Dielectric spectroscopy study of composite PEO/E8 (polymer/ liquid crystals) soft-matter thin films for flexible electronics"

1.22. Y. Dimitrova, M. Tsvetkov, D. Elenkova, "Metal-Organic Frameworks with Lanthanoid Ions and Trimesic Acid, as Sensors for Water Pollutants"

1.23. P. Karakashkova, A. Eliyas, S. Minkovska, "Photodegradation of adipic acid in aqueous solution by Au and Pd doped TiO_2 nanocomposite catalysts under UV irradiation"

1.24. K. Esmeryan, S. Vargas, S. Gyoshev, C. Castano, "Impact dynamics of water droplets on pre-frosted superhydrophobic carbon soot coatings"

1.25. R. Gergova, K. Lovchinov, G. Alexieva, "Investigation of Al-doped ZnO thin films prepared by electrochemical deposition method for gas-sensing applications"

1.26. P. Kolev, G. Dyankov, T. Eftimov, "Spectral polarimetry applied for magnetic field detection"

1.27. M. Petrov, T. Stankulov, B. Karamanova, A. Stoyanova, K. Lovchinov, "Study of the properties of supercapacitors derived from soot treated with perchlorethylene"

1.28. S. Santalla, E. Korutcheva, K. Koroutchev, H. Chamati, J. Rodríguez-Laguna, "The restricted Boltzmann machine ansatz for quantum spin-glass system"

1.29. E. Stoyanova, P. Levicharov, K. Antonova, I. Miloushev, T. Tenev, "Design and Elaboration of Various Multilayer Beamsplitters"

1.30. H. Solunov, "On the relation of the potential energy landscape and the cooperatively rearranging region"

2. SECOND POSTER SESSION, August 31st (Wednesday)

2.1. Sv. Baranovskii, "Light-Induced Nucleation and Optical Absorption in Metallic Vapors"

2.2. D. Spassov, A. Paskaleva, B. Blagoev, V. Mehandzhiev, "Electric characterization of transition metal (Co, Ni, Fe) doped ZnO thin layers prepared by atomic layer deposition"

2.3. V. Donchev, S. Georgiev, A. Bojar, D. Regaldo, M. da Lisca, J. Alvarez, J.-P. Kleider, "Surface photovoltage study of metal halide perovskites deposited directly on crystalline silicon"

2.4. B. Georgieva, K. Lovchinov, L. Slavov, G. Alexieva, Ch. Angelov, "Characterization and gas sensing properties of ZnO and ZrO_2 layers electrochemically-synthesized on quartz resonators"

2.5. D. Ivanova, N. Kaneva, "Improvement of the photocatalytic properties of ZnO thin films by co-catalytic modifying for the degradation of Paracetamol"

2.6. G. Alexieva, N. Tyutyundzhiev, R. Gergova, M. Petrov, K. Lovchinov, "Impact of the deposition temperature on morphological and gas sensing properties of electrochemically grown ZrO_2 layers"

2.7. L. Slavov, K. Lovchinov, B. Georgieva, G. Alexieva, P. Ivanov, "Influence of the substrate on the structural and optical properties of ZrO_2 layers deposited by electrochemical process"

2.8. P. Ivanov, K. Lovchinov, R. Gergova, G. Marinov, P. Petrova, B. Greorgieva, "Study of spectrofluorometric sensitivity and structural properties of electrochemical ZrO_2 layers"

2.9. P. Petrova, K. Lovchinov, G. Alexieva, R. Georgiev, R. Ivanova, V. Strijkova, "Structural and gas sensing properties of nanostructured ZrO_2 layers deposited electrochemically at different times"

2.10. S. Stankova, H. Dikov, E. Radeva, M. Ganchev, "Preparation and characterization of RF sputtered ZnO layers for application in thin films solar cells"

2.11. R. Gegova-Dzhurkova, D. Nesheva, I. Stambolova, K. Zaharieva, P. Terziyska, I. Miloushev, V. Dzhurkov, "Optical and photocatalytic properties of ZnO thin films prepared by modified sol-gel method"

2.12. V. Dzhurkov, Z. Levi, D. Nesheva, T. Hristova-Vasileva, P. Terzyiska, I. Miloushev, T. Tenev, "Investigation of porous ZnSe thin films prepared by thermal evaporation"

2.13. A. Atanasova, V. Katrova, R. Todorov, T. Hristova-Vasileva, G. Milushev, "Surface plasmon-like properties of one dimensional photonic crystal and its application in surface-enhanced luminescence"

2.14. R. Todorov, V. Katrova, T. Hristova-Vasileva, A. Atanasova, G. Milushev, "Structural and optical characterization of thin films from Bimetallic Au-Sb system as tunable plasmonic material for UV spectral range"

2.15. V. Katrova, A. Atanasova, R. Todorov, T. Hristova-Vasileva, V. Strijkova, "Thickness dependence of the optical properties of thin Ag-Bi films and their surface plasmon-enhanced photoluminescence capability"

2.16. Y. Karmakov, A. Paskaleva, D. Spassov, "Interfaces in very thin ALD Al_2O_3/HfO_2 stacks studied by ellipsometry"

2.17. E. Kotlikov, N. Lavrovskaya, I. Miloushev, T. Tenev, "Investigation of optical constants of Al_2O_3 films in the spectral range 0.2 - 0.8 microns"

2.18. D. Spassov, A. Paskaleva, E. Guziewicz, T. Stanchev, Tz. Ivanov, "Charge trapping effects in nonvolatile memory cells with HfO2/Al2O3 nanolaminated trapping layer"

2.19. D. Spassov, A. Paskaleva, E. Guziewicz, Tz. Ivanov, T. Stanchev, "Electric breakdown characteristics of ALD HfO_2/Al_2O_3-based memory capacitors"

2.20. M. Beshkova, B. Blagoev, V. Mehandzhiev, R. Yakimova, I. Avramova, P. Terziyska, V. Strijkova, "AlN films grown by plasma enhanced atomic layer deposition"

2.21. N. Nedyalkov, Rosen Nikov, Rumen Nikov, L. Aleksandrov, M. Milanova, A. Yordanova, R. Iordanova, "Effect of Ag on the glass formation ability and luminescence properties of Eu^{3+} doped $ZnO-B_2O_3-WO_3-Nb_2O_5$ glasses"

2.22. I. Avramova, I. Mihailova, R. Harizanova, G. Avdeev, "X-ray photoelectron spectroscopy investigation on thermally treated iron-rich oxide glasses"

2.23. I. Mihailova, R. Harizanova, N. Shtapleva, T. Tasheva, "Physicochemical and structural characterization of silicate glasses and glass-ceramics containing iron oxides"

2.24. R. Harizanova, M. Pernikov, I. Mihailova, D. Tatchev, G. Avdeev, I. Avramova, C. Rüssel, "Phase composition and microstructure characterization of strontium-modified barium titanate glass-ceramics"

2.25. Ch. Ghelev, B. Georgieva, S. Kolev, P. Peneva, K. Krezhov, D. Kovacheva, B. Vertruyen, R. Closset, L. M. Tran, M. Babij, A. Zaleski, T. Koutzarova, "Influence of Al-substitution on the Structure and Magnetic Properties of $BaFe_{12}O_{19}$ Obtained by Modified Co-precipitation Methods"

2.26. B. Blagoev, V. Mehandzhiev, P. Terziyska, I. Avramova, P. Tzvetkov, D. Kovacheva, A. Paskaleva, "Growth of Fe Oxide Nanofilms by Atomic Layer Deposition"

2.27. Ch. Angelov, N. Tyutyundzhiev, T. Arsov, H. Nitchev, K. Lovchinov, "Variation of UV-A/UV-B daily profiles depending on location and altitude"

2.28. Ch. Angelov, N. Tyutyundzhiev, T. Arsov, K. Lovchinov, A. Mitafov, "Remote datalogging of solar UV irradiation using open-source ESP32 platform and MQTT protocol"

2.29. S. Karatodorov, M. Shehadi, L. Stoychev, D. Tsankov, B. Shivachev, T. Petrov, "Laser-Induced Periodic Surface Structuring of Wide Bandgap Transparent Materials"

ABSTRACTS OF INVITED LECTURES

GEORGI NADJAKOV MEMORIAL LECTURE

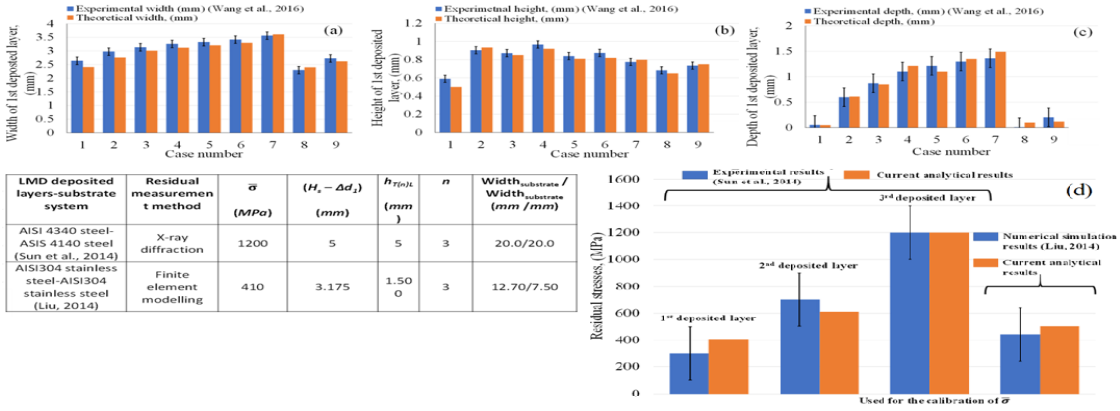
Direct Energy Deposition of Functional Materials via Laser Additive Manufacturing: Process Modeling versus Experimental Verification

Ion N. Mihăilescu[1], Muhammad Arif Mahmood[2], Carmen Ristoscu[1], Mihai Oane[1], Sinziana Anghel[1,3], Andrei Popescu[1], Diana Chioibașu[1], Cristian Mihailescu[1,*]

[1] Laser Department, National Institute for Laser, Plasma and Radiation Physics (INFLPR), Ilfov-Magurele, 077125, Romania
[2] Mechanical Engineering Program, Texas A &M University at Qatar, P.O. Box 23874, Doha, Qatar
[3] Faculty of Physics, University of Bucharest, Magurele, Ilfov, RO-077125 Muntenia, Romania

* cristi.mihailescu@inflpr.ro@inflpr.ro

Direct energy deposition (DED) is a fast-emerging technology for manufacturing near-net-shaped parts. The printed layers' characteristics and induced residual and thermal stresses determine the parts' quality and mechanical-physical properties [1]. Three user-defined analytical models are reviewed. Initially, the printed layer's geometrical characteristics of the 1st layer are estimated based on the parameters involved in the DED process, which was transformed into multiple layers via a hatch distance that controls the re-melting depth. The model's output described above was next linked with the 2nd model to estimate the residual stresses within the substrate and deposited layers. An experimental [2] verification is presented in the case of AISI 316L powder on AISI 321 substrate, which resulted in a solution with an accuracy of 10-15 % mean absolute deviation (Fig. 1).



LMD deposited layers-substrate system	Residual measurement method	$\bar{\sigma}$ (MPa)	$(H_s - \Delta d_s)$ (mm)	$h_{T(n)L}$ (mm)	n	$Width_{substrate}$ / $Width_{substrate}$ (mm /mm)
AISI 4340 steel-ASIS 4140 steel (Sun et al., 2014)	X-ray diffraction	1200	5	5	3	20.0/20.0
AISI304 stainless steel-AISI304 stainless steel (Liu, 2014)	Finite element modelling	410	3.175	1.500	3	12.70/7.50

Figure 1. Experimental vs. simulation: for 1st deposited clad geometry **(a)** width, **(b)** height, **(c)** depth in the case of DED of AISI 316L powder on AISI 321 substrate [3], and **(d)** residual stress analyses [4,5].

With the 3rd model, the thermal history predicted, when the laser moves along with the simultaneous addition of powder, has been described with the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model to estimate the average grain size across the printed layer. According to the Hall Patch relationship, the mechanical properties, including ultimate tensile strength, yield strength, and hardness, can be estimated using the average grain size. The developed method was validated for single depositions of AISI 304 powder on a steel substrate in the DED process. The average grain size was quantified using SEM images and the "Image-J" software. The mechanical properties predicted by the simulation model were cross-verified with Vickers hardness tests, which resulted in a strong correlation between experiments and computations, within the range of 10-15 % (grain size estimation), and 8-10 % (medical properties calculation) [6].

The defined models could assist experimentalists in quantifying and controlling the DED process for the future large-scale, scientifical and industrial applications.

References:

1. Laser Coatings via State-of-the-Art Additive Manufacturing: A Review. Coatings. 11(3):296 (2021).
2. Estimation of clad geometry and corresponding residual stress distribution in laser melting deposition: analytical modeling and experimental correlations. Int J Adv Manuf Technol 111, 77–91 (2020).
3. Effects of mass energy and line mass on characteristics of the direct laser fabrication parts, Rapid prototying, vol. 24, pp. 270-275 (2016)
4. Evaluation of defect density, microstructure, residual stress, elastic modulus, hardness and strength of laser-deposited AISI 4340 steel, Acta materialia, vol. 84, pp. 172–89 (2015).
5. Numerical analysis of thermal stress and deformation in multi-layer laser metal deposition process. Masters Theses 2014.
6. Grain refinement and mechanical properties for AISI304 stainless steel single-tracks by laser melting deposition: Mathematical modelling versus experimental results, Results in Physics, 22, 103880, (2021).

Carrier Transport and Dielectric Properties of Methylammonium Lead Halide Perovskite Single Crystals

Steve Reynolds*

University of Dundee, School of Science and Engineering, Dundee DD1 4HN, UK.

* s.z.reynolds@dundee.ac.uk

Organic-inorganic lead halide perovskites such as methylammonium lead iodide (MAPI) have attracted much attention over the past decade as efficient solar cell absorber layers, both individually (approaching 25%) [1] and in combination with crystalline silicon in tandem cells (approaching 30%) [2]. Perovskite formulations possess several key properties including large optical absorption coefficients across a wide spectral range, long carrier diffusion lengths, good ambipolar carrier transport properties and, despite quite basic preparation and deposition processes, remarkably low densities of carrier traps [3].

Following a brief review of the present status of this technology, we will discuss some of the methods that have been used to assess the density of trap states in MAPI and related materials, particularly steady-state conductivity, transient and modulated photocurrent density of states (DOS) spectroscopy [4] and space-charge limited currents (SCLC) [5]. SCLC is a long-standing technique for the estimation of defect densities in semiconductors. With reference to measurements on single-crystals, we demonstrate that the complex impedance of MAPI is strongly frequency-dependent and that I-V characteristics are sweep-rate dependent, which makes defect interpretation more challenging. Given the strongly ionic nature of MAPI, we suggest that SCLC measurements require careful interpretation. Photo-dependence of dielectric properties [6] and hysteresis effects [7] may also affect the credibility of DOS spectroscopies.

References:

1. H. Min, D.Y. Lee, J. Kim et al., *Nature* **598**, 444 (2021).
2. A. Al-Ashouri, E. Köhnen, Bor Li et al, *Science* **370,** 1300 (2020).
3. K.X. Steirer, P. Schulz, G. Teeter et al, *ACS Energy Lett.* **1**, 360 (2016).
4. S. Reynolds, M. Brinza, M.L. Benkhedir, G.J. Adriaenssens (2017). Photoconductivity in Materials Research. In: S. Kasap, P. Capper (eds) *Springer Handbook of Electronic and Photonic Materials*. Springer Handbooks. Springer, Cham.
5. M. Saidaminov, A. Abdelhady, B. Murali et al, *Nat Commun* **6**, 7586 (2015).
6. E.J. Juarez-Perez, R.S. Sanchez, L. Badia et al, *J. Phys. Chem. Lett.* **5**, 2390 (2014).
7. M. Berruet, J.C. Pérez-Martínez, B. Romero et al, *ACS Energy Lett.* **7** 1214 (2022).

AFM and XRD - the powerful combination for nanostructured thin films characterization

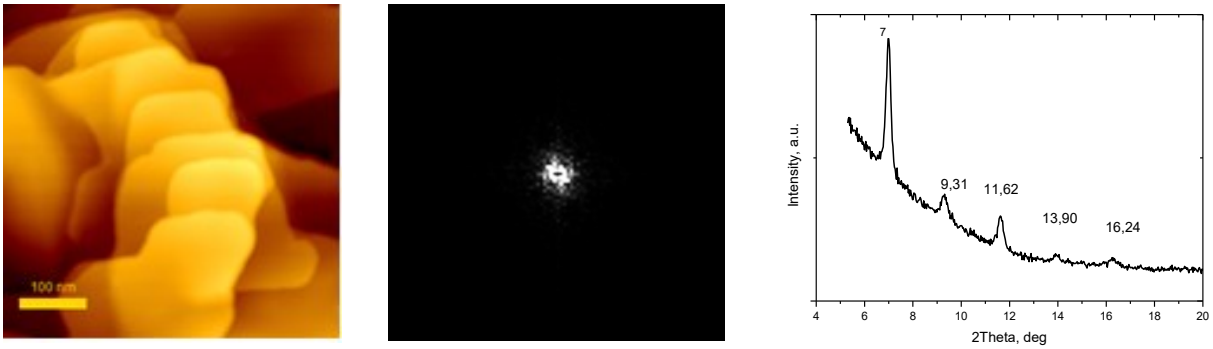
Irina Bineva*

Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

* irka@issp.bas.bg

Atomic Force Microscopy (AFM) is one of the most powerful tools for the characterization of surfaces at the nanoscale, offering possibilities for the investigation of the surface texture, roughness, nanoparticles and voids size and distribution. The insight provided by X-ray Diffraction techniques(XRD) into both the underlying crystal structure and the local environments of surface atoms is critical for the understanding of nanostructured thin films. Both techniques very often go together for the characterization of thin films and nanostructured surfaces. While usually they complement each other some discrepancies are possible when interpreting the results. The most common artefacts and mistakes mainly due to the post-processing and some typical examples for the investigation of the nanocrystalline thin films are regarded – the proper size determination, phase analysis, surface roughness, dislocations and superstructures.

The potential of AFM to provide useful information on fractals and superstructures that may coexist in the nanostructured thin films is shown by means of the fractal dimension and 2D fast Fourier transform (2DFTT) analysis.



AFM Height and 2DFTT image and GIRXD spectra of self-organized layered structure of $Zn_xCd_{1-x}Se$

Domain-like structures in physical fields

Juš Polanšek[1], Arbresha Hölbl[1], Samo Kralj[1,2,*]

[1] Faculty of Natural Sciences and Mathematics, University of Maribor, Koroška cesta 160, 2000 Maribor, Slovenia

[2] Solid State Department, Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia

* samo.kralj@um.si

We consider history-dependent behavior in domain-type configurations in physical fields exhibiting orientational order that are formed in configurations reached via continuous symmetry-breaking phase transitions. In equilibrium, these systems exhibit in absence of impurities a spatially homogeneous order. We focus on cases where domains are formed via (i) Kibble-Zurek mechanism [1] in fast enough quenches or by (ii) Kibble mechanism [2] in strongly supercooled phases. These mechanisms were originally introduced to model coarsening dynamics of the Higgs field in the early universe. In both cases, domains could be arrested due to pinned topological defects (TDs) that are formed at domain walls. TDs refer to localized field distortions that are topologically protected. Note, that TDs in a relevant physical field might correspond to "fundamental particles" if fields represent fundamental natural entities. In systems exhibiting polar or quadrupolar order point and line defects (disclinations) dominate, respectively. In particular, the disclinations could form complex entangled structures and are more efficient in stabilizing domains. Domain patterns formed by fast quenches could be arrested by impurities imposing a strong enough random-field type disorder, as suggested by the universal Imry-Ma theorem [3]. On the other hand, domains formed in supercooled systems could be also formed if large enough energy barriers arresting domains are established due to large enough systems' stiffness. The resulting effective interactions in established domain-type patterns could be described by random matrices. The resulting eigenvectors reveal expected structural excitations formed in such structures. The most important role is commonly played by the random matrix largest eigenvector. Qualitatively different behavior is expected if this eigenvector exhibits a localized or extended character. In the former case, one expects a gradual, non-critical-type transition into a glass-type structure. However, in the latter case, a critical-like phase behavior could be observed.

References:

1. W. H. Zurek, Cosmological experiments in superfluid helium? Nature 317, 1985, 505-508.
2. T. W. B. Kibble, Topology of cosmic domains and strings, J. Phys. A: Math. Gen. 9, 1976, 1387-1389.
3. Y. Imry, S. Ma, Random-field instability of the ordered state of continuous symmetry, Phys. Rev. Lett 35, 1975, 1399-1401.

Archaeolipids and their potential use as a coating material

Nataša Poklar Ulrih*

Biotechnical Faculty, University of Ljubljana, Jamnikarjeva 101, 1000 Ljubljana, Slovenia

* natasa.poklar@bf.uni-lj.si

Archaeosomes are liposomes prepared from archaeal lipids. They are characterized by remarkable thermostability, resistant to enzymatic degradation, stable over extended periods of time, and possess immunomodulatory properties.

The isolated core lipids of *Aeropyrum pernix* K1 consist exclusively of glycerol ether lipids with isoprenoid groups attached to glycerol via ether linkages. The two major polar lipids extracted from the membranes are C25,25-achaetidyl(glucosyl)inositol (AGI) and C25,25-achaetidylinositol (AI). These lipids differ from those of anaerobic sulfur-dependent hyperthermophiles in the absence of tetraether lipids and the direct linkage of inositol and sugar moieties.

The effects of temperature and pH on the stability, structural organization, fluidity, permeability, and cytotoxicity of pure C25 archaeosomes (SUVs) were investigated by a combination of fluorescence emission spectroscopy, electron paramagnetic resonance (EPR), differential scanning calorimetry (DSC), and confocal microscopy. In addition, the effect of archaeal lipids on the physicochemical properties of conventional liposomes made from DPPC or sphyngomyelin and cholesterol will be discussed with respect to their potential use as coating materials or targeted drug delivery systems.

References:

1. Gmajner D., Ota A., Šentjurc M., Poklar Ulrih N. Stability of diether C25,25 liposomes from the hyperthermophilic Archaeon Aeropyrum pernix K1. Chemistry and physics of lipids 164 (2011) 236-245.
2. Gmajner D., Ahlin Grabnar P., Tušek-Žnidaršič M., Štrus J., Šentjurc M., Poklar Ulrih N. Structural characterization of liposomes made of diether archaeal lipids and dipalmitoyl-L-[alpha]-phosphatidylcholine. Biophysical chemistry 158 (2011) 150-156.
3. Gmajner D., Poklar Ulrih N. Thermotropic phase behaviour of mixed liposomes consist of archaeal diether and conventional diester lipids. Journal of thermal analysis and calorimetry 106 (2011) 255-260.
4. Batista Napotnik T., Valant J., Gmajner D., Passamonti S., Miklavčič D., Poklar Ulrih N. Cytotoxicity and uptake of archaeosomes prepared from Aeropyrum pernix lipids. Human and experimental toxicology 32 (2013) 950-959.

Acknowledgements:

To Slovenian Research Agency for financial support through the research program P4-0121.

Archaeosomes: Next-generation liposomes based on archaeal lipids for drug delivery and biomedical applications

Poornima Budime Santhosh*, Julia Genova, Hassan Chamati

Institute of Solid State Physics, Bulgarian Academy of Sciences,
Tzarigradsko Chaussee 72, 1784 Sofia, Bulgaria

* poorni@issp.bas.bg

Archaea represents a domain of single-celled microorganisms that possess unique membrane lipids with isoprenoid hydrocarbon side chains attached via ether linkage to the glycerol-phosphate backbone. The self-assembled vesicles prepared from the archaeal membrane lipids called "Archaeosomes" represent the next generation of liposomes that exhibit high stability under various extreme environmental conditions such as high temperature, pH, and pressure [1-2]. Therefore, they have gained importance as a multifunctional system to carry and deliver various cargos such as drugs, peptides, nanoparticles, etc. (Figure 1). The present study aims to prepare archaeosomes entrapped with different concentrations (0.5, 1, and 2 w %) of hydrophobic gold nanoparticles (AuNPs) and analyze the influence of AuNPs on the fluidity, thermal and structural properties of archaeal lipid membranes using a series of techniques such as fluorescent spectroscopy, differential scanning calorimetry, Fourier transform infrared spectroscopy and Raman spectroscopy, respectively. The experimental results have shown that the entrapped AuNPs did not cause a significant alteration in the fluidity, phase transition temperature, and structural properties of archaeosomes. Considering the biocompatibility of AuNPs with lipid membranes, these results suggest that archaeosomes can serve as a safe and potential system for drug delivery and various biomedical applications.

Keywords: archaeosomes, gold nanoparticles, lipid membranes, phase transition, fluidity

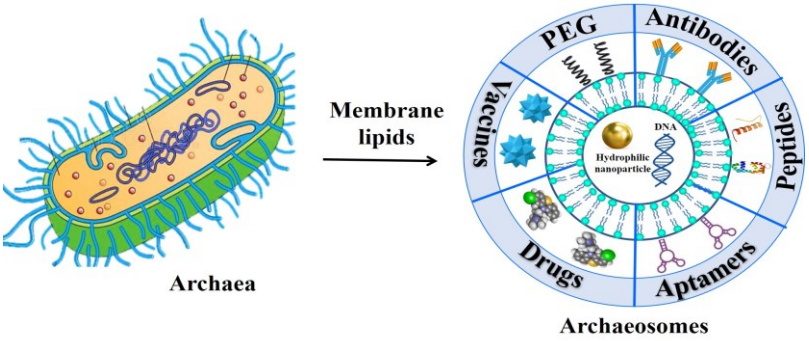


Figure 1. Schematic representation of archaeosomes prepared from archaeal membrane lipids and ability of archaeosomes to load various molecules for biomedical applications.

References:

1. Adamiak N, Krawczyk K, Locht C, Kowalewicz-Kulbat M. Archaeosomes and Gas Vesicles as Tools for Vaccine Development. Frontiers in Immunology, 2021, 12.
2. Kaur G, Garg T, Rath G, Goyal AK. Archaeosomes: an excellent carrier for drug and cell delivery. Drug Delivery, 2016, 23: 2497-2512.

Acknowledgements: The authors acknowledge financial support from the project AuLip KP-06-DB-8/01.12.2020 from the Bulgarian National Science Fund under the National Scientific Program P. Beron 2020.

The Future is Vast: Regenerative Medicine Perspectives and Technology Trends in Advance Implantable Biomaterial Strategies

E. Iordanova* and G. Yankov

Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tsarigradsko Chaussee blvd.,1784 Sofia, Bulgaria

* eiordanova@issp.bas.bg

The current need for organ and tissue replacement, repair and regeneration for patients is continually growing such that supply is not meeting the high demand primarily due to a tenuity of donors. In an effort to overcome these drawbacks, scientists working in the field of tissue engineering and regenerative medicine have investigated the use of biopolymer films and scaffolds as an alternative to transplantation. At present, biomaterials have been widely used in skin, cartilage, bone, tendon, vessels, nerves, bladder, and liver tissue engineering. Thanks to the complexity of any process involved in the preparation of bio-implants, such as synthesis, micro- and nano-structuring, cell culture, in-vivo, in-vitro assays, an in-depth study and research of the interaction mechanism bioenvironment - biomaterial is required. Furthermore, optimization of morphology, topography and physico-chemical composition of the contact surface should be carried on. The implementation of a new effective method will open new directions, both in the fundamental description of the properties of biocompatible systems and in the development of new applications.

Biomedical applications involving phenomena from the receptor scale of ~10 nm up to implantable 3D scaffolds with cross-sections >1 cm require adequate biocompatible materials and processing approaches to structure them. Laser processing with ultrashort laser pulses can address this challenge from the resolution, productivity, and materials points of view. Processing of materials by ultrashort laser pulses has evolved significantly over the last decade and is starting to reveal its scientific, technological, and industrial potential. In ultrafast laser manufacturing, optical energy of tightly focused fs laser pulses can be delivered to precisely defined positions on a timescale much faster than thermal energy exchange occurs. Control of photoionization and thermal processes with the highest precision has been achieved. State-of-the-art ultrashort laser processing techniques exploit high 0.1–1 μm spatial resolution and almost unrestricted three-dimensional structuring capability. The possibility of three-dimensional (3D) writing in polymers using tightly focused femtosecond (fs) laser pulses has attracted attention in a wide range of areas related to academic research and engineering, among them in tissue engineering and regenerative medicine.

Acknowledgements:

The authors express their acknowledgments to the financial support of BNSF under the project №КП-06-Н38/5 2019 and Grant No Д01-74 (19.05.2022) from the Ministry of Education of Bulgaria.

Hydrothermally synthesized TiO_2 nanostructures

Niharika Rawat[1], Ita Junkar[2], Metka Benčina[1,2], Ekaterina Gongadze[1], Veronika Kralj-Iglič, Aleš Iglič[1,*]

[1] Laboratory of Physics, Faculty of Electrical Engineering, University of Ljubljana, Tržaška 25, SI-1000, Ljublja-na, Slovenia
[2] Department of Surface Engineering, Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

* ales.iglic@fe.uni-lj.si

Various surface modification techniques, for instance electrochemical anodisation [1], hydrothermal treatment [2], etc. have been proposed in order to enhance biocompatibility of metallic materials used as implants. It has been shown that alteration of surface physicochemical properties, e.g. morphology, surface chemistry and wettability, influences the biological response [3,4]. In present contribution we describe the synthesis of different nanostructures by using the hydrothermal method on the surface of titanium (Ti)-based substrates. The morphology, surface chemistry and wettability of as-prepared surfaces were analysed by scanning electron microscopy combined with energy dispersive X-ray spectroscopy (SEM-EDX), X-ray photoemission spectroscopy (XPS) and water contact angle analysis (WCA). The efficacy of the hydrothermal treatment of Ti-based substrates has been established through hemocompatibility studies. It has been shown that the adhesion and activation of blood platelets is reduced on hydrothermally treated samples in comparison with Ti substrate used as control. The corresponding theoretical analysis of experimental results is also presented.

References:

1. Kulkarni, M., Patil-Sen, Y., Junkar, I., Kulkarni, C. V., Lorenzetti, M., & Iglič, A. (2015). Wettability studies of topologically distinct titanium surfaces. Colloids and Surfaces B: Biointerfaces, 129, 47-53.
2. Benčina, M., Rawat, N., Lakota, K., Sodin-Šemrl, S., Iglič, A., & Junkar, I. (2021). Bio-Performance of Hydrothermally and Plasma-Treated Titanium: The New Generation of Vascular Stents. International Journal of Molecular Sciences, 22(21), 11858.
3. Junkar, I., Kulkarni, M., Humpolíček, P., Capáková, Z., Burja, B., Mazare, A., ... & Sodin-Semrl, S. (2017). Could titanium dioxide nanotubes represent a viable support system for appropriate cells in vascular implants?. In Advances in Biomembranes and Lipid Self-Assembly (Vol. 25, pp. 1-39). Academic Press.
4. Junkar, I., Kulkarni, M., Drašler, B., Rugelj, N., Recek, N., Drobne, D., ... & Mozetič, M. (2016). Enhanced biocompatibility of TiO_2 surfaces by highly reactive plasma. Journal of Physics D: Applied Physics, 49(24), 244002.

Challenges and solutions for high performance green nanoelectronics devices and materials

Francis Balestra

Univ. Grenoble Alpes, CNRS, Grenoble INP, IMEP-LAHC & Sinano Institute, Grenoble, France

For future sustainable societies, a holistic approach is needed with the combination of two pillars: Digitalization of many domains to reduce footprint, and Sustainable Electronics, including innovative materials, devices, circuits and systems.

The substantial increase of electronic systems and IoT devices, the exponential augmentation of computing power for AI training, the strong growth of ICT share in electrical energy consumption, the problem of E-waste, and the lack of material availability put forward the need of substitution of critical (scarce, toxic) materials, the reduction of energy consumption in electronic systems, and the development of alternative architectures.

This paper presents promising solutions for overcoming these challenges in the areas of nanodevices and nanomaterials, which are at the core of future ICT systems. Nanowires, ultrathin films, gate-all-around structures, advanced materials such as 1D or 2D, alternative device architectures such as steep slope switches, heterostructures, and ultimate nanodevices are highlighted, which will be able to reach the ambitious targets of the IRDS Roadmap for the next decades [1-16].

References:

1. F. Balestra, Nanoscale CMOS: Innovative Materials, Modeling and Characterization, Francis Balestra Ed., ISTE-Wiley (2010).
2. F. Balestra, Beyond CMOS Nanodevices (tomes 1 & 2), Francis Balestra Ed., ISTE-Wiley (2014).
3. F. Balestra, Challenges for high performance and very low power operation at the end of the Roadmap, Solid-State Electronics, Volume 155, May 2019, pp. 27-31.
4. F. Balestra, Advanced technologies for future materials and devices, Chapter in Springer Handbook of Semiconductor Devices, to be published, 2022.
5. S.B. Deasy et al, Science, Vol. 354, Issue 6308, pp. 99-102, 2016.
6. W. Chung, IEDM 2017, p. 365.
7. A. Saeidi, IEEE EDL, VOL. 38, No. 10, p.1487, Oct. 2017.
8. M.H. Lee, IEDM 18, p. 735.
9. Z. Yu, IEDM 18, p. 524.
10. A. Saeidi, IEDM 18, p. 304.
11. E.A. Casu., IEDM 16, p. 19.3.1.
12. S. Lim, IEDM 16, p. 34.7.1.
13. C.-H. Yeh et al, DOI: 10.1109/IEDM19573.2019.8993600, IEDM 2019.
14. D. Akinwande et al, doi: 10.1038/s41586-019-1573-9, Nature, Sept. 2019.
15. I. Asselberghs, DOI: 10.1109/IEDM13553.2020.9371926, IEDM 2020.
16. International Roadmap for Devices and Systems, IEEE/IRDS, 2022.

Acknowledgements:

The author would like to thank all the Sinano Institute Members for their strong involvement in this research area.

Hierarchical Integration of Electrospinning and 3D/4D Printing Process for Prototyping of Smart Structures

Ashok Vaseashta Prof. Dr. Acad.

Office of Applied Research, International Clean Water Institute, Manassas, VA, USA
Professor, Transylvania University of Brasov, Brasov, ROMANIA
IEEN Chaired Professor of Nanotechnology, Academy of Sciences of Moldova, Chisinau, MOLDOVA
Academician, Euro Mediterranean Academy of Arts and Sciences.

Electrospinning is an effective and versatile technique used to produce porous structures ranging from submicron to nanometer diameters. Using a variety of high-performance polymers and blends, several porous structure configurations have become possible for applications in tactile sensing, energy harvesting, filtration, and biomedical applications, however, the structures lack mechanical complexity, conformity, and desired three-dimensional single/multi-material constructs necessary to mimic desired structures. A simple, yet versatile, strategy is through employing digitally-controlled fabrication of shape-morphing by combining two promising technologies, viz., electrospinning and 3D printing/additive manufacturing process. Using hierarchical integration of configurations, elaborate shapes and patterns are printed on mesostructured stimuli-responsive electrospun membranes, modulating in-plane and interlayer internal stresses induced by swelling/shrinkage mismatch, and thus guiding morphing behaviors of electrospun membranes to adapt to changes of the environment. Recent progress in 3D/4D printing/additive manufacturing processes includes materials and scaffold constructs for tactile and wearable sensors, filtration structures, sensors for structural health monitoring, biomedical scaffolds, tissue engineering, and optical patterning, among many other applications to support the vision of synthetically prepared material systems that mimic many of the structural aspects with digital precision. A novel technology called 3D jet writing was recently reported that catapults electrospinning to adaptive technologies for the manufacturing of scaffolds according to user-defined specifications of the shape and size of both the pores and the overall geometric footprint. This chapter reviews the hierarchical synergy between electrospinning and 3D printing as part of precision micromanufacturing for rapid prototyping of structures that are likely to evolve next-generation structures into reality.

Keywords: electrospinning, 3D printing, 4D printing, prototyping, jet printing

Characterization of functional materials using coherence scanning interferometry and environmental chambers

P.C. Montgomery[1,*], M. Flury[1], F. Anstotz[1], H. Mukhtar[1, 2], A. Rubin[3], A. Shpiruk[3], M. Del Nero[4], R. Barillon[4]

[1] *Laboratoire des Sciences de l'Ingénieur, de l'Informatique et de l'Imagerie (ICube), University of Strasbourg - CNRS - INSA, 300 Boulevard Sébastien Brand, F-67412 ILLKIRCH, France*
[2] *School of Electrical Engineering, Telkom University, Indonesia*
[3] *Institut Charles Sadron-CNRS, 23 rue du Loess, 67037 Strasbourg, F-67034 Cedex 2, France*
[4] *Institut Pluridisciplinaire Hubert Curien (IPHC) – CNRS – University of Strasbourg, 23 rue du Loess, 67037 Strasbourg, France*

* paul.montgomery@unistra.fr

Interference microscopy is a useful technique for characterizing functional materials, providing rapid and quantitative measurements of microscopic surface topography. The technique has since been extended for measuring changing surfaces in real time, defects in transparent layers, inhomogeneous materials using local spectroscopy and details with higher lateral resolution using microspheres placed near to the sample.

Another challenge in materials science is the measurement of materials in controlled environments. In this paper we present some initial results of several microscope systems that have been combined with environmental chambers. The first one uses control of the pressure, temperature and humidity for measuring the mechanical properties of nanometric polymer films, in the "nanobubble" project (Figure 1) [1]. The second one uses the automatic control of the deposition of polymer microdroplets for measuring drying properties. The final one uses an immersion system for studying changes in colloidal layers immersed in water in the presence of heavy metals with an application in the study of pollution of the environment [2].

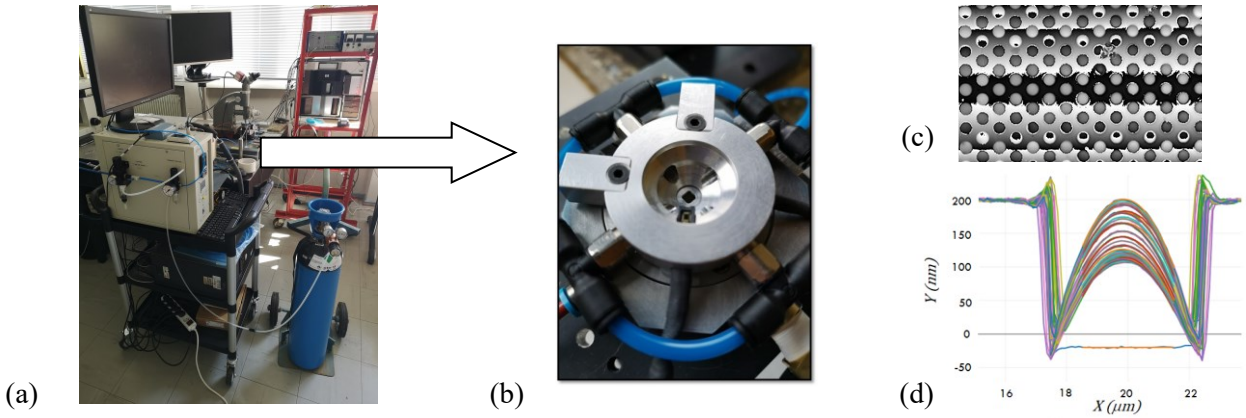


Figure 1: Interference microscope system (a), environmental chamber (b), PSM measurements (c) and series of profiles of relaxation of polymer film (d) in "nanobubble" project.

References:

1. Chapuis P., Montgomery P.C., Anstotz F., Leong-Hoï A., Gauthier C., Baschnagel J., Reiter G., McKenna G.B. and Rubin A., *A novel interferometric method for the study of the viscoelastic properties of ultra-thin polymer films determined from nanobubble inflation*, Review of Scientific Instruments, **88**(9), 2017, p. 093901.
2. Mukhtar H., Montgomery P., Anstotz F., Barillon R., Rubin A., Immersion white light scanning interferometry using elastic polymer path length compensation, Proc. SPIE 10678, 2018, p. 10678L.

Nanomaterials at interfaces for optical sensing

Peter Petrik[1,2,*]

[1] *Institute for Technical Physics and Materials Science, Centre for Energy Research, Konkoly-Thege Rd. 29-33, 1121 Budapest, Hungary*
[2] *Department of Electrical and Electronic Engineering, Institute of Physics, Faculty of Science and Technology, University of Debrecen, 4032 Debrecen, Hungary*

* petrik.peter@ek-cer.hu

Optical sensors are gaining increasing attention due to their high sensitivity, stability, speed, and versatile configuration opportunities. The interface nanostructures and layers for optical sensors need to be suitable in terms of both chemical properties and optical enhancement. There is a large variety of possible materials and structures including plasmon resonance [1], multi-layers [2], scanning resonance by lateral grading [3], or periodic lateral structures (Fig. 1B) utilizing the Kretschmann-Raether arrangement (Fig. 1A) for in-situ spectroscopic ellipsometry at solid-liquid interfaces. Special features, benefits and future opportunities of different surface designs will be discussed. For more information see http://www.ellipsometry.hu

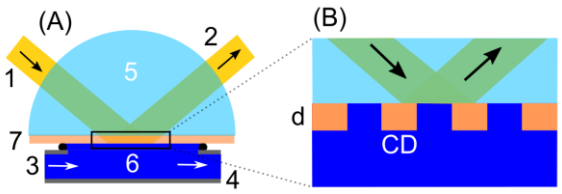


Figure 1. (A) Optical setup using the Kretschmann-Raether arrangement. The numbered components are the following. 1: incoming light, 2: reflected light leaving the system, 3: incoming liquid, 4: outgoing liquid, 5: body of the cell, 6: liquid volume of the cell, 7: sample. (B) Interface structure based on a grating with a thickness of d and critical dimension of CD.

References:

1. J. Nador, B. Kalas, A. Saftics, E. Agocs, P. Kozma, L. Korosi, I. Szekacs, M. Fried, R. Horvath, P. Petrik, Plasmon-enhanced two-channel in situ Kretschmann ellipsometry of protein adsorption, cellular adhesion and polyelectrolyte deposition on titania nanostructures, Opt. Express. 24 (2016) 4812. https://doi.org/10.1364/OE.24.004812.
2. B. Kalas, K. Ferencz, A. Saftics, Z. Czigany, M. Fried, P. Petrik, Bloch surface waves biosensing in the ultraviolet wavelength range – Bragg structure design for investigating protein adsorption by in situ Kretschmann-Raether ellipsometry, Applied Surface Science. 536 (2021) 147869. https://doi.org/10.1016/j.apsusc.2020.147869.
3. B. Kalas, G. Safran, M. Serenyi, M. Fried, P. Petrik, Scanning-resonance optical sensing based on a laterally graded plasmonic Ag_xAl_{1-x} structure, under submission.

Acknowledgements:

Supports from the OTKA-k131515 and TKP2021-EGA-04 Hungarian NRDI funds as well as from the H2020 POLight European grant are gratefully acknowledged.

Joule resistive heating of a shape memory composite: some design rules to predict the temperature in samples with rectangular cross-section

Clara Pereira Sánchez[1], Maxime Houbben[2], Jean-François Fagnard[1], Philippe Laurent[1], Christine Jérôme[2], Ludovic Noels[3], Philippe Vanderbemden[1,*]

[1] Department of Electrical Engineering and Computer Science, Montefiore Institute, University of Liege, 4000 Liège, Belgium
[2] CERM, CESAM-RU, University of Liège, 4000 Liège, Belgium
[3] Department of Aerospace and Mechanical Engineering, University of Liège, Liège, Belgium

* Philippe.Vanderbemden@uliege.be

Shape memory polymers (SMP) and their composites (SMC) are materials exhibiting morphing capabilities that can be applied to numerous applications, including aerospace or biomedical engineering. The changes of shape of the material are triggered by modifying its temperature. Amongst the possible activation methods, Joule resistive heating occurring when an electric current is injected directly in the material is particularly attractive since it is fast and does not require an external heating source. This method, however, requires the electrical resistivity of the polymer to be decreased by the use of conductive fillers. In addition, a suitable activation requires the temperature increase of the sample to be predicted accurately. In this work we establish and investigate the different analytical expressions that can be used to predict the characteristics of the resistive heating of an electroactive shape memory composite with rectangular cross-section [1]. We determine the parameters that are important to understand the temperature increase that happens either when a constant current is injected in the sample or when this current is injected at constant power. The results are compared to measurements of the temperature distribution at the surface of a conductive shape memory composite consisting of covalent poly(ε-caprolactone) matrix filled with 3 wt% of multiwall carbon nanotubes [1]. The experimental temperature distribution across the sample can be reproduced using the analytical expressions, which can then be used to predict the temperature increase for samples of various sizes and properties.

References:

1. Clara Pereira Sánchez et al. *Resistive heating of a shape memory composite: analytical, numerical and experimental study* (2022) *Smart Mater. Struct.* **31** 025003.

Acknowledgements:

This study is supported through the 'Actions de recherche concertées 2017 *Synthesis, Characterization, and MultiScale Model of Smart composite Materials* (S3CM3) 17/21-07' financed by the 'Direction générale de l'Enseignement non obligatoire de la Recherche scientifique, Direction de la Recherche scientifique, Communauté française de Belgique, et octroyées par l'Académie Universitaire Wallonie-Europe.

Phase Transitions in Magneto-Electric Hexaferrites

Tatyana Koutzarova[1,*], Svetoslav Kolev[1,2], Kiril Krezhov[1], Borislava Georgieva[1]

[1] *Institute of Electronics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria*
[2] *Neofit Rilski South-Western University, 66 Ivan Mihailov Str., 2700 Blagoevgrad, Bulgaria*

* tanya@ie.bas.bg, tatyana_koutzarova@yahoo.com,

Hexaferrites have been intensively studied for many years as materials for permanent magnets, high-density recording media, microwave devices, biomedical applications, etc. In recent years, research has been focused on the appearance of the magneto-electric effect in some hexaferrite systems and the possibility of their use as single-phase multiferroic and magnetoelectric materials. Theoretical analyses have shown that the large magneto-electric effect originates from the strong interplay between magnetization and electric polarization existing in insulating systems with non-collinear magnetic structures. This contribuyion is focused on the structural properties and magnetic phase transition of hexaferrites. The magnetic structure in the hexaferrites and especially the particular magnetic spin order are key factors for the observation of magneto-electric phases in hexaferrites. Some of the magnetoelectric phases are metastable, making it difficult to transfer them to applications. But in the phase diagrams of the hexaferrites, a large variety of non-collinear stable magnetic phases can be realized by chemical doping. As the magnetoelectric effect is related to the magnetic spin ordering, it is very important to investigate the influence of cation substitutions on the magnetic phase transition temperature. Here we present recent advances in the study of the magnetic phase transitions in Y- and Z-type hexaferrites. In particular, the influence of substituting the non-magnetic cations with magnetic cations, and of the magnetic Fe^{3+} cations with non-magnetic ones in Y-type hexaferrites on their magnetic properties and magnetic-phase transitions will be exemplified.

Acknowledgements:

The work was supported by the Bulgarian National Science Fund under contract KP-06-N48/5 and KP-06-India-2 (for Y type hexaferrites), by a joint research project between the Bulgarian Academy of Sciences and WBI, Belgium, and by a joint research project between the Bulgarian Academy of Sciences and the Institute of Low Temperature and Structure Research, Polish Academy of Sciences.

Effects of Alloy Disorder in Organic and Inorganic Semiconductors

Sergei Baranovskii[1,2,*], Florian Gebhard[1], Dirk Hertel[2], Klaus Meerholz[2]

[1] Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Marburg 35032, Germany
[2] Department für Chemie, Universität zu Köln, Luxemburger Strasse 116, 50939 Köln, Germany

* sergei.baranovski@physik.uni-marburg.de

Alloying of semiconductors is often used to tune the material properties desired for device applications. For instance, alloyed lead-tin perovskites exhibit lower bandgaps than the compositions with only lead, or only tin metal cations [1]. This feature makes alloys promising for applications in tandem solar cells to absorb the broad portions of the solar spectrum. The concept of the band structure engineering has recently been applied also to organic semiconductors in order to improve the device features of organic solar cells, organic light-emitting diodes, and organic field-effect transistors [2].

The price for the band structure tunability is an extra disorder caused by alloying. In order to reveal the features of the disorder potential in alloys of atomically thin transition-metal dichalcogenides (TMDs) such as $Mo_xW_{1-x}Se_2$, the exciton photoluminescence has been recently measured in a broad temperature range between 10 and 200 K [3]. In contrast to the binary materials, $MoSe_2$ and WSe_2, the ternary system demonstrated non-monotonous temperature dependences of the luminescence Stokes shift and of the luminescence linewidth. Such behaviour is a strong indication of a disorder potential that creates localized states for excitons and affects the exciton dynamics responsible for the observed non-monotonous temperature dependences [4].

A comparison between the experimental data and the results obtained by Monte Carlo computer simulations provides information on the energy scale of the disorder potential and on the shape of the density of localized states created by disorder. Statistical spatial fluctuations in the distribution of the chemically different material constituents were revealed to cause the disorder potential responsible for the observed effects [3].

Experimental studies on a series of $FAPb_{1-x}Sn_xI_3$ alloys showed that the impact of disorder is maximal around alloy compositions $x < 0.25$ and $x > 0.85$, as evidenced by the contributions of the disorder potential to the luminescence linewidth and to the luminescence Stokes shift [1]. This observation perfectly agrees with the theoretical predictions for the statistically random spatial fluctuations in the distribution of the chemically different material constituents [5].

References:

1. E. S. Parrott, T. Green, R. L. Milot, M. B. Johnston, H. J. Snaith, and L. M. Herz, “Interplay of Structural and Optoelectronic Properties in Formamidinium Mixed Tin–Lead Triiodide Perovskites”, Adv. Funct. Mater. 28 (2018) 1802803.
2. M. Schwarze, W. Tress, B. Beyer, F. Gao, R. Scholz, C. Poelking, K. Ortstein, A. A. Günther, D. Kasemann, D. Andrienko, K. Leo, “Band structure engineering in organic semiconductors“, Science 352 (2016) 1446.
3. H. Masenda, L. M. Schneider, M. A. Aly, S. J. Machchhar, A. Usman, K. Meerholz, F. Gebhard, S. D. Baranovskii, and M. Koch, “Energy Scaling of Compositional Disorder in Transition-Metal Dichalcogenide Monolayers”, Adv. Electron. Mater. 2100196 (2021).
4. S. D. Baranovskii, R. Eichmann, P. Thomas, "Temperature-dependent Exciton Luminescence in Quantum Wells: Computer Simulation" Phys. Rev. B 58 (1998) 13081.
5. S. D. Baranovskii, P. Höhbusch, A. V. Nenashev, A. V. Dvurechenskii, M. Gerhard, M. Koch, D. Hertel, K. Meerholz, and F. Gebhard1, “Comment on “Interplay of Structural and Optoelectronic Properties in Formamidinium Mixed Tin-Lead Triiodide Perovskites", Adv. Funct. Mater. 28 (2022) 2201309.

Controlling High Speed Mach Zehnder Modulator Quadrature Bias Point Using Si PIN Diode Phase-Shifter

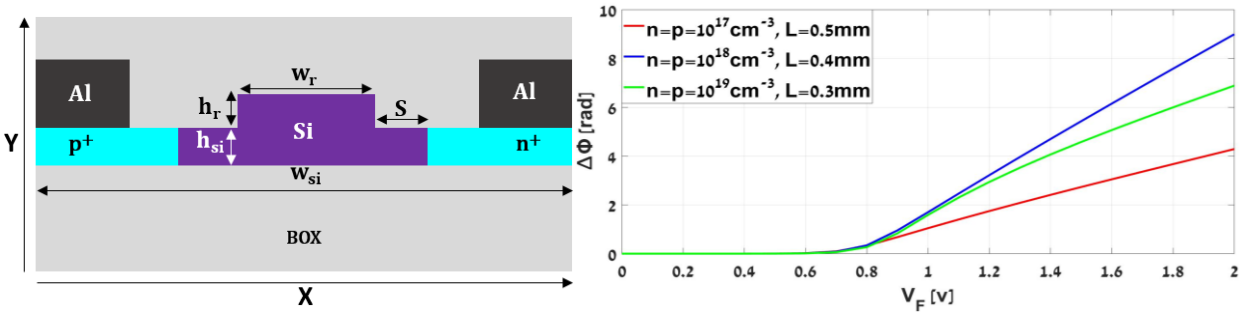
Dror Malka*

Faculty of Engineering, Holon Institute of Technology (HIT), Holon 5810201, Israel

* drorm@hit.ac.il

Commercial high-speed silicon (Si) Mach-Zehnder modulator (MZM) [1] required to be active around the quadrature bias point (linear transmission area) with low power consumption, small footprint, and small drive voltage. The bias controlling is done by an optical phase-shifter (PS). However, the accuracy is limited by the drive voltage, laser thermal drift, and fabrication errors. To overcome these problems, we propose in this paper the study and analysis of Si PIN diode PS under forward biasing at 1550 nm wavelength using the standard 220 nm substrate silicon-on-insulator (SOI) rib waveguide technology. Numerical investigations were carried out on the key geometrical parameters, doping concentration, doping locations, operating wavelength, biasing level. Results show that the optimal design can be operated with a lower voltage (V_π=1.629 v), lower attenuation (α=28.985 dB/cm), and short device length with an extremely small voltage-length product $V_\pi L$=0.815 vmm. Thus, this PS can be used for designing an efficiency high-speed MZM and to obtain better performances in the optical commutation system.

Figure 1(a) shows the Si rib waveguide structure at the x-y plane. In this figure, the purple color area represents pure Si, gray color areas represent silica, black color areas represent aluminum (Al) and doping areas (n^+/p^+) represent light blue color. The PS width is w_{si}, h_r is the etching depth, h_{si} is the slab thickness, S is the distance between the rib waveguide core and the doping concentration area, w_r is the rib waveguide core width. The Si rib waveguide based on SOI substrate with a 220 nm top Si layer and a 2μm buried oxide (BOX) layer. Figure 1(b) shows the optimizations of the doping concentrations and phase-shifter lengths for finding the optimal driver voltage.



(a) **(b)**

Figure 1. Si PIN rib waveguide. (a) Schematic sketch. (b). ΔΦ as a function of V_F at different doping concentrations and phase-shifter lengths.

The numerical optimizations of Si PIN phase-shifter based on forwarding biased PIN diode using a commercial 220 nm SOI rib waveguide technology has been reported. This study shows how to design a phase-shifter that can fulfill the high-speed Mach Zehnder modulator conditions with a very low optical and electrical energy consumption.

References:

1. G. T. Reed, G. Z. Mashanovich, F. Y. Gardes, M. Nedeljkovic, Y. Hu, D. J. Thomson, K. Li, P. R. Wilson, S.-W. Chen, and S. S. Hsu, "Recent breakthroughs in carrier depletion based silicon optical modulators" Nanophotonics 3, 229-245 (2014).

Silver and gold containing compounds of *p*-block elements as perspective materials for plasmonics

R. Todorov[1], T. Hristova-Vasileva[1,2,*], V. Katrova[1], A. Atanasova[1]

[1] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, 1113 Sofia, Bulgaria
[2] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* teddie@issp.bas.bg

A review on the preparation and optical properties of bimetallic alloys and compounds based on silver and gold with *p*-block metals in the Periodic table of chemical elements is presented. Together with the boundary solid solutions, already reported as perspective for plasmonic applications due to the fluent tuning of the plasma frequency, the phase diagrams of the different bimetallic systems show two additional groups of promising materials - intermetallic compounds, exhibiting new properties, and continuous rows of inhomogeneous binary alloys, representing a mixture of both materials used. The formation of intermetallic phases in many of the Ag(Au) – *p*-block systems is related to the Hume-Rothery rule, which points out dependence on the number of valence electrons per atom.

A short review of the different methods for synthesis of alloys with *p*-block metals from the Periodic table of chemical elements is considered. The bimetal alloys and solid solutions in the Ag-Au, Ag-Cu and Au-Cu systems are well-known plasmonic materials that allow variation of the plasma frequency between those of the single metals. Existing literature data show that the addition of Cd, Al and In reduces the band gap for interband transitions associated with 4*d* and 5*d* electronic states of silver and gold atoms, respectively. As a result, this effect reduces the value of the imaginary part of the complex permittivity in the ultraviolet spectral range and increases the efficiency of the localized surface plasmon resonance (Q_{LSPR}) in this region, respectively. Unfortunately, the increase of the structural disorder in the crystal lattice of silver at concentrations greater than 10 at. % of p-block metal causes reduction of the Q_{LSPR} value.

On the other hand, the intermetallic compounds offer a well-ordered crystalline structure together with a good conductivity level, but heretofore, their optical properties have been less investigated. Studies of the band structure of intermetallic compounds from the AgM_2 and AuM_2 (where M = Ga, In and Al) type show that the density of their electron states is greater than zero at the Fermi level, which shows that these compounds have a metallic character, well described by '*nearly free electron model*'. Based on the existing conductivity data, they show a reduced value of the damping parameter in the Drude dispersion model, which implies higher Q_{LSPR} values compared to strongly doped solid solutions.

Based on the existing data on the complex dielectric function, extinction calculations and scattering cross-sections, local field enhancement of spherical nanoparticles from intermetallic Ag_xM_y and Au_xM_y compounds was determined and the plasmon activity was evaluated.

Acknowledgements:

This work is financially supported by contract KP-06-N38/8 - 05.12.2019 with the Bulgarian National Science Fund.

Acceptor Doping of Zinc Oxide – Defect Complexes in Nanoscale

Oksana Volnianska, Sushma Mishra, Elżbieta Guziewicz*

Institute of Physics Polish Academy of Sciences: Al. Lotników 32/46, Warsaw, Poland, 02 668

* guzel@ifpan.edu.pl

The problem with achieving repeatable and stable *p*-type conductivity of ZnO is still not resolved. The undoped material is highly *n*-type, and defect levels of substitutional acceptor dopants are deep. According to present knowledge, acceptor states are provided by complexes of a dopant, native defects and/or hydrogen.

We will present recent cathodoluminescence studies on *p*-type polycrystalline ZnO:N films that revealed a separation the donor-related and the acceptor-related luminescence, i.e. some columns showing only acceptor-, while other donor-related CL. The scanning photoelectron microscopy (SPEM) study were conducted at the ESCA microscopy beamline at the Elettra synchrotron (Trieste, Italy). The SPEM enables to probe the electronic structure at submicron scale (130 nm resolution) and thus to obtain the photoemission spectroscopy signal from a single column of growth. The measurements, performed on the ZnO and ZnO:N film cross-section, revealed two types of crystallites with a different valence band electronic structure in the valence band region. Density Functional Theory (DFT) calculations show that the complexes involving

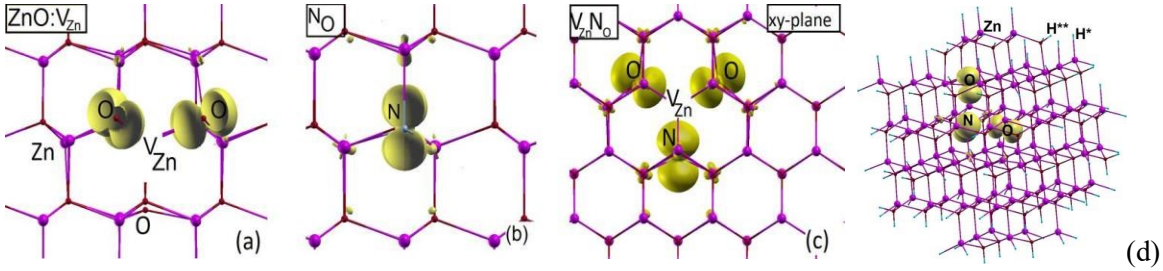


Figure 1. Isosurfaces of spin density distribution for the empty orbitals in the defect states. (a)-(c) bulk, (d) defect states in QDs.

zinc vacancy (V_{Zn}), hydrogen and nitrogen (in the case of ZnO:N), which provide complexes-related acceptor states, modify density of states in the valence band region of bulk and QDs and are easily formed under O-rich conditions. According to this, the experimentally observed differences in photoelectron spectra evidence the grouping of acceptor and donor complexes in separate crystallites. Hydrogen, which in many cases is abundant during the growth process, stabilizes formation of the $V_{Zn}N_O$ complex, but the appearing $V_{Zn}N_OH$ complex is found to be a deep acceptor. As the formation of acceptor complexes involves distortion of the crystal lattice, it may be assumed that microstrain may play an important role in grouping of acceptors and donors in crystallites with different orientation (Fig.1).

References:

1. E. Guziewicz, E. Przezdziecka et al., ACS Appl. Mat. Interfaces 9, 26143-26150 (2017).
2. E. Guziewicz, O. Volnianska et al., Valence Band Electronic Structure of ZnO and ZnO:N –Experimental and Theoretical Evidence of Defect Complexes, Phys. Rev. Appl. (under revision).

Acknowledgements:

The work was supported by the Polish NCN Project DEC-2018/07/B/ST3/03576.

Designing Electrode Architectures across Length Scales: Some Lessons Learned from Li-ion and "Beyond Li" Chemistries

Sarbajit Banerjee[1,2,*]

[1] *Department of Chemistry, Texas A&M University*
[2] *Department of Materials Science & Engineering, Texas A&M University*

* banerjee@chem.tamu.edu

The design and operation of rechargeable batteries is predicated on directing flows of mass, charge, and energy across multiple interfaces. Understanding such flows requires knowledge of atomistic and mesoscale diffusion pathways and the coupling of ion transport with electron conduction and stress gradients across length scales. Using multiple polymorphs of V_2O_5 as model systems, I will discuss our efforts to develop an Angstrom-level view of diffusion pathways using single-crystal X-ray diffraction studies of topochemical transformations. I will further discuss the accumulative results of atomic scale inhomogeneities at single-particle and particle ensemble levels based on scanning transmission X-ray microscopy and X-ray ptychography measurements of lithiation inhomogeneities and stress gradients. The mitigation of diffusion impediments will be discussed with reference to two distinct approaches: (a) utilization of Riemann manifolds as a geometric design principle for electrode architectures and (b) the atomistic design of polymorphs with well-defined diffusion pathways that provide frustrated coordination. Finally, I will discuss the role of chemical substitution and the extent to which it can be considered a proxy for stress modification.

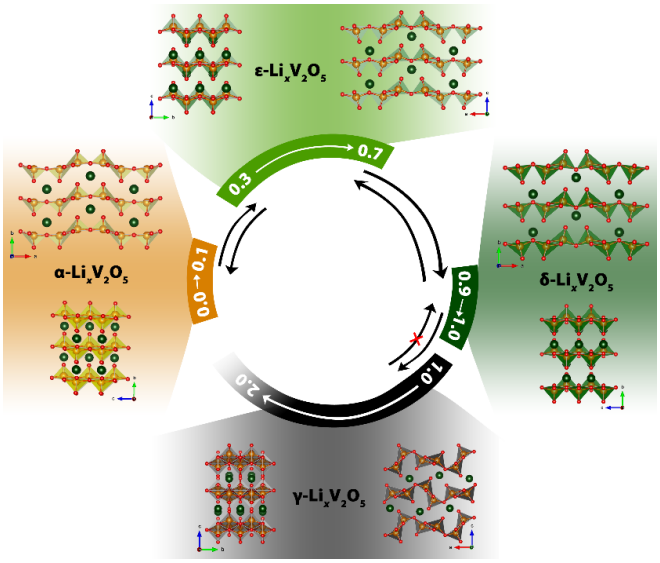


Figure 1. Intercalation-induced phase transformations in V_2O_5

References:

1. J. Andrews, *et al. Matter* 3: 1754-1773 (2020), DOI: 10.1016/j.matt.2020.08.030.
2. Y. Luo, *et al. Nature Materials* 21: 217-227 (2022), DOI: 10.1038/s41563-021-01151-8.
3. J. Handy, *et al. Angewandte Chemie International Edition* 60: 15582-15589 (2021), DOI: 10.1002/anie.202104231.

Acknowledgements:

We are grateful to the NSF for support under DMR 1809877.

Investigation of the surface reactivity of a carbon steel container exposed to different types of environments and conditions

Margit Fabian*, Istvan Tolnai, Otto Czompoly, Janos Osan

Centre for Energy Research, 1121 Budapest, Konkoly Thege st 29-33, Hungary

* fabian.margit@ek-cer.hu

All states that engage in any kind of nuclear application must consider the management of radioactive waste and make sure it is handled in a safe manner, with due regard to the level of radioactivity and in compliance with national/international regulations. There is a broad consensus that the preferred method of ensuring long term safety for high level radioactive waste (HLW) is isolation in a deep geological repository (DGR), which will provide passive multibarrier isolation of radioactive materials. The vitrified HLW form in a steel canister is specifically designed for long term durability in storage and disposal [1]. The requirements for container lifetime and integrity depend on the DGR concept and the chosen geological medium.

The focus of the interface scale is on two materials in contact to obtain information on the geochemical evolution close to an interface in terms of chemical variables and alteration in solid phase composition at a detailed small scale. The study concerns steel in contact with clay and concrete with attention to the effect of degradation products from one material on the other.

We built a scale model system where close to real conditions were used (temperature, porewater composition). The main goal was to understand the characteristics, applicability and stability of the whole system, from the physical properties of the steel to the clay/concrete response in the repository. We have been conducted a triplicate steel (S235JR carbon steel)/clay (crushed rock from Boda Claystone Formation) and steel/concrete experiments using synthetic porewater [2,3] for saturation. The corrosion potential was continuously monitored (container vs Pt electrode in clay). All containers were kept in an incubator at 80 °C. After 3, 7 and 12 months a container was opened for post-mortem characterization. With SEM/EDX investigations we focused on the composition and nature of alteration products formed on the steel and within the clay/concrete. Formation of 30-40 µm long Fe-oxide ingrowths were detected and confirmed by micro-Raman investigations. The main corrosion products contain hematite, magnetite and ferrihydrite in different ratios. The soaking liquid was characterized using ICP-OES/IC after 3, 7 and 12 months. The measured B, Ca, K and Na concentration increased, while the Mg, and Si concentration decreased with time. Concentrations of Cl^- and SO_4^{2-} ions as determined by ion chromatography in the final porewater are close to the starting concentrations, the increase was less than 10% for chloride but higher for sulfate.

Details of the phase characteristics and trends of the dissolution rates will be presented.

References:

1. L. W. Hill Shannon, The corrosion of carbon steel under deep geological nuclear waste disposal conditions, Electronic Thesis and Dissertation Rep. 3820 (2016).
2. M. M. Fernandes, N. Ver, B. Baeyens, Applied Geochemistry 59 (2015) 189–199.
3. D. Breitner, J. Osan, M. Fabian, P. Zagyvai, C. Szabo, R. Dahn, M. M. Fernandes, I. Sajo, Z. Mate, S. Torok, Environmental Earth Sciences 73(1) (2015) 209-219.

Acknowledgements:

The research activities presented were supported by the H2020 project EURAD-847593.

Single-molecule magnets: The huge zero-field splitting revisited

Miroslav Georgiev* **and Hassan Chamati**

Institute of Solid State Physics, Bulgarian Academy of Sciences
Tsarigradsko Chaussee 72, 1784 Sofia, Bulgaria

* mgeorgiev@issp.bas.bg

Single-molecule magnets are a particular type of molecules that exhibit an energy barrier to the reversal of magnetization and a suppressed tunnelling effect. The barrier's height and profile are intrinsic features of an anisotropy energy that leads to a magnetic hysteresis of pure molecular nature. This magnetic anisotropy attracts the attention of all researchers in the field of molecular magnetism. Single-molecule magnets have the potential to pave the road to the application of adatoms in future technologies. Single-ion magnets that possess a high energy barrier [1-3] are among the most reliable candidates for implementation as high density information storage devices. Their successful application, however, is closely linked to the knowledge of their underlying electronic structure and the way the crystal field, spin exchange, spin-orbit and spin-spin dipole interactions interplay. At present, a comprehensive analysis of the contribution of all aforementioned interactions remains beyond reach. The absence of a consistent theory rises a confusion about the true effect of spin-orbit interactions and hence the misinterpretation of crystal field splitting as a zero-field one. Furthermore, it leads to incorrect association of the zero-field splitting parameters as magnetic anisotropy ones [4]. Elaborating in that direction, we demonstrate how an ab initio approach based on the multi-configurational self-consistent field method has the advantage to shed light on the contribution of all relevant interaction terms and the origin of the fine structure promoting the single-molecule magnet behavior. Here we focus on the emergence of the unexpected large and huge zero-field splitting in $3d^8$ single-ion magnets.

References:

1. Ruamps, R., Maurice, R., Batchelor, L., Boggio-Pasqua, M., Guillot, R.; Barra, A. L., Liu, J., Bendeif, E.-E., Pillet, S., Hill, S., Mallah, T., Guihéry, N. Giant Ising-Type Magnetic Anisotropy in Trigonal Bipyramidal Ni(II) Complexes: Experiment and Theory. *J. Am. Chem. Soc.* **2013**, *135* (8), 3017–3026.
2. Blagg, R. J., Muryn, C. A., McInnes, E. J. L., Tuna, F., Winpenny, R. E. P. Single Pyramid Magnets: Dy5 Pyramids with Slow Magnetic Relaxation to 40 K. *Angew. Chem. Int. Ed.* **2011**, *50* (29), 6530–6533.
3. Marriott, K. E. R., Bhaskaran, L., Wilson, C., Medarde, M., Ochsenbein, S. T., Hill, S., Murrie, M. Pushing the Limits of Magnetic Anisotropy in Trigonal Bipyramidal Ni(II). *Chem. Sci.* **2015**, *6* (12), 6823–6828.
4. Rudowicz, C., Karbowiak, M. Disentangling Intricate Web of Interrelated Notions at the Interface between the Physical (Crystal Field) Hamiltonians and the Effective (Spin) Hamiltonians. *Coord. Chem. Rev.* **2015**, *287*, 28–63.

Acknowledgements:

This work was supported by the Bulgarian National Science Fund under grant No КП-06-Н38/6.

Star polymer chains in confined geometries: theory and simulations

Zoriana Danel[1,*], Joanna Hałun[2], Paweł Karbowniczek[1]

[1] *Faculty of Materials Engineering and Physics, Cracow University of Technology, 30-084 Cracow, Poland*
[2] *Institute of Nuclear Physics, Polish Academy of Sciences, 31-342 Cracow, Poland*

* zoriana.danel@pk.edu.pl

The investigation of the influence of the star polymer topology on the depletion interaction potentials, the depletion forces and the monomer density profiles was investigated analytically in the framework of the Gaussian model and by molecular dynamic simulations. The calculations of the dimensionless depletion interaction potentials, dimensionless depletion forces and the layer monomer density profiles for a dilute solution of ideal star polymers with f = 3,4,5 arms in a Θ-solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the mixed case of one repulsive and the other inert surface were performed. Furthermore, taking into account the Derjaguin approximation, the dimensionless layer monomer density profiles for ideal star polymers with different number of armss f = 3,4,5 immersed in a dilute solution of big colloidal particles with different adsorbing or repelling properties with respect to polymers were calculated. The density-force relation for the above-mentioned cases was analysed. Taking into account the small sphere expansion allowed to obtain the monomer density profiles for a dilute solution of ideal star polymers with different number of arms immersed in a solution of small spherical particles, or nano-particles of finite size, which are much smaller than the polymer size and the other characteristic mesoscopic length of the system. Besides, we performed molecular dynamics simulation of a dilute solution of star-shaped polymers with N = 901 (3 × 300 + 1-star polymer with three arms), 1201 (4 × 300 + 1-star polymer with four arms) and 1501 (5 × 300 + 1-star polymer with five arms) beads accordingly. The obtained analytical and numerical results for star polymers are compared with the results for linear polymer chains in confined geometries. The obtained results indicate that a dilute solution of star polymer chains can be used for the production of new functional materials because the behaviour of these solutions depends on the topology of polymers, as well as on the nature and geometry of confined surfaces. These properties can find wide practical application in nanotechnology, as well as in biotechnology for drug and gene transmission.

The Hubbard model and optics of 2D materials

Vladan Celebonovic*

Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

* vladan@ipb.ac.rs

Materials being able to fulfill several functions simulaniously are usually called multifunctional materials. Their parameters can be chosen either experimentally (trial and error) or theoretically, within a given theoretical model of the material under study.

In the present paper the well known Hubbard model (HM) of 1D and 2D solids will be used. The aim of the paper is to calculate the reflectivity of 1D and 2D materials, and explore the influence of the elasticity of materials on their reflectivity.

Reference:

1. Celebonovic V. and Nikolic, M. G.: 2022, Some Ideas onTheoretically Choosing Multifunctional Materials: A Modelling Approach in Resarch Trends and Challnges in Physical Science, vol.7, pp.42 -51., ed by George, Th. F., published by B. P. International, Hooghly, India.

ABSTRACTS OF ORAL PRESENTATIONS

Magneto-optical and multiferroic properties of transition-metal (Fe, Co or Ni)-doped ZnO layers deposited by ALD

Albena Paskaleva[1], Armando Galluzzi[2,3], Krastyo Buchkov[1,4,*], Dencho Spassov[1], Tzvetan Ivanov[1], Blagoy Blagoev[1], Vladimir Mehandzhiev[1], Ivalina Avramova[5], Penka Terzyiska[1], Peter Tzvetkov[5], Daniela Kovacheva[5], Massimiliano Polichetti[2,3]

[1] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee blvd., 1784 Sofia, Bulgaria
[2] Department of Physics "E.R. Caianiello", University of Salerno, via Giovanni Paolo II, 132, Fisciano (SALERNO), I-84084, Italy
[3] CNR-SPIN Salerno, via Giovanni Paolo II, 132, Fisciano (SALERNO), I-84084, Italy
[4] Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev Str, bl.109, Sofia, BG-1113, Bulgaria
[5] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl.10, Sofia, BG-1113 Bulgaria

* buchkov@issp.bas.bg

The present study provides an extended analysis of magneto-optical MO Kerr effect and the ferroelectric state in transition-metal (TM) (Co, Fe or Ni)-doped ZnO films prepared by Atomic Layer Deposition (ALD). The structural, chemical, magneto-optical and dielectric properties were considered in relation to the technological details of the ALD process and the corresponding dopant effects. The doped samples show sophisticated MO Kerr behavior with strong magnetization response and very high values of the Kerr polarization angle, especially in the case of ZnO/Fe (Fig. 1). In addition, it is established that the doped ZnO demonstrate ferroelectric behavior. In this context the observed rich and versatile physical nature and functionality opens-up new prospects for application of these nanostructured materials in advanced electronic, spintronic and optical devices.

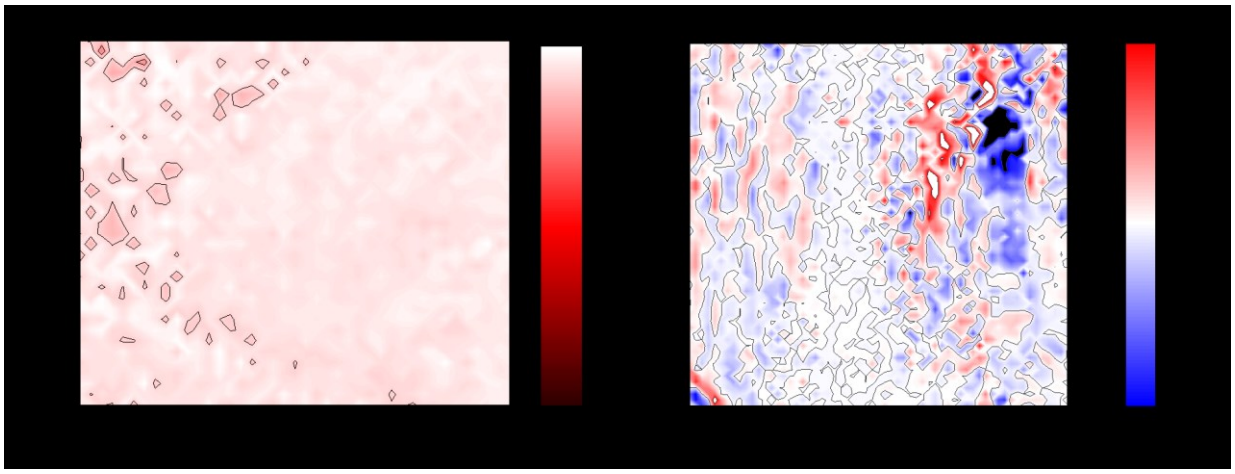


Figure 1. Maps of the variations of the MO Kerr rotation angle for ZnO and ZnO/Fe ALD films.

Acknowledgements:

This study was supported in part by the Bulgarian National Science Fund, Project KP-06-H28/9 and inter-academic Italian-Bulgarian research project (Department of Physics "E.R. Caianiello" CNR-SPIN unit, University of Salerno, and the Institute of Solid State Physics "Georgi Nadjakov," Bulgarian Academy of Sciences).

An Electrochemical Impedance Spectroscopy Study of the Influence of Miltefosine on Lung Cancer Cells and Endothelial Cells

D. Georgieva[1], I. Georgieva[2], B. Borisova[2], R. Tzoneva[2] and L. Vladimirova-Mihaleva[1]

[1]Sofia University "St. Kliment Ohridski", Faculty of Physics, Department of Optics and Spectroscopy, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria
[2]Institute of Biophysics and Biomedical Engineering, Bulgarian Academy of Sciences, Akad. G. Bonchev str., Bl. 21, 1113 Sofia, Bulgaria

* vladimirova@phys.uni-sofia.bg

Electrochemical impedance spectroscopy is a fast and non-invasive electrochemical method with a rapidly increasing use in studying the behaviour of cancer cells in the last years. In this paper we present the opportunity to use the impedance spectroscopy as a technique for lung cancer cells studies and the effect of the anti-cancer agent Miltefosine (n-hexadecylphosphocholine) on such cells.

The obtained results showed the manner of initial cell attachment of HUVEC and A549 cells in real-time. The data was used to evaluate the development of the cytotoxic effect of Miltefosine on cancer cells.

Investigations of zirconium layers obtained by electrochemical process at different temperatures

K. Lovchinov[1,*], R. Gergova[2], R. Georgiev[1], P. Petrova[1], K. Lazarova[1]

[1] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 109, 1113 Sofia, Bulgaria.
[2] Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee blvd., 1784 Sofia, Bulgaria

* lovchinov@iomt.bas.bg

The results in this work represent the influence of the deposition temperature of the aqueous solution (containing $ZrOCl_2$ – 5×10^{-3} M and KCl – 0.1 M) on the properties of ZrO_2 films obtained by electrochemical deposition on SnO2 covered glass substrates is studied. Temperatures of the deposited layers are 60, 65, 70, 75 and 80 °C. Through the implementation of X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), optical profilometry, UV-VIS-NIR and photoluminescence spectroscopy, the temperature dependence of ZnO films properties is revealed. The XRD spectra show the polycrystalline nature of the films at all studied deposition substrate with the typical characteristic reflexes of the ZrO_2. Calculations for the size of the crystallites from the diffraction maxima and the average roughness show that no dependence is observed between them and the deposition temperature. The SEM micrographs show that the ZrO_2 layers are composed mainly of grains of relatively regular shape, as their size increases with increasing deposition temperature. It is demonstrated that the deposition temperature almost no effect on the reflectance and transmittance spectra of the ZrO_2 layers. The low values of the diffuse reflectance and transmittance in the spectral range from 380 to 800 nm could be beneficial for application of similar films as antireflective layers of thin films solar cells.

Acknowledgements:

This research is funded by Bulgarian National Science Fund (BNSF) under the project КП – 06 – Н38/7 (12.2019). Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

Mixed-spin kagome strips

N. B. Ivanov[1,*], F. Liedeker[2], J. Schnack[2], J. Richter[3]

[1] Institute of Solid State Physics, Sofia, Bulgaria
[2] Universitaet Bielefeld, Germany
[3] Universitaet Magdeburg, Germany

* ivanov@issp.bas.bg

Based on analytical strong-coupling expansions, as well as numerical exact diagonalization and DMRG simulations, we study the quantum phase diagram of a Heisenberg kagome strip containing two types of site spins with quantum spin numbers S=1 and σ=1/2 and two different exchange constants (J_1 =J cos θ and J_2=J sin θ) for the nearest-neighbor S-σ and σ-σ bonds, respectively. The system can be regarded as one-dimensional cutting of the kagome lattice composed of spin clusters with a central S spin and four corner s spins. The model is a natural generalization of the spin-1/2 kagome strip [1] and exhibits a rich quantum phase diagram in the semicircle 0< θ< π: For J_2>0 two Haldane-type phases with effective site spins S+4σ and S-4σ are stabilized close to the end points θ=0 and θ=π, respectively. Another spin-1 Haldane state occupies a small region around the point J_1=0. Finally, two different spin-liquid phases, related to the macroscopically degenerate classical canted state, appear between the regions occupied by the above spin-1 phase around J_1=0 and the Haldane-type phases with effective site spins S+4σ and S-4σ [2].

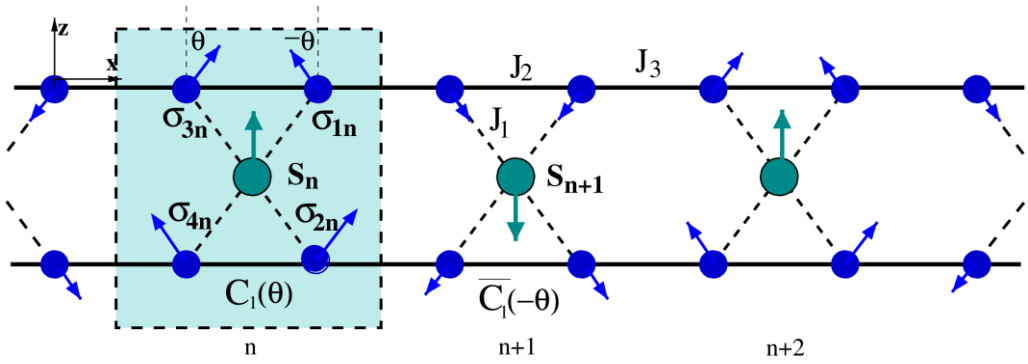


Figure 1. Sketch of the mixed-spin kagome strip

References

1. P. Azaria et al., Phys. Rev. Lett. **81**, 1694 (1998); S. K. Pati, R. R. P. Singh, Phys. Rev. B **60**, 7695 (1999); S. R. White, R. R. P. Singh, Phys. Rev. Lett. **85**, 3330 (2000); A. A. Donkov, N. B. Ivanov, J. Richter, AIP Conf. Proc., **2075**, 020015 (2019).
2. S. I. Petrova, N. B. Ivanov \& J. Schnack, Acta Phys. Pol. A **137**, 976 (2020); N. B. Ivanov, F. Liedeker, J. Schnack \& J. Richter, to be published.

Acknowledgements:

This research was supported by the National Science Foundation of Bulgaria (Grant КП-06-Н38/6/05.12.2019)

Physical properties of SOPC at low temperatures through the Slipid force field

N. Ivanova[1, 2,*] and H. Chamati[2,*]

[1] Department of Physical Chemistry, University of Chemical Technology and Metallurgy, 8 Kliment Ohridski Boulevard, 1756 Sofia, Bulgaria
[2] Institute of Solid State Physics, Bulgarian Academy of Sciences, Tzarigradsko Chaussée 72, 1784 Sofia, Bulgaria

* n.ivanova@uctm.edu, chamati@issp.bas.bg

Slipid (Stockholm lipids) force field is suitable for the description of the physical properties of biological membranes composed of phospholipids at room temperature [1,2]. So far, its accuracy to reproduce the behavior of the thermodynamic and structural quantities of membranes at low temperatures has not yet been tested in sufficient details. In the present study, we compute some characteristic quantities of SOPC (1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine) using GROMACS in conjunction with Slipid force field. The initial configuration of the SOPC system composed of 128 lipid molecules distributed equally in each monolayer and 5120 water molecules was generated with the aid of CHARMM-GUI [2]. Atomistic molecular dynamic (MD) simulations were performed at several temperatures. By virtue of a statistical analysis of trajectories, we computed the main structural parameters of the lipid molecules and thermodynamic quantities characterizing the phase behavior of the bilayer. The results are compared to available experimental data, as well as theoretical predictions. The Slipid force field was found to describe fairly well the structural behavior of the lipids at low temperatures.

References:

1. F. Grote, A.P. Lyubartsev, Optimization of Slipids Force Field Parameters Describing Headgroups of Phospholipids, J. Phys. Chem. B 124, 2020, 8784–8793.
2. N. Ivanova, J. Genova and H. Chamati, Physical properties of SOPC lipid membranes containing cholesterol by molecular dynamics simulation, Adv. Biomembr. Lipid Self-Assem. 34, 2021, 1-30.
3. S. Jo, T. Kim, V.G. Iyer, W. Im, CHARMM-GUI: A web-based graphical user interface for CHARMM, J. Comp. Chem. 29 (11), 2008, 1859-1865.

Acknowledgments:

We acknowledge the financial support from Joint Institute for Nuclear Research (JINR), Dubna, Russian Federation – THEME04-4-1133-2018/2023 and Grant No Д01-229/27.10.2021г. of the Ministry of Education and Science of Bulgaria, as well as the access to the e-infrastructure of the NCHDC part of the Bulgarian National Roadmap on RIs, with the financial support by the Grant No D1-271/16.12.2019.

Dynamic simulation of the quasiparticle excitations spectra in the magnetic bcc iron

Elena Angelova* **and Hassan Chamati**

Institute of Solid State Physics, Bulgarian Academy of Sciences,
Tsarigradsko Chaussee 72, 1784 Sofia, Bulgaria

* angelova@issp.bas.bg

We used the symplectic and scalable LAMMPS algorithm for spin - lattice dynamics to model the coupled relaxation processes of the spin and lattice subsystems to investigate the phonon and magnon dispersion laws of bcc Fe at T=300 K. The atomic interactions were modeled via three semi-empirical many-body potentials of Chamati, Chiesa and Olsson within the embedded atom method (EAM) approach. In the state of mutual equilibrium of the spin and atom ensembles, we have calculated the dynamical matrix of the phonons, the intermediate scattering function, the dynamical structure factor and finally the phonon and magnon spectra in bcc – iron. We found that for a small to moderate wavevector absolute values, the phonon dispersion curves calculated with the use of different approaches agree well with the experimental results obtained from inelastic neutron scattering, while discrepancies between theory and experiment were observed for larger wavevector values, particularly near the zone boundaries (Figure 1).

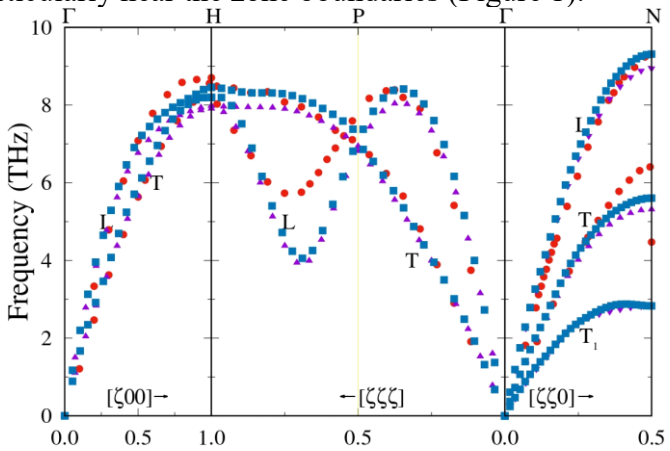


Figure 1. Phonon dispersion curves obtained via molecular and spin dynamics simulation (blue squares) and pure molecular dynamics simulation (purple triangles) of a periodic block of bcc Fe atoms with the aid of Chamati EAM potential. For comparison purposes, the experimental results obtained from inelastic neutron scattering are also plotted with red dots.

References:

1. Elena L. Angelova, Hassan Chamati. Dynamic simulation of the energy spectrum of phonons in the magnetic bcc iron. Comptes rendus de l'Academie bulgare des Sciences, Tome 75, N 2, 2022, P. 197 - 206.

Acknowledgments:

This work was supported by the Joint Institute for Nuclear Research, Dubna, Russian Federation – THEME 01-3-1137-2019/2023 and Grant No D01-229/27.10.2021 of the Ministry of Education and Science of Bulgaria.

Stabilization and characterization of simulated liquid radioactive waste in a new type of cement mixture

Istvan Tolnai*, Margit Fabian, Zoltan Kis, Veronika Szilagyi

Centre for Energy Research, Konkoly-Thege st. 29-33., Budapest, 1121, Hungary

* tolnai.istvan@ek-cer.hu

Boric acid is commonly used as a neutron absorber in pressurized water reactors, with a measurable concentration of up to 16 kg/m^3 in liquid radioactive waste, thus significantly determining their physical and chemical properties. Boric acid waste most often contains radionuclides ^{90}Sr, ^{137}Cs, ^{51}Cr and ^{60}Co. The management of large volumes of liquid radioactive waste poses a significant technological challenge and its environmental impacts must be considered. Safe and long-term inert matrix materials are needed to stabilize the radioactive isotopes in liquid waste. Cement is often used to stabilize intermediate-level liquid waste, in which even the presence of small amounts of boric acid can substantially increase the curing time. During this period radionuclides can easily escape from the system. Additives are used to optimize the curing time. In this work, we investigated a new type of cement mixture for the solidification of liquid radioactive waste and performed its application-oriented analysis [1].

An admixture was added to Portland based cement that changed the macro/micropore ratio of normal concrete from 70/30 to 3/97, increasing chemical stability. To test for boric acid absorption, 50 cm^3 of cylindrical concrete samples were made using different concentrations of boric acid (50g/l, 150g/l and 250g/l) and kept at 20°C for 28 days during the cementation process. Leaching test was conducted on the samples according to ASTM-C1308 [2], and the analysis of the leachates was performed on an inductively coupled plasma optical emission spectrometer (ICP-OES). Mechanical characteristics were determined during compressive strength testing. The distribution of boric acid in the cement samples was assessed by neutron tomography measurements. All the measurements were performed on both the initial specimens and the soaked specimens after the leaching test.

The elemental analysis of the leachates showed an increasing trend for the boron fraction according to the initial boric acid concentration. All three-sample series are characterized by a plateau curve. The results of compressive strength of the concrete bodies before and after the leaching test suggest that the increasing boron concentration is coupled with higher compressive strength. Mechanical tests before and after leaching did not show any detectable difference in strength. The imaging artifact due to beam hardening during the reconstruction of tomogprahic slices was corrected by a function calculated from neutron radiographic transmission measurements on specimens of different heights. The correction function was determined for the 250g/l sample and the results showed a uniform distribution of boron in the volume. In the case of the leached samples, the neutron attenuation coefficient is significantly decreased, however, the magnitude of the decreasing far exceeds the solely effect from the loss of boron, because it also includes the effect of significant water loss. Similar conclusions are expected for different boric acid concentrations.

Based on our studies, Portland cement mixed with water-resistant admixture solidifies liquid boric acid of various concentrations in an even distribution, which can also ensure uniform radionuclide binding.

References:

1. Bruggeman, A., Dubost, E., Ekenved, M., Hooper, E. W., Houbetsov, E. B., Kallonen, I., Lucas, M., Luo, S., Sen Gupta, S. K., Timulak, J., Tsarenko, A. F., Ojovan, M., Viszlay, J., Processing of nuclear power plant waste streams containing boric acid, IAEA-TECDOC-911, 2, 1996, 1-67.
2. ASTM C-1308-21, Standard Test Method for Accelerated Leach Test for Measuring Contaminant Releases From Solidified Waste, ASTM International, 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428–2959, United States (2021).

Measurement of Nonlinear Optical Characteristics of GaN using Femtosecond Z-scan Technique

Mariam Shehadi[1,*], Stefan Karatodorov[1], Lyubomir Stoychev[1], Georgi Yankov[1], Docho Tsankov[2], Boris Shivachev[3], Todor Petrov[1,2]

[1] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784, Sofia, Bulgaria
[2] Technical University of Sofia, 8, Kliment Ohridski St. Sofia-1000, Bulgaria
[3] Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

***** mshehadi@issp.bas.bg

Gallium nitride GaN is a widely used third generation semiconductor with wide bandgap (E_{gap}= 3.4 eV), it has many applications in the field of optoelectronics such as Blue/UV solid state lighting and lasers, optical switching, short wavelength detectors and optical storage devices. The successful implementation of GaN for optoelectronic applications depends strongly on detailed knowledge of its optical properties.

In this work, we measured the third order nonlinear optical characteristics of GaN - nonlinear refractive index n_2 and two-photon absorption coefficient β. The experiment is done employing modified femtosecond z-scan technique [1] at room temperature and at cryogenic temperatures using specially designed crystal cooling system. The obtained results in each regime are discussed.

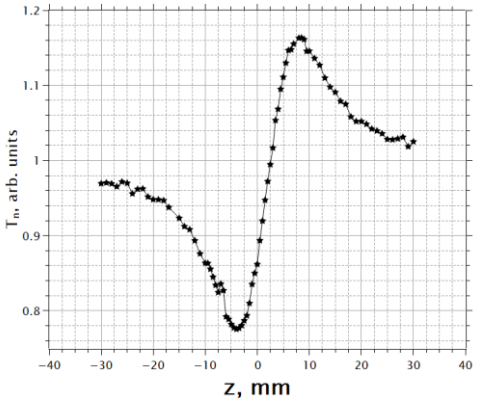


Figure 1. Closed aperture z-scan measurement of the transmittance of GaN as a function of its translation along z-axis in room temperature.

References:

1. M.Sheik-Bahae, A. Said, T. Wei, D. Hagan and W. V. Stryland, Sensitive Measurement of Optical Nonlinearities Using a Single Beam. IEEE JOURNAL OF QUANTUM ELECTRONICS 26, 4, 1990 760-769.

Acknowledgments:

The research is funded by projects: Bulgarian Science Fund DN – 18/7 -10.12.2017, BG05M2OP001-1.001-0008 National center of Mechatronics and Clean Technologies Operational Program: Science and Education for Smart Growth 2014-2020 and ELI "Extreme Light" (Extreme Light Infrastructure BG) D01– 401/18.12.2020.

Ablation damage and threshold in transparent media - case study at ns, ps and fs laser pulses

G. Yankov, S. Karatodorov, V. Mihailov, V. Tankova, E. Iordanova*

Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tsarigradsko Chaussee blvd.,1784 Sofia, Bulgaria

* eiordanova@issp.bas.bg

The present work is a case study of a project concerning investigation on in-depth extensive fundamental research on the plasma formation and dynamics induced by femtosecond infrared laser pulses in solid transparent media. The motivation of the research is based on the specific properties of transparent media after laser irradiation and its applications. Further contributing to the clarification of the mechanism of interactions between laser irradiation and solid transparent materials leading to growth in the development of applications such as surface modification, nanostructure generation, bioimaging and 5D data storage. The dependence of the laser pulse duration as a function of the ablation process is investigated. The experiments are performed on a wide range of processing parameters, including laser power and laser pulses duration. Three types of laser processing are considered including cases of nanosecond picosecond and femtosecond duration of the laser pulses. The applied laser energy is varied from 5 μJ to 250 μJ. The used pulse durations are 35 fs, 100 ns, and 170 ps. The laser ablation measurements are applied on glass samples with dopped silver nanoparticles before and after annealing and ion concentration of 0.1%. The effects of the applied single laser pulses and their consequence laser induced modifications, damages and ablation thresholds are observed and compared.

Acknowledgements: The authors express their acknowledgments to the financial support of: BNSF under the project **КП-06 ПН58/7-2021** entitled “Plasma dynamics and formation induced by femtosecond infrared laser pulses in transparent media”.

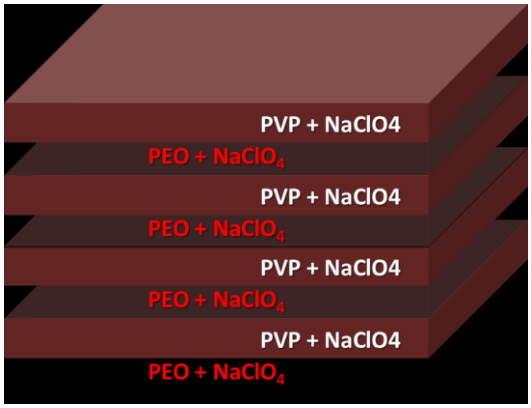
Optical properties of multi-layers structured PEO/PVP solid polymer membranes doped with sodium perchlorate

Hari Krishna Koduru[1,*], Nicola Scaramuzza[2], Tihomir K. Tenev[1], Ilko K. Miloushev[1], Yordan G. Marinov[1]

[1] Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee, Sofia 1784, Bulgaria.
[2] Dipartimento di Fisica, Università degli Studi della Calabria, Via P. Bucci, Cubo 33B - 87036 Rende (CS) – Italy

* koduru@issp.bas.bg

In this present research work, fabrication of multi-layers structured (MLS) polymer membranes has been proposed to understand the variation of the optical bandgap and determine the types of electronic transitions as a function of sodium salt doping concentration[1]. Solid MLS polymer membranes based on PEO/PVP have been prepared by the well-known solution cast technique. The recorded absorption, transmittance and reflectance spectra revealed that, incident energy absorption increased upon increase of salt dopant concentration and a shift of absorption edge towards lower energy region suggests the good complexation between the host polymers and dissociated salt (Na^+, ClO_4^-) ions, which in turn the energy bandgap decrement expected. A detailed investigation has been carried out on the variation of refractive index of all the MLS polymer membranes as a function of salt doping concentration. The miscibility between the sodium salt and the individual polymers present in MLS polymer membranes can be understood from the linear relationship between the refractive index and the volume fraction of the added salt. The increase of extinction coefficient at high wavelengths was observed. The optical band gap measured from the plots of $(\alpha h\upsilon)^x$ versus photon energy ($h\upsilon$) was compared to that determined from the optical dielectric loss. The Urbach energy was found to vary with as a function of sodium salt concentration.



Schematic representation for the proposed multi-layers structured 'PEO/PVP/$NaClO_4$' based polymer electrolyte membrane.

Reference:

1. Ho Mei Law, Jing Yu, etc. A hybrid dual-salt polymer electrolyte for sodium metal batteries with stable room temperature cycling performance. Energy Storage Materials 46 (2022) 182 – 191.

Acknowledgments:

The authors would like to acknowledge the financial support by the BNSF of Bulgaria, under National Scientific Program "Petar Beron i NIE" (P. Beron) contract № KP-06-DB-1/16.12.2019.

Lead Oxide X-ray photoconductive layers for application in direct conversion medical imaging detectors

Oleksandr Grynko[1] and Alla Reznik[1,2,*]

[1] Physics Department, Lakehead University, 955 Oliver Road
Thunder Bay, ON, Canada P7B 5E1
[2] Advanced Detector Devices, Thunder Bay Regional Health Research Institute,
1040 Oliver Rd, Thunder Bay, ON Canada P7B 7A5

* areznik@lakeheadu.ca

X-ray imaging detectors rely on either indirect or direct conversion of X-ray quanta to an electrical signal, with the indirect method most commonly used in commercial systems. In the indirect scheme, the multi-stage conversion process begins with a scintillator converting X-ray quanta into optical photons. The optical photons in turn diffuse through a phosphor and then are converted to electrons by an array of photodiodes. In the direct method, the X-ray quanta are absorbed in a photoconductor that directly creates electron-hole pairs. The electrons and holes are then separated by a bias electric field to generate an electrical signal in the imaging array. With the right photoconductor, the direct conversion scheme offers high spatial resolution, limited only by the pixel size of the imaging array and improved dose efficiency down to the lowest required radiation exposure.

Here we present the results of the ongoing into new X-ray photoconductive structures based on two different polymorphs of Lead Oxide (PbO) photoconductors for application in direct conversion X-ray detectors, namely, polycrystalline Lead Oxide (poly-PbO) and amorphous Lead Oxide (a-PbO) [1-3]. Optimization of PbO technology was focused on improving the collection of the X-ray–generated charge and solving the problem of signal lag, that is, the residual signal after the end of X-ray exposure. The latter is one of the main obstacles to the use of disordered semiconductors as X-ray–to–charge transducers since the presence of signal lag limits the application of direct conversion detectors to static imaging only and obscures the full potential of this detection method in diagnostic imaging. The approaches we have taken to improve the X-ray performance of PbO-based photoconductive structures can be applied to other promising materials to solve the problems common to disordered photoconductors, paving a way for their use in practical detectors.

Reference:

1. O. Grynko, T. Thibault, E. Pineau, A. Reznik. Engineering of a Blocking Layer Structure for Low-Lag Operation of the a-PbO Based X-ray Detector. IEEE Transactions on Electron Devices. 68(5), (2021) 2335-2341.
2. O. Grynko, A. Reznik. (2022). Progress in Lead Oxide X-ray Photoconductive Layers. Edited by Safa O. Kasap. Photoconductivity and Photoconductive Materials 2 V Set.: 20, Wiley, United States.
3. O. Grynko, T. Thibault, E. Pineau, G. Juska, A. Reznik, A. Bilayer lead oxideX-ray photoconductor for lag-free operation. Nature Scientific Reports. 10(1) (2020) 20117.

Acknowledgments:

Research was funded by Teledyne DALSA, the Natural Sciences and Engineering Research Council (NSERC), and MITACS programs.

ABSTRACTS OF FIRST POSTER SESSION

1.1. Effect of the nanofiller concentration on its dispersion in a system of liquid crystalline SB(3R)-11 and single wall carbon nanotubes

Ginka Exner[1,*], Yordan Marinov[2], Bhyranalyar Veerabhadraswamy[3], Channabasaveshwar Yelamaggad[3], Peter Rafailov[2], Veselina Georgieva[1]

[1]Faculty of Physics and Technology, Plovdiv University "Paisii Hilendarski", 24 Tsar Asen Str., Plovdiv 4000, Bulgaria
[2]Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., Sofia 1784, Bulgaria
[3]Centre for Nano and Soft Matter Sciences, Arkavathi Campus, Survey 7, Shivanapura, Dasanapura Hobli, Bangalore – 562162, India

* ginka.exner@gmail.com

Designing materials with new or altered properties is on demand nowadays. One way of developing new materials is to prepare composites. A lot of research has been devoted to nanocomposites containing single wall carbon nanotubes (SWCNTs) due to their attractive electrical, optical, thermal and mechanical properties. The main challenge when employing SWCNTs as a nanofiller is still their homogeneous dispersion in the main matrix because of the strong tendency of aggregation and the difficult alignment [1]. This problem can be overcome in composites with liquid crystals (LC). Such an approach would lead to double gain – to alignment of both- SWCNT and LC molecules - and an opportunity to tune the properties by means of the nanofiller concentration and/or by external stimuli (electric field, temperature, light and etc.).

In the present work, nanocomposites from recently synthesized ferroelectric and optically active liquid crystal SB(3R)-11 and SWCNTs have been investigated. The effect of the nanofiller concentration was studied in the range from 0.01 up to 10 wt.%. Differential scanning microscopy (DSC), Polarized optical microscopy (POM), and Raman spectroscopy (RS) were involved in the tests. The DSC results show clear differences between the neat SB(3R)-11 and the nanocomposites. The POM results confirm a good dispersion in all cases. A new finding is that SB(3R)-11 tolerates a dispersion of as high as 10 wt% of SWCNTs. This is believed to be facilitated by the existence of preordered states in the solution, where SB(3R)-11 molecules are attached onto the SWCNTs surface so that LC decorated SWCNT fibres are formed. The fibres prevent the aggregation at elevated temperatures, after the solvent evaporation, thus improving greatly the dispersion. The existence of such interactions on a molecular level between SB(3R)-11 and SWCNTs was confirmed by RS.

References:

1. S. B. Sumandra, B. Mahendra, F. Nugroho, Y. Yusuf, Alignment of carbon nanotubes under the influences of nematic liquid crystals and electric fields — an analytical study, Int. J. Comput. Mater. Sci. Eng. (2022), 11(2), art.n. 2150033.

Acknowledgment:

This work was supported by the National Science Fund of Bulgaria, the Ministry of Education and Science, contract No. KP-06-N58/6/2021, "Structural and functional investigations of liquid-crystal nanocomposites for applications in photonics, sensorics, and biomedicine".

1.2. Investigation of ideal star polymers in confined geometries

J. Halun[1,*] and Z. Danel[2]

[1] *Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland*
[2] *Faculty of Materials Engeeniring and Physics,*
Cracow University of Technology, Kraków, Poland

* joanna.halun@ifj.edu.pl

Taking into consideration the well known polymer–magnet analogy developed by de Gennes [1] the calculations of the depletion interaction potentials, the depletion forces and the monomer density profiles for a dilute solution of phantom ideal star-shaped polymers with 3,4,5 – arms in a Θ−solvent confined in a slit geometry of two parallel repulsive walls and for the mixed case of one repulsive and the other one inert wall were performed. Furthermore, taking into account the Derjaguin approximation [2] the monomer density profiles for phantom ideal star-shaped polymers confined in a solution of big colloidal particles with different adsorbing or repelling properties were calculated. Moreover we investigate a dilute polymer solution between wall and small particle. Our calculations are concentrated on the case of small colloidal particle of size R much smaller than typical polymer lenght, such as the radius of gyration Rg; $R \ll Rg$. The obtained results are in good qualitative agreement with numerical results obtained by molecular dynamics simulation [3].

References:

1. P.G. de Gennes, Scaling Concepts in Polymer Physics (Cornell University Press, Ithaca, NY, 1979).
2. B.V. Derjaguin, Kolloid-Z. 69 (1934) 155.
3. J. Halun, P. Karbowniczek, P. Kuterba, Z. Danel, Entropy (2021).

1.3. PEO/Starch-nanocrystals based Solid Polymer Electrolyte Membranes for Magnesium – Ion Conducting Applications

Yordan G. Marinov[1,*], Hari Krishna Koduru[1], Ginka K. Exner[2], Nicola Scaramuzza[3]

[1] Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., Sofia 1784, Bulgaria
[2] Faculty of Physics and Technology, Plovdiv University "Paisii Hilendarski", 24 Tsar Asen Str., 4000, Plovdiv, Bulgaria
[3] Dipartimento di Fisica, Università degli Studi della Calabria, Via P. Bucci, Cubo 33B – 87036, Rende (CS) – Italy

* ymarinov@issp.bas.bg

The pursuit of significant improvements in the field of flexible electronic devices necessitate for the development of advanced technologies for flexible batteries in order to meet the requirements of next generation devices with required safety attributes [1]. Currently, there is a continuous increase of publications on the fabrication of novel solid polymer electrolytes (SPEs) membranes for their effective utilization in super capacitors, fuel cells, energy storage devices and dye sensitized solar cells [2]. In our study we will present PEO/SNCs (Starch-nanocrystals) based nanocomposite electrolyte membrane complexed with $MgBr_2$ salt (15 wt.%) and fabricated by following conventional solution casting technique. The effect of incorporation of salt ions on microstructural properties of host matrix of 'PEO/SNCs' were investigated by means of XRD, FTIR, DSC studies. The modifications in nature of diffraction peaks and vibrational modes of nanocomposites reveled the formation of strong hydrogen bondings and cross links between SNCs and salt ions. A decrease of melting and glass trasnition temperatures of host matrix was noticed as a result of salt doping. The complex electrochemical impedance measurements were carriedout in the applied frequency range of 0.1 Hz – 1 MHz and in the temperature range of 303 K – 373 K. The 'PEO/SNCs' composite complexed with 15 wt.% salt was demonstred room temperature ionic conducvity of 7.8×10^{-8} S/cm.

References:

1. G. Qian, X. Liao, Y. Zhu, F. Pan, Xi Chen, Y. Yang. Designing Flexible Lithium-Ion Batteries by Structural Engineering. ACS Energy Lett. 03 2019, 690.
2. K. Fu, Y.H. Gong, J.Q. Dai, A. Gong, X.G. Han, Y.G. Yao, C.W. Wang, Y.B. Wang, Y.N. Chen, C.Y. Yan, Y.J. Li, E.D. Wachsman. Flexible, solid-state, ion-conducting membrane with 3D garnet nanofiber networks for lithium batteries. Proceedings of the National Academy of Sciences of the United States of America 113 2016, 7094.

Acknowledgements:

This work was supported by the BNSF of Bulgaria under National Scientific Program "Petar Beron i NIE", contract № KP-06-DB-1/16.12.2019.

1.4. Volatile organic compound vapor sensing with nano-thin Langmuir-Blodgett phospholipide monolayer

Yordan G. Marinov*, Todor E. Vlakhov, Georgi B. Hadjichristov

Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria

* ymarinov@issp.bas.bg

We report electrical sensor composed of phospholipidic Langmuir-Blodgett (LB) monolayer. The sensing element was developed for detecting vapors of volatile organic compounds (VOCs) such as methanol, ethanol, hexane, cyclohexane, chloroform, tetrachloromethane, and petroleum ether, at concentrations up to 0.8 g/dm^3. Due to their high vapor pressure, VOCs are readily transformed to the vapor phase. Such vapors (gases) may often be hazardous to human health, even being as air pollutants at relatively low concentration.

In our work, we used nano-thin (~ 6 nm thickness) sensing LB molecular monolayer of phospholipid dipalmitoyl-phosphatidyl-ethanolamine (DPPE) [1] that was deposited on micro-patterned interdigital electrodes [1]. The electrical response of the assembled sensor element was measured by means of complex electrical impedance spectroscopy (EIS) in the frequency range 0.1 Hz – 3 MHz of the applied electrical field. The gas/vapor in-field sensing was achieved in-plane of the LB monolayer. Due to the gas/vapor sorption by the DPPE LB monolayer (a mass-change effect), the impedimetric response of the LB monolayer is changed. The analyses of the VOC vapor-induced change of both real and imaginary parts of impedance spectra of DPPE LB monolayer can be used for quantitative determination of the VOC concentration.

The obtained results show that in this way one can reliably detect vapors of various VOCs. The suitability of the investigated DPPE LB film for practical sensing of VOC vapors at room temperature was demonstrated. The impedimetric behavior of phospholipid DPPE LB monolayer deposited on interdigital electrodes was extremely sensitive to the electrostatic interaction of DPPE phospolipid LB monolayer with VOC vapors. Thus, DPPE lipid LB monolayers and EIS can be used in electrically functional portable impedance biosensors of VOC vapors with in-field real-time monitoring, e.g., electronic microdevices for security and ecological monitoring.

References:

1. G. B. Hadjichristov, Y. G. Marinov, T. E. Vlakhov, N. Scaramuzza. Phospholipid Langmuir-Blodgett nano-thin monolayers: electrical response to Cadmium ions and harmful volatile organic compounds. Advances in Biomembranes and Lipid Self-Assembly 34, 2021, Chapter 5, pp.129–172.

Acknowledgements:

Work supported by the Ministry of Education and Science (the National Science Fund of Bulgaria) – research project "New effects in nano-thin ordered organic films (Langmuir and Langmuir-Blodgett) and their use for conceptual development of a new generation of biosensors for working in a fluid environment at ambient conditions and real-time monitoring of hard-to-find water pollutants (anti-terrorism) or early diagnosis by tumor markers (acronym NanoBioSensors)" - contract № KP-06-OPR 03/9).

1.5. Formulation and characterization of Benzydamine loaded casein/chitosan nanocomplexes

Maria Marudova[1,*], Sofia Milenkova[1], Nikolay Zahariev[2,3], Bissera Pilicheva[2,3]

[1] Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski", 24 Tsar Asen Str.,4000 Plovdiv, Bulgaria
[2] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Medical University of Plovdiv, 15A Vassil Aprilov Blvd, 4002 Plovdiv, Bulgaria
[3] Research Institute, Medical University of Plovdiv, 15A Vassil Aprilov Blvd, 4002 Plovdiv, Bulgaria

* marudova@uni-plovdiv.net

The objectives of the present study were to synthesize casein/chitosan nanocomplexes, which are able to immobilize and release Benzydamine in a controlled manner, and to investigate the influence of casein/chitosan ratio on the their morphological, physico-chemical and drug career characteristics. The complexes were obtained by electrostatic interaction at pH 6, at which casein in negatively charged (isoelectric point is 4.6) and chitosan is protonated (pKa = 6.5). The yield of the complexation was the lowest for chitosan excess particles (18.4%) and increased to 83.5% for casein excess particles. The particle size was examined by dynamic light scattering (DLS) method and depending on the casein/chitosan ratio varied in the range from 400 nm to several microns. Atomic force microscopy (AFM) was used to assess the morphological properties of the nanocomplexes. It was found that the Benzydamine loading was minimal (15%) in the stoichiometric complex maximal (30%) in complexes with casein/chitosan ratio 5:1. The mechanism of Benzydamine release was defined as diffusion and significantly depended on the swelling of the complexes.

Acknowledgements:

The authors gratefully acknowledge the financial support of the project MU21-FTF-003, Department of Scientific Research at the Plovdiv University.

1.6. Numerical calculations of the monomer density profiles of real ring polymer chains in a slit geometry of two parallel walls with mixed b.c.

Piotr Kuterba[1,*], Zoriana Danel[2], Wolfhard Janke[3], Henrik Christiansen[3]

[1] *Institute of Theoretical Physics, Jagiellonian University*
[2] *Faculty of Materials Engineering and Physics, Cracow University of Technology*
[3] *Institut für Theoretische Physik, Universität Leipzig*

* piotr.kuterba@uj.edu.pl

We have used molecular dynamics simulations to obtain the monomer density profiles for real linear and ring polymer chains of 360 monomers length with different topological structures such as: 0_1, 3_1, 6_1, 7_1 and 9_1 in a slit geometry of two parallel walls with one attractive and another repulsive surface. We have used Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software to perform simulations with Verlet integration algorithm. The interactions between monomers were simulated as Lennard-Jones 12-6 potential, for bonds we have used Finitely Extensible Nonlinear Ellastic (FENE) potential and the interaction with the walls was taken into account via Lennard-Jones 9-3 potential. We observed that the number of adsorbed monomers on the surface decreases with increasing entanglement of polymer. Polymer chains start desorbing from the surface of the wall with higher temperatures as the fluctuations of the polymers increase. These results are important for better understanding the nature of the depletion forces which arise in a slit geometry of two parallel walls with mixed b.c. Besides, we discuss potential applications of such models in the context of the polymer abundance and size.

1.7. Benzydamine hydrochloride immobilization in multilayer structures based on lyophilized polylactic acid and poly(ε-caprolactone)

A. Grigorov*, A. Viraneva, M. Marudova, T. Yovcheva

Department of Physics, University of Plovdiv, 24, Tzar Assen, str, 4000, Plovdiv, Bulgaria

* aleksandar.grigorov@abv.bg

The present article examines the immobilization and release of a model drug benzydamine hydrochloride from polyelectrolyte multilayers (PEMs), created on the surface of corona charged lyophilized films from polylactic acid (PDLA) and poly(ε-caprolactone) (PEC). The base lyophilized substrates were charged under either positive or negative corona discharge for 1 minute with 5kV voltage applied to the corona electrode and 1kV voltage of the same polarity applied to the grid. The time dependences of the normalized surface potential for both types of lyophilized substrates, charged either positively or negatively, were determined. Solutions of 1% casein in phosphate buffer (pH 8) and 0.1% chitosan in acetate buffer (pH 5) with added benzydamine hydrochloride were prepared. The multilayers were created with the use of a Layer-by-Layer (LbL) deposition technique, with the first deposited layer always possessing different charge to that of the base substrate. The loading efficiency and drug release kinetics of the chosen model drug were carried out spectrophotometrically.

Acknowledgements:

The authors gratefully acknowledge the support of the project BG05M20P001-1.002-0005, Personalized Innovative Medicine Competence Center (PERIMED).

1.8. Graphene oxide induced sub-structures of bi-tilted smectic CG in dimer liquid crystals

B. Katranchev*, M. Petrov, H. Naradikian, P. Rafailov

Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* boykopk@issp.bas.bg

A series of nanocomposites, built of hydrogen-bonded in dimmer liquid crystal (HBDLC) p-n-heptyloxybenzoic acid (7OBA) and Graphene oxide (GO) exhibiting a cascade of phase transitions and phases not typical for pristine 7OBA, were observed and investigated by optical polarization microtexture analysis and confirmed by temperature-dependent Raman spectroscopy, as well as by differential scanning calorimetry. GO is an useful and promising nanomaterial for graphene based applications in electronic, photonics and biology. Unlike conventional graphene it provides wide range of chemical methods for attachment of various functional groups to its surface for control optical transparency, electrical and thermal conductance. We use such effective functionalizing properties of GO to study the generation and development of smectic CG phase in its bi-tilted configuration, exposed by two detached sub-structures denoted as CGcl (clinic) and CGln (leaning), in nanocomposites of 7OBA with admixture of GO. For the appearance of the CG phase with its substructures we propose an explanation based on the π–π interaction of the 7OBA dimmer's and biphenyl molecular rings with graphene hexagons, attended by hydrogen bonding of dimmers, in closed and open conformations, with hydroxyl functional groups, located on the periphery of the GO sheets. Due to these complex interactions the dimmer molecule bend and passes in 3D different coupling combinations of the clinic and leaning degree of freedom of the doubly tilted molecular geometry in the CG ordering. We propose molecular and macroscopic models for the 7OBA ordering in the substructures CGcl and CGln. We also demonstrate that bent-dimer domination produces a triclinic tilted smectic-CG phase, in its two sub-structures, with C1 symmetry being chiral, biaxial, and exhibiting anisotropic in-layer fluidity. The electro-optical investigations in low frequency ac and dc electric fields of this phase indicate that it possesses a permanent ferroelectric polarization (polar vector) in a direction oblique to the layers. In combination with the established helical properties, expressed by left and right handedness, this confirms that the liquid CG phase, is ferroelectric in the bulk, like that in solid ferroelectrics, thus reminding for controllable photonic functional devices.

Acknowledgements:

This work was supported by the National Science Fund of Bulgaria, the Ministry of Education and Science, contract No. KP-06-N58/6/2021, "Structural and functional investigations of liquid-crystal nanocomposites for applications in photonics, sensorics and biomedicine".

1.9. Surface Modification of Polyethersulfon Nanofiltration Membrane for Improving Water-Ethanol Separation

Darinka Christova[1,*], Maya Staneva[1], Sijka Ivanova[1], Mariela Alexandrova[1], Philip Ublekov[1], Maria Dencheva-Zarkova[2], Julia Genova[2], Irene Tsibranska[3], Bartosz Tylkowski[4]

[1] *Institute of Polymers, Bulgarian Academy of Sciences, Akad. G. Bonchev St., Block 103A, 1113 Sofia, Bulgaria*
[2] *Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria*
[3] *Institute of Chemical Engineering, Bulgarian Academy of Sciences, Akad. G. Bonchev St., Block 103B, 1113 Sofia, Bulgaria*
[4] *Centre Tecnològic de la Química de Catalunya, Carrer de Marcel·lí Domingo, 43007 Tarragona, Spain*

* dchristo@polymer.bas.bg

Nowadays membrane technologies play a key role in the attempts for turning many industrial processes green. Recent advances in the development of innovative extraction and separation methods in winemaking industry are mainly related to membrane technology and utilization of various synthetic polymer membranes due to the low operating and maintenance costs, mild operating conditions of temperature and pressure, easy control and scale-up, and high selective separations. In this context surface properties of the membrane are of great importance especially when aiming at higher permeability and selectivity together with preserving bioactive components. This paper reports on the surface modification of a commercial Microdyn Nadir polyethersulfon membrane (NP030P) aiming at improved water-ethanol separation. To achieve this, three types of poly(vinyl alcohol) (PVA) copolymers of varied hydrophilic-lipophilic balance were synthesized and tested as modifiers: wholly hydrophilic PVA graft copolymer with poly(N,N-dimethyl acrylamide) side chains (PVA-*g*-PDMAAm), amphiphilic poly(vinyl alcohol-*co*-vinyl acetal)s (PVA-Ac) with different chemical composition, as well as highly hydrophobic PVA copolymer with grafted poly(methyl methacrylate) chains (PVA-*g*-PMMA). Copolymers' chemical structure and composition as well as properties in aqueous and mixed organic solvent solutions were evaluated by conventional analytical techniques. Methods for thin film deposition including spin-coating and phase inversion were applied for membrane modification. Alteration of the hydrophilic-lipophilic balance at the membrane surface was studied by contact angle measurements whereas the surface microstructure was characterized by attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) and optical and scanning electron microscopy. The feasibility of tailoring membrane surface to specific requirements by using PVA-based copolymer was assessed and the influence of copolymer structure and composition on the membrane properties was considered.

Acknowledgements:

This work was supported by the Bulgarian National Science Fund under the grant agreement no. КП-06-Н47/1/26.11.2020. We thank Assoc. Prof. Dr. Karekin Esmeryan for contact angle measurements.

1.10. On the Critical Specific Heat Capacity of a Model of Structural Phase Transitions with Long-range Interaction

Ekaterina S. Pisanova*

Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski", 24 Tzar Assen Str., BG-4000 Plovdiv, Bulgaria

* katia_pisanova@abv.bg

An exactly solvable lattice model describing structural phase transitions in an anharmonic crystal with long-range interaction (decreasing at large distances r as $r^{-d-\sigma}$, where d is the space dimensionality and $0<\sigma\leq 2$) [1, 2, 3] is considered near to its classical critical point T_c. The behaviour of the bulk critical specific heat capacity c of the model is studied at temperatures $T\to T_c^{\pm}$, i.e. in both the disordered phase ($T>T_c$) and the ordered phase ($T<T_c$). For $\sigma<d<2\sigma$ at $T\to T_c^{+}$, i.e. in the disordered phase, we derive $c(T)\approx 1-D(T/T_c-1)^{-\alpha_s}$, where both the coefficient D and the critical exponent α_s depend only on the ratio d/σ. From the result obtained one can see that for fixed $d/\sigma=x$ $(1<x<2)$ the temperature dependence of the critical specific heat capacity is the same for chain ($d=1$ and $\sigma=1/x$), thin layer ($d=2$ and $\sigma=2/x$) and 3-dimensional system ($d=3$ and $\sigma=3/x$), as the cases with $\sigma\geq 2$ correspond to short-range interaction. The obtained here critical exponent $\alpha_s<0$ coincides with this one of the classical mean spherical model [3] which belongs to the same universality class. For arbitrary d at all temperatures $T\leq T_c$, it is shown that the specific heat capacity keeps its maximum value $c(T)=1$ and the Dulong – Petit law of the classical thermodynamics holds in both the classical critical point T_c and the ordered phase.

References:

1. T. Schneider, E. Stall and H. Beck, Exactly soluble models for distortive structural phase transitions, Physica A 79 (1975) 201.
2. N. M. Plakida, A. Radosz and N. S. Tonchev, Exactly solvable model of a structural phase transition, Phase Transitions 29 (1991) 179.
3. J. G. Brankov, D. M. Danchev and N. S. Tonchev, The Theory of Critical Phenomena in Finite-Size Systems – Scaling and Quantum Effects, Vol. 9 of Series in Modern Condensed Matter Physics (World Scientific, Singapore, 2000).

1.11. Thin films of nanocomposites from glassy-state tris(keto-hydrozone) discotic liquid crystals and single-walled carbon nanotubes, for optoelectronics

Georgi B. Hadjichristov*, Yordan G. Marinov, Todor E. Vlakhov

Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria

* georgibh@issp.bas.bg

Discotic liquid crystals (DLCs) have disk-like molecules, consisting of a mesogenic core and flexible tails. As a new field of scientific and commercial interest, DLCs are used in nanocomposite design by combination of DLCs with nano-sized species [1]. Such novel multifunctional nanocomposite liquid-crystalline (LC) materials have found diverse applications in organic electronics, biosensing, energy storage, etc. [2]. Here we study photoresponsive thin films (thickness 3 μm) based on star-shaped tris-hydrazone discotic mesogen LTTH6 – a macromolecular DLC structure with three branches [3]. In this DLC were incorporated single-walled carbon nanotubes (SWCNTs) with diameter of 1.5 nm, at concentration of 1 wt.%. The SWCNT/LTTH6 films were characterized by UV-Vis-NIR spectroscopy and polarizing optical microscopy. The studied nanocomposite exhibits a columnar LC phase at room temperature that is a valuable property for practical application, e.g., in organic optoelectronics and sensorics.

Upon illumination of SWCNT/LTTH6 films with a low-intensity (~ 1 mW/cm^2) continuous light in the visible spectral range, their photo-electrical response was analyzed by complex electrical impedance spectroscopy in the frequency range from 1 Hz to 1 MHz of the applied electric field. The results obtained show that the electrical conductivity of the SWCNT/LTTH6 films can be controlled by light, utilizing the controllable intrinsic thermal behavour of the electrical conductivity of SWCNTs and SWCNT network formed in the SWCNT/LTTH6 nanocomposite. The photo-controllable effect observed by glassy-like columnar state of considered DLC nanocomposites is reversible. This property would be of practical interest for optoelectronic applications, and the studied SWCNT/LTTH6 nanocomposites will be capable of serving as active layers for sensors and organo-electronic devices at ambient temperature.

References:

1. S. Kumar. Investigations on discotic liquid crystals. Liquid Crystals 47(8), 2020, 1195–1203.
2. A. Joshi, V. Manjuladevi, R. K. Gupta, S. Kumar. Morphological transformation in supramolecular assembly of discotic liquid crystal molecules by silver nanoparticles and its sensing application. Nanotechnology 31(36), 2020, Art. No. 365605.
3. G. K. Exner, Y. G. Marinov, G. B. Hadjichristov. Novel nanocomposites of single wall carbon nanotubes and discotic mesogen with tris(keto-hydrozone) core. Compt. Rend. Acad. Bulg. Sci. 73(9), 2020, 1217–1224.

Acknowledgements:

This work was supported by the Ministry of Education and Science of Bulgaria, through the National Science Fund of Bulgaria (research project No. KP-06-N58/6/2021, “Structural and functional investigations of liquid-crystal nanocomposites for applications in photonics, sensorics and biomedicine”).

1.12. Gas Sensing of Volatile Organic Compounds by Arachidic Acid Langmuir-Blodgett Sensing Layers and Electrical Impedance Spectroscopy

George R. Ivanov[1], Todor Vlakhov[2], Evgenia Bogdanova[1], Georgi B. Hadjichristov[2], Yordan G. Marinov[2,*]

[1] University Laboratory "Nanoscience and Nanotechnology", University of Architecture, Civil Engineering and Geodesy, blvd. Hr. Smirnenski, 1, 1064 Sofia, Bulgaria
[2] Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria

* ymarinov@issp.bas.bg

Volatile Organic Compounds (VOCs) like acetone, ethanol, chloroform and others, can contaminate the environment and human health, therefore it is necessary their detection. Their reliable detection can also help in e.g. disease diagnosis or test the fruit freshness. However, some of them are difficult to detect because are inert, highly dilute and volatile, and their sticking activity to various types of surfaces is low. In this study we use one of the most well studied molecules in the area of Langmuir-Blodgett (LB) films – Arachidic Acid (AA) as a sensing coating, deposited on the surface of 434 MHz Surface Acoustic Wave Resonator (SAWR). The gravimetric sensor response of such assembly was very efficient. Additionally, the interdigitated electrodes on the surface of the SAWR were used to measure the impact of the vapors of six VOCs, applying Electrical Impedance Spectroscopy (EIS) (Figure 1). In air, AA is an excellent dielectric with resistance in the TΩ range. When subjected to VOC vapors and water tested here, the resistance of the AA LB films is changed and can go down to MΩ range. We have measured also the kinetics of such change, which is especially dramatic for the polar molecule of methanol. Combining gravimetric and electrical characterization with EIS on a single device gives additional selectivity option. One transduction method can give similar results, while the other method can differentiate the analyte. Besides VOC detection, the proposed sensing element coated with different number of AA LB layers in different phase of the AA LB layer, can provide multifunctional applications.

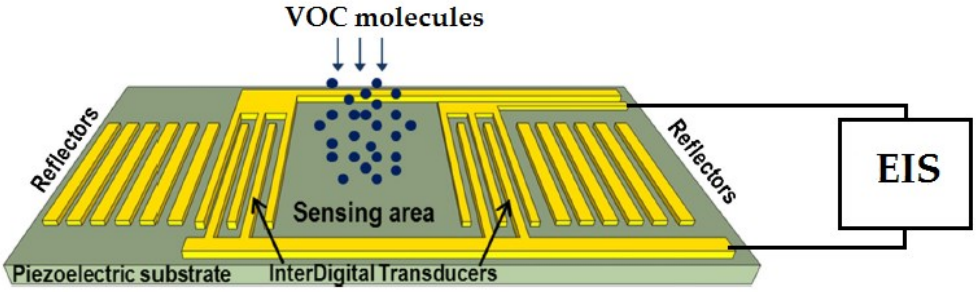


Figure 1. Schematic of measurement with EIS and by SAWR device coated with AA LB film.

Acknowledgements:

This research was funded by the Bulgarian National Science Foundation, grant numbers: KP-06-OPR 03/9 and KP-06-Russia/8. Work supported by the BNSF of Bulgaria contract No. KP-06-N58/6/2021.

1.13. Comparative Study of Protective Coating Properties of CR-39 Based Ophthalmic Lenses

Gergana Mihova*, Andreana Andreeva, Nikolay Zografov

Faculty of Physics, Sofia University, 5 J. Bourchier Blvd, 1164 Sofia, Bulgaria

* gerganamm@uni-sofia.bg

This research aimed to study the mechanical durability and contamination resistance of organic spectacle lenses for everyday use, based on CR-39 (Poly(allyl diglycol carbonate) (PADC).

The widely used in the past mineral lenses are being replaced by new organic materials [1], which are significantly lighter, but at the same time more vulnerable to scratches and chemical substances. Their disadvantages are overcome by applying special protective surface coatings [1,2]. The most common ones are Hard Multilayer Coatings (HMC). The protective coatings offer better mechanical properties due to mineral particle additives, improved anti-reflective properties, as well as additional hydrophobic, lipophobic, dust-resistant layers, infrared and blue light filters, etc. Comparisons of their optical properties have been made [3], but there is a lack of data on their mechanical properties [4]. This determines the main goal of the presented research, to obtain systematic data about the mechanical properties of various HMC applied to the widely used polymer CR-39 with application in eyeglass lenses [1] and to provide comparative analysis, based on the conducted experiments and measurements.

The objects of this research are selected corrective lenses from three different manufacturers. Each brand is represented by a reference uncoated lens and three other lenses with different types of protective coating. Each sample has been characterized experimentally in our laboratory conditions according to three indicators of the surface coating: microhardness, roughness, and wetting properties.

The results of this study allow the eye specialists to be able to make an objective and informed comparison of different factors that are important for the daily usage of the spectacles, in order to select the most suitable product for their needs.

References:

1. R. Pillay, R. Hansraj, N. Rampersad. Historical Development, Applications and Advances in Materials Used in Spectacle Lenses and Contact Lenses. Clinical Optometry 12, 2020 157-167.
2. F. Samson. Ophthalmic Lens Coatings. Surface and Coatings Technology 81, 1996 79-86.
3. M. Schubert, D. Poxson, F. Mont, J. K. Kim, E. Schubert. Performance of Antireflection Coatings Consisting of Multiple Discrete Layers and Comparison with Continuously Graded Antireflection Coatings. Applied Physics Express 3, 2010 082502.
4. J. Caro, N. Cuadrado, I. González, D. Casellas, J.M. Prado, A. Vilajoana, P. Artús, S. Peris, A. Carrilero, J.C. Dürsteler. Microscratch Resistance of Ophthalmic Coatings on Organic Lenses. Surface and Coatings Technology 205, 2011 5040–5052.

Acknowledgements:

This study is supported by the Bulgarian State Budget and Sofia University "St. Kliment Ohridski" under project 80-10-124/16.5.2022. The laboratory is supported by the project CoE "National center of mechatronics and clean technologies" BG05M2OP001-1.001-0008-C01.

1.14. Chitosan/grapeseed oil multicomponent edible films – design and properties

Biser Gechev[1], Gabor Zsivanovits[2,*], Angel Iliev[2], Maria Marudova[1]

[1] Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski", 24 Tsar Asen Str.,4000 Plovdiv, Bulgaria
[2] Institute of Food Preservation and Quality, Plovdiv, Agricultural Academy of Bulgaria, 153 Vassil Aprilov Blvd, Plovdiv, Bulgaria

* g.zsivanovits@canri.org

Physical and antioxidant properties of edible chitosan films, formed by casting method, were investigated. The films were loaded with grapeseed oil (GsO), which is a strong antioxidant, contains vitamin E and protects human cells against cancer. The mechanical tensile and puncture characteristics, colour, thickness, water uptake, barrier, antioxidant (DPPH and FRAP assay) and swelling properties of the films were investigated. The results showed that the addition of GsO to chitosan film improved the gas barrier and the mechanical properties. The increased antioxidant activity of the films is a prerequisite for extending the shelf life of food products packaged in them.

Keywords: chitosan, grapes seed oil, physical properties, antioxidant properties, mechanical characteristics, swelling

Acknowledgements:

This research was funded by the Bulgarian Ministry of Education and Science under the National Research Programme "Healthy Foods for a Strong Bio-Economy and Quality of Life" approved by DCM # 577 / 17.08.2018" and by Bulgarian National Science Fund (BNSF), grant number KP-06-N37/29". "Innovative packaging, extending the shelf life of fruits and vegetables by multicomponent edible coatings (ECOATFRUIT)".

1.15. Effect of pressure and cross-flow velocity on membrane behavior in red wine nanofiltration

M. J. Dencheva-Zarkova[1], J. L. Genova[1,*], I. Tsibranska[2]

[1] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee, Blvd., 1784 Sofia, Bulgaria
[2] Institute of Chemical Engineering, Bulgarian Academy of Sciences, Acad. G. Bonchev Str. Bl. 103, 1113 Sofia, Bulgaria

* ulia@issp.bas.bg

Nanofiltration has found numerous applications in winemaking industry as an effective separation technology, allowing for the recovery and concentration of valuable bioactive compounds from wine/grape by-products, as well as for wine dealcoholization. However, the assessment of membrane fouling remains essential for a stable and sustainable membrane operation. Because of its complex nature, wine components (colloids and solutes such as polysaccharides, polyphenols, proteins) contribute to different mechanisms of fouling. The increase of fouling propensity as well as the conditions that contribute to it - transmembrane pressure and cross-flow velocity – are studied in the present study. Quantitative characteristics as fouling indices are discussed. Results with red wine (Mavrud) nanofiltration are obtained using two NF membranes - NADIR NP030 P (asymmetric sulfonated PES, MWCO 400-500 Da) and Alfa Laval NF99HF (thin film composite polyester, MWCO 200 Da). Nanofiltration runs were carried out by a constant-pressure cross-flow filtration system MaxiMem, Prozesstechnik GmbH with a rectangular flat-sheet membrane of 215 cm^2 active area.

Effect of transmembrane pressure (TMP) (10 to 50 bar) and cross-flow rate (1-3 l/min) on the permeate flux are discussed in view of membrane fouling. Higher operating pressures enhance the permeate flux but may also lead to increased fouling. The two membranes show very different permeate fluxes, the ones measured with NF9HF being 10-20 times higher. Increase in cross-flow velocity improves the hydrodynamic conditions such as shear stress field close to the membrane. The expected positive effect on permeate flux is the more noticeable the more pronounced the fouling. This was shown by two polymer membranes of different molecular weight cut-off exhibiting different susceptibility to fouling.

Acknowledgements:

The authors acknowledge with gratitude the financial support from the Bulgarian Science Fund, Ministry of Education and Science under Contract No KP-06-N47/1/26.11.2020.

1.16. Effect of Driving Pressure and Flux Rate on Red Wine Nanofiltration

M. Lazarova[1,*], M. Dencheva-Zarkova[2], D. Yankov[1], J. Genova[2]

[1] Institute of Chemical Engineering – Bulgarian Academy of Sciences, Acad. G. Bonchev Str., Bldg. 103, 1113 Sofia, Bulgaria
[2] Georgi Nadjakov Institute of Solid State Physics – Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* m.lazarova@iche.bas.bg

Red wine contains many bioactive components, such as phenolics, which are responsible for important sensory qualities of wine and also play a beneficial role on human health. Membrane technology offers advantages compared to the traditional methods used for polyphenols extraction in terms of high recovery/removal efficiency, no phase transition and mild operating conditions.

In this study, a MaxiMem membrane filtration system (PS Prozesstechnik GmbH) was used to perform wine nanofiltration empoying the membrane Microdyn Nadir™ NP030 (MWCO 500 Da). Mavrud red wine vintage 2020 was provided by the Bulgaran wine cellar, Harmanli, Bulgaria. The effects of the operating parameters (transmembrane pressure and flux rate) on the retention of bioactive compounds in wine were investigated. The phenolic amount of the obtained wine after nanofiltration was evaluated and compared with the data of the original wine.

It was found out that the examined nanofiltration membrane can be effectively used for concentration of phenolics in wine. Optimal results with comparable phenolic concentrations were obtained applying two sets of pressure and flux rate, namely 40 bars and 1.2 L/min, and 30 bars and 3 L/min.

Acknowledgements:

This work was financially supported by the National Science Fund of Bulgaria [project No KP-06-N47/1/26.11.2020].

1.17. Soliton dynamics in two ferromagnetic chains coupled through interactions between opposite and diagonal spins

R. S. Kamburova*, M. Danev and M. T. Primatarowa

Georgi Nadjakov Institute of Solid State Physics
Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria

* krad@issp.bas.bg

A system of two anisotropic ferromagnetic chains coupled through the interactions between both opposite and diagonal spins is investigated. For the easy-axis on-site anisotropy the system possesses bright soliton solutions. We studied the influence of the coupling constants on the soliton parameters. We obtained that the coupling between opposite spins does not change the soliton parameters while the coupling between diagonal spins has influence on the form and the velocity of the soliton. Further we considered the propagation of a soliton excitation launched in one of the chains and obtained the condition for its perfect switching. The possibility for a compensation between the two coupling mechanisms is analysed.

Acknowledgements:

This work is supported by the Bulgarian National Science Fund under Grant No. КП-06-Н38/6 from 05.12.2019, by the Joint Institute for Nuclear Research, Dubna, Russian Federation – THEME 01-3-1137-2019/2023 and Grant No Д01-229/27.10.2021 of the Ministry of Education and Science of Bulgaria.

1.18. Doping of dilute nitride compounds grown by liquid phase epitaxy

M. Milanova[1], S. Georgiev[2], V. Donchev[2,*]

[1] Central Laboratory of Applied Physics, Bulgarian Academy of Sciences, 61, St. Petersburg blvd., 4000 Plovdiv, Bulgaria
[2] Faculty of Physics, Sofia University, 5, blvd. J. Bourchier, BG-1164, Sofia, Bulgaria

* vtd@phys.uni-sofia.bg

The doping of dilute nitrides is an important point of the growth and processing technology for different optoelectronic devices based on these compounds. In this paper, both intentional and nonintentional doping of GaAsN, InGaAsN and GaAsSbN have been investigated by temperature-dependent Hall-effect measurements. Dilute nitrides layers have been grown by low-temperature (T_{cryst} < 600 °C) liquid-phase epitaxy (LPE). The chemical elements Sn and Mg have been chosen as *n*-type and *p*-type dopants, respectively. All nominally undoped GaAsN and InGaAsN layers are n-type with free carrier concentration about one order of magnitude higher in comparison to corresponding layers not containing nitrogen grown by LPE. This makes it difficult to obtain epitaxial layers with p-type conductivity with these compounds. However, for GaAsSbN our experiments on doping have shown that high-quality *n*-type, *p*-type and nearly compensated layers have been successfully grown covering a large range of carrier concentrations from 10^{15} to 6×10^{18} cm^{-3}. The quality of the GaAsSbN layers has been evidenced by a good photoresponse with a low energy threshold down to 1.2 eV obtained by surface photovoltage spectroscopy.

1.19. Chitosan-based particles by emulsion crosslinking

Sofia Milenkova[1], Maria Marudova[1,*], Nikolay Zahariev[2,3], Bissera Pilicheva[2,3]

[1] Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski", 24 Tsar Asen Str.,4000 Plovdiv, Bulgaria
[2] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Medical University of Plovdiv, 15A Vassil Aprilov Blvd, 4002 Plovdiv, Bulgaria
[3] Research Institute, Medical University of Plovdiv, 15A Vassil Aprilov Blvd, 4002 Plovdiv, Bulgaria

* marudova@uni-plovdiv.net

In the present study, biopolymer-based particles were formulated with the aim of using them as drug delivery system. They were obtained by applying the water-in-oil emulsion technique in the presence of surfactant. The chosen polymer was chitosan due to its natural biodegradation and antimicrobial properties, along with its mucoadhesion properties. Systems with different polymer concentrations and amount of the crosslinking agent, namely sodium trypolyposphate (NaTPP) were obtained by applying the 3^2 factorial design. Laser difraction technique was applied to observe the sizes of the spheres, together with additional study of their surface morphology. The yield of the formulation process of all of the formulations was also calculated. Swelling properties and mucoadhesion of the formed particles were examined in order to confirm their potential as drug delivery system for orally applied active pharmaceutical substances.

Acknowledgements:

The authors gratefully acknowledge the financial support of the projects MU21-FTF-003, Department of Scientific Research at the Plovdiv University and BG05M20P001-1.002-0005, Personalized Innovative Medicine Competence Center (PERIMED).

1.20. Photoswitchable photochromic fluorescent spirooxazine derivative for metal ions sensing: Photopysical properties and quantum-chemical calculations

Stela Minkovska[1,*], Georgi B. Hadjichristov[2], Andreea Neacsu[3], Viorel Chihaia[3], Yury V. Fedorov[4]

[1] *Institute of Catalysis, Bulgarian Academy of Sciences, Acad. G. Bonchev Srt., Bl.11, BG-1113, Sofia, Bulgaria*
[2] *Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria*
[3] *Institute of Physical Chemistry "Ilie Murgulescu", Romanian Academy of Sciences, Spl. Independentei 202, Bucharest 060021, Romania*
[4] *A. N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Vavilova str., 28, Moscow, 119991, Russia*

* stelamin@ic.bas.bg

The production of stable and efficient photochromic systems is of increasing scientific and practical interest because of their present and future applications in advanced technologies, such as data recording and storage, all-optical switching, displays and nonlinear optics. In view of practical applications, we have synthesized a novel spirooxazine bearing sulfobutyl substituent on the indoline part of the molecule. The photochromic properties of this compound and its complex formation with metal ions were studied. The produced merocyanine exhibits an efficient and reversible photo-chemical isomerization into open or closed molecular forms. This is attractive for advanced applications such as photo-controllable chemical sensing, bio-analytical assays and bioimaging, and for photo-controllable photonic-logic devices.

The fluorescent properties and photo-switching behavior of the synthesized spirooxazine derivative in solution were studied upon photoexcitation with a low-intensity (~ 10 mW/cm^2) continuous light in the UV spectral region, as well as by a red portion of the visible. The light-induced broadband fluorescence emission from the examined solutions was centered in the green spectral region. The fluorescence was excited by UV illumination centered at 310 nm, 365 nm and 385 nm. The most favorable UV excitation was established in order to achieve an optimal photo-switching of the fluorescence. Interaction of spirooxazine with Mg^{2+}, Ca^{2+}, Cd^{2+}, Zn^{2+} or Pb^{2+} ions in the dark leads to the formation of complexes of merocyanine form. As a result, both absorption and fluorescence spectra of these compounds in solution have considerably changed.

The obtained photo-physical characteristics highlight the picture of the photo-chemical mechanism of the phototransformations of the involved molecular species, which might enable various channels of their photo-controllable applications. Complementary to the optical characterization of the considered spirooxazine derivative and its supramolecular complexes with metal ions, quantum-chemical calculations were performed to optimize the electronic and stereo-chemical structure of the spirooxazine compound, and the synthesis route accordingly. By that, experimental FT-IR spectral data were compared with FT-IR data obtained by theoretical calculations. The results show that by a specific structure modification of the spirooxazine derivative under study, its fluorescence and photo-switching performance could be improved.

Acknowledgements:

The work was supported by the Ministry of Education and Science of Bulgaria, through the National Science Fund of Bulgaria (research project No. KP-06-4), as well as by the Russian Foundation for Basic Research (RFBR) - research project No. 19-53-18010.

1.21. Dielectric spectroscopy study of composite PEO/E8 (polymer/ liquid crystals) soft-matter thin films for flexible electronics

Todor E. Vlakhov, Georgi B. Hadjichristov*, Yordan G. Marinov

Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria

* georgibh@issp.bas.bg

In the last decade, numerous composites or blends from polymers and liquid crystals have been developed and thoroughly investigated due to their important properties [1, 2]. Such multifunctional mixed soft-solid materials have found a wide variety of applications, the most popular being the electrically-controllable large scale displays, projection systems, switchable windows (smart windows) and light shutters.

We will present a study on the temperature-dependent dielectric properties of flexible composite dielectric materials produced from polymer poly(ethylene oxide) (PEO) and nematic liquid crystals E8 (in compositional ratio PEO:E8 = 70:30 wt%). Self-supported flexible thin films (150 μm-thick) of PEO/E8 were prepared by using standard solution cast technique [3]. They were characterized by means of complex dielectric spectroscopy in the frequency range from 1 Hz to 1 MHz of the applied electric field. The frequency behaviors of both complex electric modulus and dielectric permittivity of the PEO/E8 films were analyzed, since they are of practical interest. Information about the dielectric relaxation processes relevant to electric field-responsive applications of the PEO/E8 (polymer/liquid crystal) dielectric composite material was obtained. The results show that the examined ion-conducting dielectric soft-solid material is promising for use in flexible organic electronics and in dielectric devices, utilizing the unique properties of nematic liquid crystals upon electro-magnetic fields.

References:

1. X. M. Liu, B. B. Zhang, Z. Y. Niu, M. Z. Du, S. X. Li. Research progress of liquid crystal polymer composites in augmented and virtual reality. Sci. Adv. Mater. 13(4) 2021, 522–529.
2. G. B. Hadjichristov, T. E. Vlakhov, Y. G. Marinov, N. Scaramuzza. Ion-conducting flexible thin films of composites from poly(ethylene oxide) and nematic liquid crystals E8 – characterization by impedance and dielectric relaxation spectroscopy. Polymers 13(24) 2021, art. no. 4465 (pp.1–27).
3. G. B. Hadjichristov, Y. G. Marinov, Tz. E. Ivanov, H. K. Koduru, N. Scaramuzza. PEO/E8 Polymer-Liquid Crystal Flexible Complex Blend Electrolyte System for Na Ions. In: Liquid and Single Crystals: Properties, Manufacturing and Uses, Jai Goosen (Ed.), Nova Science Publ., Series: Chemistry Research and Applications, New York, 2020, Chapter 1, pp. 1–64.

Acknowledgements:

This work was supported by the Ministry of Education and Science of Bulgaria, through the National Science Fund of Bulgaria (research project No. KP-06-N58/6/2021, “Structural and functional investigations of liquid-crystal nanocomposites for applications in photonics, sensorics and biomedicine”).

1.22. Metal-Organic Frameworks with Lanthanoid Ions and Trimesic Acid, as Sensors for Water Pollutants

Yana Dimitrova*, Martin Tsvetkov, Denitsa Elenkova

Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski", 1. J. Bourchier, 1164-Sofia, Bulgaria

* yanadim123@gmail.com

Metal-organic frameworks (MOFs) are coordinated compounds of metal ions correlated to often rigid organic molecules to form one-, two- or three- dimensional structures that can be porous. When the ions are lanthanoids the resulting Ln-MOFs can possess luminescent properties and be used as sensors for water pollutants [1,2]. The biggest advantages of lanthanoid-based MOFs are the fast response and the high sensitivity to specific pollutants.

The current work is mainly focused on solvothermal synthesis of Ln-MOFs with trimesic acid and Eu(III), Tb(III), Dy(III) and Sm(III) as metal ions. All chosen ions can emit in the visible region of light. In addition trimesic acid is a well-known linker that can both enhance the luminescence of Ln(III) and lead to multi-dimensional porous structures [3,4]. Attempt to combine the trimesic acid with different linkers is also done. All samples are characterized so the structures to be determined. Fluorescent properties are investigated and most promising samples are tested as sensor in water. The determination of the possibilities for detection of pollutants in water was carried out by a fluorescence titration process.

References:

1. Zhao, X.Y.; Wang, J.; Hao, H.G.; Yang, H.; Yang, Q.S.; Zhao, W.Y. A water-stable europium-MOF sensor for the selective, sensitive ratiometric fluorescence detection of anthrax biomarker. *Microchem. J.* **2021**, *166*.
2. Sun, Y.; Zhang, N.; Guan, Q.L.; Liu, C.H.; Li, B.; Zhang, K.Y.; Li, G.H.; Xing, Y.H.; Bai, F.Y.; Sun, L.X. Sensing of Fe3+ and Cr2O72- in Water and White Light: Synthesis, Characterization, and Fluorescence Properties of a Crystalline Bismuth-1,3,5-benzenetricarboxylic Acid Framework. *Cryst. Growth Des.* **2019**, *19*, 7217–7229.
3. Lucena, M.A.M.; Oliveira, M.F.L.; Arouca, A.M.; Talhavini, M.; Ferreira, E.A.; Alves, S.; Veiga-Souza, F.H.; Weber, I.T. Application of the Metal-Organic Framework [Eu(BTC)] as a Luminescent Marker for Gunshot Residues: A Synthesis, Characterization, and Toxicity Study. *ACS Appl. Mater. Interfaces* **2017**, *9*, 4684–4691.
4. Aswin Kumar, I.; Jeyaseelan, A.; Viswanathan, N.; Naushad, M.; Valente, A.J.M. Fabrication of lanthanum linked trimesic acid as porous metal organic frameworks for effective nitrate and phosphate adsorption. *J. Solid State Chem.* **2021**, *302*, 122446.

Acknowledgements:

The financial support of project № 80-10-7 from 10.05.22 is acknowledged.

1.23. Photodegradation of adipic acid in aqueous solution by Au and Pd doped TiO_2 nanocomposite catalysts under UV irradiation

P.A. Karakashkova[1,*], A.E. Eliyas[1], S. I. Minkovska [1]

[1] *Institute of Catalysis, Bulgarian Academy of Sciences, Sofia 1113, Bulgaria*

* petia.karakashkova@gmail.com

Palladium and gold modified TiO_2 (Degussa P25) under the effect of feeding oxygen and ozone containing mixture to the reactor under UV-A and UV-C irradiation were examined for their catalytic activity in the reaction of adipic acid oxidation. The samples were synthesized by extractive-pyrolytic method by loading 0.5% of the active metal having particles size varying from 7 to 12 nm. The XRD, TEM and BET methods were employed for their structural and chemical characterization. The reaction rate constants under monochromatic 254 nm irradiation are about 3 times higher than those evaluated with polychromatic (365 nm) light. This is due to the additional generation of HO• radicals by the ozone on the conduction band of the TiO_2 photocatalysts as well as the result of O_3 photolysis by the UV-C light photons of high energy [1].

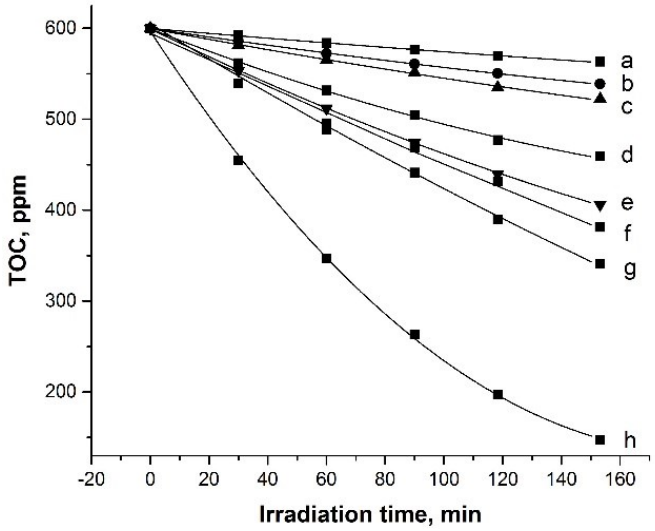


Figure 1: Total degree of mineralization of adipic acid catalyzed by: in the presence of O_2 (λ= 365 nm) – (a) TiO_2, (b) Pd/TiO_2, (c) Au/TiO_2; in the presence of O_3 (λ = 365 nm) – (d) TiO_2, (e) Pd/TiO_2, (f) Au/TiO_2; in the presence of O_3 (λ = 254 nm) – (g) TiO_2; (h) Au/TiO_2.

References:

1. V. Kalarivalappil, C. M. Divya, W. Wunderlich, Suresh C. Pillai, Steven J. Hinder, Manoj Nageri, V. Kumar, Baiju K. Vijayan, Catalysis Letters, 146, 474 (2016).

Acknowledgements:

The reported study was funded by National Science Fund of Bulgaria (NSFB) according to the research project No KP-06-4 and by Russian Foundation for Basic Research (RFBR) according to the research projects No 19-53-18010.

1.24. Impact dynamics of water droplets on pre-frosted superhydrophobic carbon soot coatings

Karekin D. Esmeryan[1,*], Santiago Vargas[2], Stanislav D. Gyoshev[3], Carlos E. Castano[2]

[1] Acoustoelectronics Laboratory, Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72, Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria
[2] Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, VA 23284, USA
[3] Department of Distributed Information and Control Systems, Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, Bl.2, 1113 Sofia, Bulgaria

* karekin_esmerian@abv.bg

The technological failure of different industrial facilities caused by freezing rain events, during which the water droplets pass through a superficial sub-freezing layer of air and transform into ice immediately upon dynamic collision with a given solid surface, could be avoided if modifying the latter with a micrometer-thick superhydrophobic soot-based coating. Such a coating converts the kinetic energy of the impinging droplets into surface energy, and vice versa, with virtually no losses and promotes water-shedding preceding the ice nucleation. However, in conditions of negative temperatures and highly humid atmosphere, the supersaturated ambient water vapor may freeze within the micro- nanocavities of the non-wettable surface and droplet bouncing associated with the superhydrophobicity cannot be sustained.

This research investigates the opportunity of developing superhydrophobic carbon soot coatings maintaining droplet rebound even if their surface is covered by frost. The analysis of the water droplet impact dynamics on two groups of frosted soot coatings, differing by morphology, roughness, surface chemistry and porosity, shows that the bouncing-pinning transition is independent of the surface morphology and topography. Instead, the dynamic collisions with a frosted soot-coated surface could or could not instigate a complete droplet rebound depending on the preliminary laboratory adjustment of the surface chemistry and porosity. Impalement of the liquid meniscus is discerned at both low and moderate Weber numbers for soot samples comprising mainly mesopores, total pore area below 20 % and oxygen functional groups exceeding 7 % due to the excessive energy dissipation resulting from interactions with the intimately located ice (frost) bridges, whose incipiency is dictated by the hydrophilic active sites. Ensuring surface configuration supporting minimum energy losses (qualitatively defined) right after the dynamic collision, by reducing the quantity of surface nucleation sites, suppresses the heat transfer and ice incipiency at the contact interface, which paves the path for future fabrication of advanced water-repellent materials with a specially-contrived surface profile, permitting droplet rebound even in supersaturated environments – a feature with serious implications for the proper operation of renewable energy systems exposed to ice storms.

Acknowledgements:

This research was performed thanks to the financial support of Bulgarian National Science Fund under grant No. KP-06-H37/7/06.12.2019.

1.25. Investigation of Al-doped ZnO thin films prepared by electrochemical deposition method for gas-sensing applications

Rositsa Gergova[1,*], Konstantin Lovchinov[2], Gergana Alexieva[3]

[1] Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria
[2] Acad. J. Malinowski Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev St.
[3] Faculty of Physics, University of Sofia, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria

* rgergova@phys.bas.bg

ZnO thin films doped with Al were deposited on quartz resonators by electrochemical deposition method and their gas-sensing properties were investigated. Electrochemical deposition has the advantage of a low-cost technology and its relatively simple configuration makes it attractive for research of materials with possible industrial application. The influence of the concentration of the doping agent $Al_2(SO_4)_3$ on the properties of the deposited ZnO thin films was thoroughly investigated by optical profilometry, scanning electron microscopy, energy dispersive x-ray analysis and quartz crystal microbalance method. The results form optical profilometry revealed that the increase in the concentration of $Al_2(SO_4)_3$ from 0 M to $4x10^{-5}$ M leads to an increase in the average roughness of the ZnO:Al thin films. The SEM images show that the morphology of the layers changes upon increasing the dopant concentration and leads to the formation of nano-walls. The sensitivity of the electrochemically deposited layers to ammonia and ethanol was also investigated and will be presented for layers with different Al concentration.

Acknowledgements:

This research is funded by Bulgarian National Science Fund (BNSF) under the project КП–06–Н38/7 (12.2019). Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

1.26. Spectral polarimetry applied for magnetic field detection

P. Kolev[1,*], G. Dyankov[1,2], T. Eftimov[2,3]

[1] Institute of optical materials and technologies, Bulgarian Academy of Sciences, 109, Acad. G. Bonchev Str., Sofia
[2] Central Laboratory for Applied Physics, Bulgarian Academy of Sciences, 61 Sanct Petersburg Blvd, Plovdiv, Bulgaria
[3] Centre de recherche en photonique, Université du Québec en Outaouais, 101 rue Saint-Jean-Bosco, Gatineau, Québec, J8X 3X7, Canada

* p.kolev@iomt.bas.bg

The light-matter interaction, which is influenced by magnetic fields, exhibit in the so-called "Magneto-optical" effects. Historically, the first such effect observed was the Faraday (EF) effect. This effect gives impetus to create magneto-optical materials (MOM) that allow rapid modulation of the intensity and polarization of light through external fields. The FE is expressed in the rotation of the plane of polarization of light passing through MOM what change the state of polarization.

We discuss a standard application of EF - for measuring the magnetic field by detecting the polarization state. For the purpose we use the "spectral polarimetry" method [1], which is based on polarization interference to effect spectral amplitude modulation. In fact, it is an analogue of amplitude modulation. To form the carrier frequency and an amplitude-modulated signal we used two phase wave plates made of birefringent material, of different thickness and oriented below 45^0. The wave plates are followed by a polarizer oriented at 0^0. The light that is analyzed (in our case the light passing through MOM) passes through this configuration (called a "spectral polarimeter") and is received by a spectrometer. Fourier processing of the spectrum provides information about the state of polarization of the input signal.

Here we report for the first results, related to the constructed spectral polarimeter. The wave plates were fabricated by crystalline quartz having thickness ratio 3:1. The material and thickness ratio were determined according to spectral resolution of the spectrometer so that different frequencies to be spectrally resolved. Fig.1 shows the measured spectrum that illustrates the fact that the phase retardation of a thick birefringent plate change appreciably with wavelength and plays a role of variable retarder. The Fourier transform of the spectrum gives the autocorrelation function, illustrated in Fig. 2 in terms of wave plate thickness L_1 and L_2.

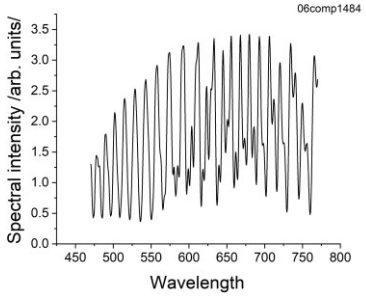


Figure 1.

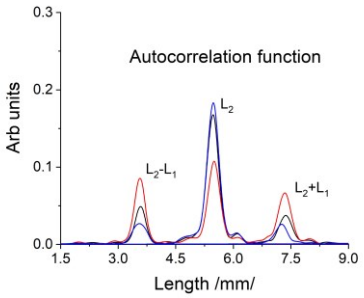


Figure 2.

Obviously, different spectral components are successfully separated. The spectral dependence of Stokes parameters, which fully characterize the polarization state, can be found from obtained spectral components by inverse Fourier transform. This is what follows in future research, as well as the studding Stokes parameters dependence on the magnetic field.

References:

1. M. W. Kudenov, D. H. Goldstein, Polarized Light, D. H. Goldstein, ed., 3rd ed. (CRC Press, 2011), pp. 401–433

Acknowledgements: The authors acknowledge the financial support of the National Scientific Fund of Bulgaria through research project КП-06-Н48/2 and КП-06-China.

1.27. Study of the properties of supercapacitors derived from soot treated with perchlorethylene

M. Petrov[1,*], T. Stankulov[2], B. Karamanova[2], A. Stoyanova[2], K. Lovchinov[3]

[1] *Institute of Electronics - Bulgarian Academy of sciences*
[2] *Institute of Electrochemistry and Energy System -Bulgarian Academy of Sciences*
[3] *Institute of Optical Materials and Technology - Bulgarian Academy of Sciences*

* petrov_80@ie.bas.bg

Due to the trend of increasing ecologic and energy requirements, the burning equipment should work in different conditions. This means lowering the temperature of the exhaust gases. It will lead to better performance but the problem appears is increased rate of soot deposition [1]. The composition of soot is known but the quantity of different compounds is varying in wide range depends on the temperature and fuel burned.

To being made of useful material the soot is collected by sweeping the chimney and subjected to treatment. The material obtained is from soot which was washed by HCl and distilled water to remove ash and subsequent draying. The following step is washing with perchlorethylene The aim of the activity is to dissolve low molecular organic compound which are useless to supercapacitors and opens the pores in black carbon matrices. The material is investigated by FTIR, Transmission Electron Microscopy (TEM), Raman Spectroscopy and XRD analysis. Supercapacitor model cell was assembled with the obtained material and tested in KOH as electrolyte.

References:

1. Zongming Yang, Victoria Kornienko, etc. Capture of Pollutants from Exhaust Gases by Low-Temperature Heating Surfaces. Energies 15(1), 2022, 120.

Acknowledgements:

This work is supported by Bulgarian National Scientific Fund, contract: КП-06-Н57/21.

1.28. The Restricted Boltzmann Machine Ansatz for Quantum Spin-Glass System

S. N. Santalla[1], E. Korutcheva[2, 4,*], K. Koroutchev[3], H. Chamati[4], J. Rodríguez-Laguna[2]

[1] Dep. de Física and Grupo Interdisciplinar de Sistemas Complejos (GISC), Universidad Carlos III de Madrid, Madrid, Spain
[2] Dep. Física Fundamental, Universidad Nacional de Educación a Distancia, Madrid, Spain
[3] Escuela Politécnica Superior, Universidad Autónoma de Madrid, Madrid, Spain
[4] Dep. Theoretical Physics. G. Nadjakov Inst. Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

* elka@fisfun.uned.es

We discuss the expressive power of the quantum restricted Boltzmann machine (QRBM) Ansatz in order to represent faithfully the operation process of a quantum spin-glass system undergoing an adiabatic quantum computation (AQC) process. We address both the representability and the trainability problems associated to the RBM Ansatz when we try to describe the Ground State (GS) of a quantum Ising spin-glass in a transverse field. In our approach, we obtain the GS of the system using exact diagonalization and find the optimal RBM. To start, we train RBM using random initial seeds in order to find how complex is the Ansatz landscape. Then, we perform classical simulations of AQC in order to better determine the optimal parameters. Our results show that due to the complex spin-glass landscape, for some topologies of the RBM, the parameters of the representation are hard to be found.

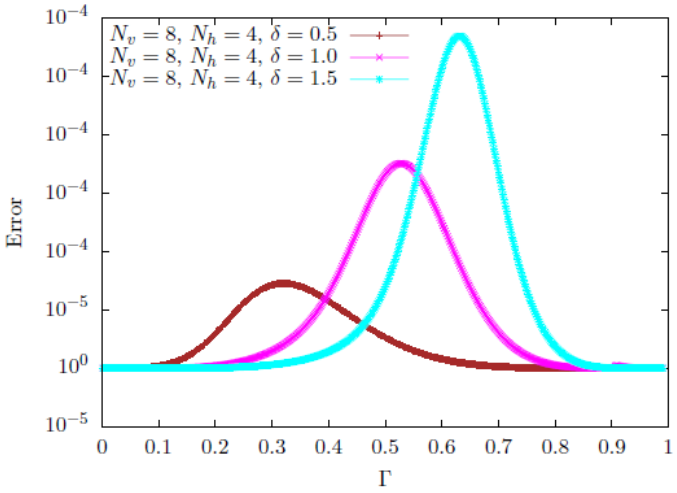


Figure 1. The error between the exact wavefunction and the RBM approximation along an AQC route, for visual units Nv=8, hidden unites Nh = 4 as a function of the transverse field for different dispersion of the random couplings.

References:

1. Melko, R.G., Carleo, G., Carrasquilla, J. et al. Restricted Boltzmann machines in quantum physics. Nat. Phys. 15, 887–892 (2019). https://doi.org/10.1038/s41567-019-0545-1.

Acknowledgements:

This work was funded by the Bulgarian National Science Fund under grant No. КП-06-Н38/6 and by the Spanish government through grants PGC2018-094763-B-I00 and PID2019-105182GB-I00.

1.29. Design and Elaboration of Various Multilayer Beamsplitters

E. Stoyanova[1,*], P. Levicharov[2], K. Antonova[1], I. Miloushev[1], T. Tenev[1]

[1] *Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee, Sofia 1784, Bulgaria*
[2] *Plovdiv University Paisij Hilendarskij, 24 ul. «Tzar Asen», Plovdiv 4000, Bulgaria*

* e.stoyanova@issp.bas.bg

Beam splitters (BS) are optical devices that are essential part in every experimental system and have a variety of applications in the instruments of high class such as medical equipment, optical telecommunication systems, laser-interferometers for nano-positioning, systems for autocollimation, etc. Their operating principle can be described as follows: the incident light beam is spatially split into two-transmitted and reflected one. Either of them can be used as a referent for mentioned precise measurements. The properties of the two beams can be controlled by altering the parameters of the multilayer mirror, which reflects the incident beam. In our work three different kinds of BS are constructed and elaborated on the base of multilayer coatings. They work in the main three aspects of the beam splitting: neutral, dichroic and polarizing, thus changing respectively the intensity, spectral composition and polarization of the output light. Usually, the multilayer coating consists of alternating thin films of materials with low (L) and high (H) refractive index. We used TiO_2 as a substance with high refraction index and SiO_2 as one with low refraction index. As well, modification of the substance optical constants can be produced *in situ* by altering the technological parameters such as temperature, evaporation velocity, different ion assistance, etc. A high class contemporary, fully automated technological equipment, SYRUS Pro 1110, Buhler, is exploited for innovative research of multilayer optical structures. It is supplied by both quartz and optical thickness control, facilities for thermal, electron gun deposition and ion assistance as well.

The realized neutral BS, splits the intensity of the incident beam into ratio Reflected:Transmitted≈ 50:50% within the 400-700 nm region. The model construction of the multilayer mirror is composed of eight non quarter wave layers deposited on the rectangular glass prism hypotenuse and a second rectangular prism is stuck on to form a cube. Thus, the angle of the incident beam is 45°.

The proposed dichroic BS, splits the incident beam into two outgoing beams selectively reflecting and transmitting particular spectral regions. The modeling 29 non quarter wave layer mirror is deposited on the glass substrate dividing the visible spectrum (entirely transmitted) from the NIR spectral region (entirely reflected). The angle of the incident beam is 0°.

The third polarizing BS splits the incident radiation into two beams of orthogonal polarization *S* and *P*. The intensity ratio of both beams ***S:P***, which determines the degree of polarization is obtained to be 1:100 in transmission for the region 550-650 nm in the visible spectrum. The model of the multilayer mirror is composed of 30 non quarter wave layers deposited on the rectangular glass prism hypotenuse and a second rectangular prism is stuck on to form a cube. The angle of the incident beam is 45°.

Acknowledgments

This work was supported from the Bulgarian Ministry of Education and Science, National Science Fund, grant No КП-06-Н57/5 (2021).

1.30. On the relation of the potential energy landscape and the cooperatively rearranging region

Hristo Solunov*

Department of physics and technology of the Plovdiv University P. Hilendarsky, Bulgaria

* solunov@uni-plovdiv.bg

In an extension of the Adam-Gibbs' theory an equation for the measuring the size of cooperatively rearranging region has been found and interpretated as the number of the beads rearranging during the time of relaxation. A relation for the partitioning the molecules to the number of the beads also have been suggested. The size of the cooperatively rearranging region. has been found as molecular base of the fragility of the glass forming liquids. In the Potential eenergy landscape, the total number of the potential minimums in the configuration space is assumed to be measure of the fragility. Here a relation between the size of the cooperatively rearranging region and the parameters in the model functions determining the total number of the potential minimums (inherent structures) is suggested. For the first time the total number of minimums per the mole molecule and per mol of the bead are compared. Two the most fragile liquids toluene and o-terphenyl are investigated and is found that, the molecular, the kinetical and the thermodynamic measure for the fragility corelated with the total number of minimums in the mol of the beads but not in the mol of the molecules.

ABSTRACTS OF SECOND POSTER SESSION

2.1. Light-Induced Nucleation and Optical Absorption in Metallic Vapors

Svetlana Baranovski*

Faculty of Physics, Philipps-Universität Marburg, Marburg 35032, Germany

* svetlana.baranovski@physik.uni-marburg.de

The features of metallic vapors desired for modern condensed matter technology are currently in the focus of intensive experimental and theoretical research. Experimental study of the spectral dependence of the nucleation of cesium vapor caused by light absorption is carried out in a diffusion cloud chamber. The spectral dependence of the nucleation rate is compared with the absorption and ionization spectra, as illustrated in Figure 1. The results evidence that the observed structure in the nucleation spectrum at photon energies above the ionization threshold is correlated with the absorption spectra and with the light-induced ionization spectra of cesium dimers.

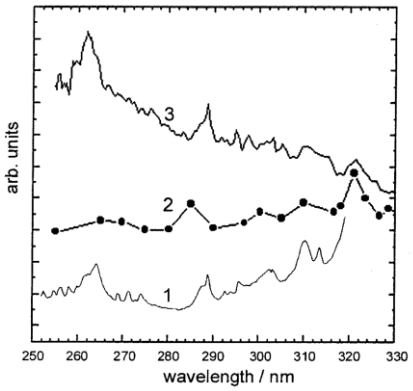


Figure 1. 1- Absorption cross-section of saturated cesium vapor at T=767 K;
2 – photoionization cross-section of cesium dimers from Ref. 3; 3 – the nucleation rate spectrum.

The spectral dependence of the nucleation rate provides a new and powerful tool to study ionization spectra of metal vapors. In addition to results obtained by conventional methods, a more consolidated insight into the energy levels of atoms and clusters under equilibrium conditions appears possible [1].

Also experimental studies for nucleation of other kinds of metal vapors in an upward thermal diffusion cloud chamber, for instance, of mercury vapors, show drastic effects of the light absorption on the nucleation rate. The rate of nucleation is greatly enhanced when the supersaturated vapor is illuminated with light absorbed by the gas molecules. In analogy to the ion-induced nucleation, the photoinduced nucleation can be explained as a general effect for all condensing atoms or molecules forming long living electronically excited states [2].

References:

1. H. Uchtmann, S. Yu. Kazitsyna, S. D. Baranovskii, and F. Hensel, “Light-induced nucleation and optical absorption in cesium vapor”, J. Chem. Phys., 113 (2000) 4171.
2. H. Uchtmann, R. Dettmer, S. D. Baranovskii, and F. Hensel, “Photoinduced nucleation in supersaturated mercury vapor “, J. Chem. Phys., 109 (1998) 9775.
3. H. R. Kratz, „The Principal Series of Potassium, Rubidium, and Cesium in Absorption”, Phys. Rev. 75 (1949) 1844.

2.2. Electric characterization of transition metal (Co, Ni, Fe) doped ZnO thin layers prepared by atomic layer deposition

D. Spassov, A. Paskaleva*, B. Blagoev, V. Mehandzhiev

Institute of Solid State Physics, Bulgarian Academy of Sciences,
Tzarigradsko Chaussee 72, Sofia 1784 Bulgaria

* paskaleva@issp.bas.bg

Amongst the oxide semiconductors, zinc oxide (ZnO) is considered as one of the most interesting because of its unique combination of properties such as low cost, wide and direct band gap of ~3.3 eV, low synthetic temperature, controllable electrical behavior, chemical stability, electrochemical activity, biocompatibility. ZnO can be grown with wide variety of morphologies and can be doped with transition metals to induce ferromagnetism at room temperature, which makes it a promising semiconductor for application in spintronics; hence there is a growing interest in this material, in which both the spin and the charge of the carriers could be exploited. The purpose of the work is to obtain by atomic layer deposition (ALD) ZnO films doped with different 3d transition metal elements (Co, Ni, Fe) and to investigate their electrical properties. Metal-ZnO-metal structures with lower electrode - TiN and upper electrode - Pt were prepared for electrical measurements and standard volt-ampere (I-V) and volt-capacitive (C-V) characteristics were measured. The C-V characteristics (Figure 1) for Fe: ZnO and Ni: ZnO demonstrate a pronounced peak revealing the semiconductor behavior of doped ZnO layers. The strong frequency dependence give evidence for polarization effects and possible ferroelectricity in the layers. Some important parameters, e.g. the concentration of major carriers N_D as well as the built-in potential V_{bi} are determined.

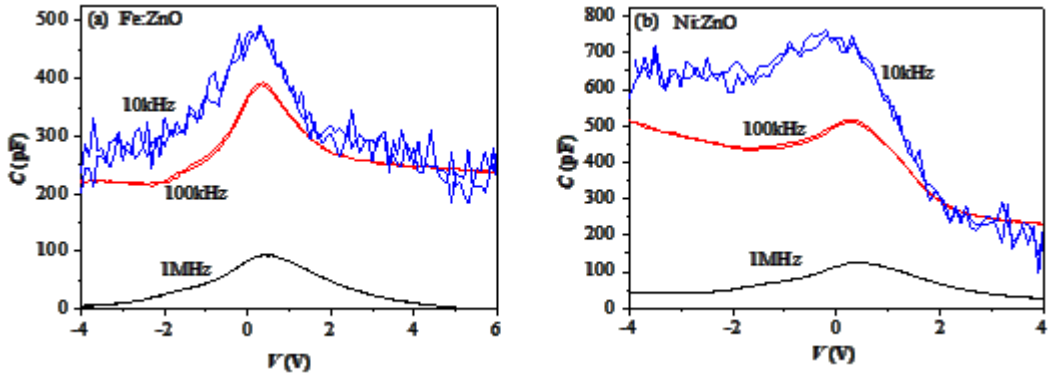


Figure 1. C-V characteristics at different frequencies of capacitors with: (a) Fe:ZnO, and (b) Ni:ZnO layers.

Acknowledgements:

The work is supported by Bulgarian National Science Fund under project KP-06-H28/9

2.3. Surface photovoltage study of metal halide perovskites deposited directly on crystalline silicon

Vesselin Donchev[1,*], Stefan Georgiev[2], Aleksandra Bojar[2,3,4], Davide Regaldo[2,3,4], Mattia da Lisca [,3,4], José Alvarez[2,3,4], Jean-Paul Kleider[2,3,4]

[1] Faculty of Physics, Sofia University, 5, blvd. J. Bourchier, BG-1164, Sofia, Bulgaria
[2] Université Paris-Saclay, CentraleSupélec, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 91192, Gif-sur-Yvette, France
[3] Sorbonne Université, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 75252, Paris, France
[4] IPVF, Institut Photovoltaïque d'Ile-de-France, 91120, Palaiseau France

* vtd@phys.uni-sofia.bg

Perovskite-silicon tandem solar cells are a prospective system for overcoming the single-cell efficiency limit. Knowledge of the carrier transport and band alignment at their interface would allow for a better understanding of their compatibility and attainable performance levels. However, in most tandem solar cell designs these two materials are not in direct contact and only a few works have dealt with a direct investigation of the perovskite-silicon interface [1].

In this work, we have studied triple cation mixed halide perovskite (PVK) films deposited directly on both p-type and n-type crystalline silicon substrates employing two different operating modes of the surface photovoltage (SPV) method: i) the metal-insulator-semiconductor (MIS) operation mode using chopped light and ii) the Kelvin probe force microscopy (KPFM) with continuous illumination. SPV-MIS amplitude and phase spectra measured at 94 and 492 Hz allowed us to study relatively fast processes of carrier generation, transport and recombination. SPV transients were recorded by KPFM over longer time scales (minutes) after switching on and off the illumination with a fixed wavelength of 980, 785 or 488 nm.

By scanning from 1300 to 500 nm in the SPV-MIS mode we have consecutively studied the optical absorption and photocarrier transport first in Si, then on both sides of the PVK/Si interface and finally in the PVK layer and its surface region. The amplitude spectra reveal the PVK optical absorption edge in the range of 1.59 – 1.61 eV in both types of samples. This is in good agreement with the determination of the bandgap at 1.63 eV from photoluminescence measurements. The combined analysis of the SPV-MIS amplitude and phase spectra has shown a downward energy band bending at the PVK surface in both types of samples. A relatively large upward band bending exists at the PVK/n-Si substrate interface. It contributes to the SPV signal down to 500 nm due to photocarriers, which reach it via diffusion. The energy band bending at the PVK/p-Si interface is found to be downward; however, it is very weak. These findings were confirmed by the SPV-KPFM transients. The slow negative transients observed by KPFM in PVK/n-Si samples after switching off the 785 and 488 nm light, were explained by the trapping of negative charges, including negative ions, at the PVK surface under illumination and their slow release in the dark.

References:

1. M. Islam Elsmani, N. Fatima, M.A. Paul Jallorina, S. Sepeai, M. Sukor Su, N. Ahmad Ludin, M. Asri Mat Teridi, K. Sopian, M. Adib Ibrahim, Recent Issues and Configuration Factors in Perovskite-Silicon Tandem Solar Cells towards Large Scaling Production, 11 (2021) 3186.

2.4. Characterization and gas sensing properties of ZnO and ZrO_2 layers electrochemically-synthesized on quartz resonators

B. Georgieva[1,*], K. Lovchinov[2], L. Slavov[1], G. Alexieva[3], Ch. Angelov[4]

[1] Institute of Electronics, Bulgarian Academy of Sciences,
72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria
[2] Institute of Optical Materials and Technologies "Acad. J. Malinowski",
Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, 1113 Sofia, Bulgaria
[3] Faculty of Physics, University of Sofia, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria
[4] Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences,
72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* b.georgiewa@abv.bg

This work presents characterization (structural and morphological) and the gas sensing properties of ZnO and ZrO_2 layers electrochemically synthesized on quartz resonators. The nanostructured ZnO and ZrO_2 layers are deposited by an electrochemical method on the Au electrodes of a quartz crystal micro-balance resonators (QCM). The deposition of the ZrO_2 and ZnO electrochemical layers is carried out in an aqueous solution of ($ZrOCl_2$ (5 mM) and KCl (100 mM) for ZrO_2 and ($ZnCl_2$ (5 mM) and KCl (100 mM) for ZnO) at 70 ºC and (vs SCE) using a three-electrode electrochemical cell. The structure of the ZrO_2 and ZnO layers deposited on the polished QCM surface is studied by scanning electron microscopy (SEM), and optical profilometry. The influence is investigated of the roughness on the ZrO_2 and ZnO layers sorption properties. For the same deposition time, the ZnO layers have a significantly higher average roughness (greater thickness) than the ZrO_2 layers. The sensitivity of the resonators with electrochemically deposited on them layers of ZrO_2 and ZnO to methanol, ethanol and ammonia is measured in a hermetic Plexiglas box with a volume of 22.5 liters. The delivery of volatile liquids in the box is carried out by means of a syringe at a step of 0.1 ml; a small fan is used to homogenize the vapor distribution. The sorption ability of the ZrO_2 and ZnO layers is determined by measuring the resonant frequency shift (Δf) of the QCM structure in the presence of different concentrations of methanol, ethanol and ammonia (2000 – 25000 ppm).

Acknowledgements:

This research is funded by the Bulgarian National Science Fund under contract КП – 06 – Н38/7 (12.2019). Research equipment of the INFRAMAT Distributed Research Infrastructure, part of the Bulgarian National Roadmap for Research Infrastructures, supported by the Bulgarian Ministry of Education and Science was used in this investigation.

2.5. Improvement of the photocatalytic properties of ZnO thin films by co-catalytic modifying for the degradation of Paracetamol

Dobrina Ivanova* **and Nina Kaneva****

Laboratory of Nanoparticle Science and Technology, Department of General and Inorganic Chemistry, Faculty of Chemistry and Pharmacy, University of Sofia, 1 James Bourchier Blvd., Sofia 1164

* dobrina.k.ivanova@gmail.com

** nina_k@abv.bg

Heterogeneous photocatalysis is one of the popular alternative treatment methods for wastewater. It utilizes semiconductor material as the catalyst and metal oxide such as zinc oxide. We report the synthesis of nanostructured silver co-catalytic modified ZnO films, using sol-gel method. The resulting films are characterized by means of X-ray diffraction analysis (XRD), Scanning electron microscopy (SEM) and UV–Vis spectroscopy. Zinc oxide exhibited hexagonal wurtzite structure and the surface is with characteristic ganglia-like structure. The photocatalytic properties of the pure and co-catalytic modified ZnO films have been investigated for the degradation of Paracetamol in distilled and tap water. The experiments are carried out under UV light and natural sunlight. The results shows that the photodegradation of the analgesic follow pseudo-first order kinetics and the lifetime of the photogenerated electron-hole pairs of ZnO is increased by the Ag modifying.

Acknowledgements:

This work is financially supported by project КП-06-Н59/11.

2.6. Impact of the deposition temperature on morphological and gas sensing properties of electrochemically grown ZrO_2 layers

Gergana Alexieva[1,*], Nikolay Tyutyundzhiev[2], Rositsa Gergova[3], Miroslav Petrov[2], Konstantin Lovchinov[4]

[1] Faculty of Physics, University of Sofia, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria
[2] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee 1784 Sofia, Bulgaria; n_tyut@ie.bas.bg
[3] Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria; rgergova@phys.bas.bg
[4] Acad. J. Malinowski Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bld. 109, 1113 Sofia, Bulgaria; lovchinov@iomt.bas.bg

* gerry@phys.uni-sofia.bg

This poster presents experimental results on the influence of deposition temperature on morphological and gas sensing properties of electrochemically deposited ZrO_2 layers. The morphology and average roughness of the layers deposited on one of the gold electrodes of AT-cut quartz resonators, vibrating at 10 MHz, were determined by Scanning Electron Microscopy (SEM) and 3D optical profilometry. The experimental results did not indicate correlation between the deposition temperature and the average roughness of the layers. The studies on the morphological properties show that there is a strong dependence of the surface morphology with the temperature change. The layers sensitivity to ethanol and ammonia gases was determined by the quartz microbalance method (QCM). The gas sensing measurements were performed in a hermetic plexiglass box at different concentrations of the analytes. It is shown that the sensitivity of the layers depends mainly on their developed surface.

Acknowledgements:
This research is funded by Bulgarian National Science Fund (BNSF) under the project КП – 06 – Н38/7 (12.2019).

2.7. Influence of the substrate on the structural and optical properties of ZrO_2 layers deposited by electrochemical process

L. Slavov[1,*], K. Lovchinov[2], B. Georgieva[1], G. Alexieva[3], P. Ivanov[2]

[1] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko chausse, Blvd. 1784, Sofia, Bulgaria
[2] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 109, 1113 Sofia, Bulgaria
[3] Faculty of Physics, University of Sofia, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria

* l_slavov@yahoo.co.uk

The influence of the substrate on the structural and optical properties of ZrO_2 layers is presented. Nanostructured layers of ZrO_2 are electrochemically deposited (on different conductive substrates) using a thermostatic bath with a three-electrode cell. The aqueous solution in the system contained $ZrOCl_2$ (5×10^{-3}M) and KCl (0,1M). The structural properties of the layers were determined by X-ray diffraction (XRD), with the spectra revealing the polycrystalline nature of the layers with the typical characteristic reflexes of ZrO_2 for all substrates studied. The average grain sizes (between 39 nm and 121 nm) were determined from the diffraction patterns for each crystallographic axis associated with a maximum. Morphological investigations by scanning electron microscopy (SEM) and optical profilometry were also carried out and the average roughness of the layers was calculated. The structures' optical properties were determined by UV-VIS-NIR and photoluminescence spectroscopies. The influence of the substrates on the ZrO2 layers' specular and total reflectance is presented and discussed. The excitation wavelength of photoluminescence spectra was 235 nm, with all samples exhibiting broad emission bands with peaks centered within the 400–430 nm range. The diffuse reflection showed high values in the spectral range 360–780 nm. Such layers are promising candidate as rear contacts of thin-film solar cells.

Acknowledgements:

This research is funded by Bulgarian National Science Fund (BNSF) under the project КП – 06 – Н38/7 (12.2019). Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

2.8. Study of spectrofluorometric sensitivity and structural properties of electrochemical ZrO_2 layers

P. Ivanov[1, *], K. Lovchinov[1], R. Gergova[2], G. Marinov[1], P. Petrova[1], B. Greorgieva[1]

[1] *Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 109, 1113 Sofia, Bulgaria.*
[2] *Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee blvd., 1784 Sofia, Bulgaria*

* petar@iomt.bas.bg

This research work represents the influence of spectrofluorometer sensitivity to volatile compounds (ethanol and ammonia). The deposition of ZrO_2 layers obtained by electrochemical process on SnO_2 covered glass substrates. The solution is aqueous (containing $ZrOCl_2$ – 5×10^{-3}M and KCl – 0.1 M) and temperatures of the deposited layers are 60, 65, 70, 75 and 80°C. To determine the structural properties and sensitivity to ethanol and ammonia were used X-ray Diffraction (XRD), optical profilometry, Scanning Electron Microscopy (SEM) and Spectrofluorometer. The XRD spectra show the polycrystalline nature of the films at all studied deposition substrate with the typical characteristic reflexes of the ZrO_2. Calculations for the size of the crystallites from the diffraction maxima and the average roughness show that no dependence is observed between them and the deposition temperature. The SEM micrographs show that the ZrO_2 layers are composed mainly of grains of relatively regular shape, as their size increases with increasing deposition temperature. It is demonstrated that the deposition temperature almost no effect on the reflectance and transmittance spectra of the ZrO_2 layers. Spectrofluorometric studies show the sensitivity of the ZrO_2 layers when exposed to ammonia.

Acknowledgements:

This research is funded by Bulgarian National Science Fund (BNSF) under the project КП – 06 – Н38/7 (12.2019). Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

2.9. Structural and gas sensing properties of nanostructured ZrO_2 layers deposited electrochemically at different times

P. Petrova[1,*], K. Lovchinov[1], G. Alexieva[2], R. Georgiev[1], R. Ivanova[1], V. Strijkova[1]

[1] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 109, 1113 Sofia, Bulgaria.
[2] Faculty of Physics, University of Sofia, 5 James Bourchier Blvd., 1164 Sofia, Bulgaria

* petia@iomt.bas.bg

This research work is focused on the influence of deposition time on structural and gas sensing properties of electrochemically deposited ZrO_2 layers. The ZrO_2 layers were deposited on gold electrodes of quartz resonators by electrochemical process (in an aqueous solution containing $ZrOCl_2$ – with concentration 5mM and KCl – with concentration 0.1 M) using a three-electrode electrochemical system. The surface morphology, structure and average roughness of the layers were determined by Scanning Electron Microscopy and 3D optical profilometry . For these layers, there is no relationship between the deposition time and the average roughness, as the layer deposited at 40 min. (the longest deposition time) has the highest average roughness. For comparison, show the average roughness of the quartz resonator on which the zirconia layers were deposited. In SEM micrographs we observe a structure composed mainly of small grains with a relatively regular shape and size between 0.3 and 2 μm. The density of the grains located on the surface of the layer increases with increasing deposition time. The layers sensitivity to VOC gases was determined by the quartz micro balance (QSM) method, measuring the resonant frequency shift (ΔF) of the quartz resonators. The measurements of sensitivity were performed in an airtight box at different concentrations.

Acknowledgements:

This research is funded by Bulgarian National Science Fund (BNSF) under the project КП – 06 – Н38/7 (12.2019). Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

2.10. Preparation and characterization of RF sputtered ZnO layers for application in thin films solar cells

S. Stankova*, Hr. Dikov, E. Radeva, M. Ganchev

Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, 72 Tzarigradsko Chausee blvd., 1784 Sofia, Bulgaria

* perovskite.psc@gmail.com

Transparent metal oxide layers find huge attention in photovoltaics as contact windows, buffer or selective blocking materials combining high optical transmittance with suitable electrical properties. Zinc oxide (ZnO) has been considered to be the most appropriate contact window in chalcopyrite [1] and Kesterite solar cells but recently attracts attention as electron selective material in organic photovoltaics (OPVs) [2,3]. Thin films ZnO was reported to be successfully applied after detailed surface engineering in planar perovskite solar cells with achieved highest efficiency up to 15.9 % [4]. Chalcopyrite based solar cells commonly consist of Cu(In,Ga)Se2 (CIGS) absorber layer and a sputter sequence of undoped and doped ZnO layers in a structure: glass/Mo/CIGS/CdS/ZnO/ZnO:Al. In some cases, ZnO plays the role of the buffer layer itself as an alternative of the mostly used toxic CdS. An advanced application of this material is considered to be involving in Organic Solar Cells (OSCs) as Electron Transporting Material (ETM). The work presents fabrication of uniform resistive thin (50-100 nm) undoped ZnO films serving as buffer layers and conductive Al-doped ZnO films (Al:ZnO) with thickness in the range of 100-500 nm. The deposits prepared are thermally stable and have good crystallinity with preferred hexagonal orientation of the c-axis as it was indicated by SEM observations. In the latter case the film thickness was optimized to combine high transmittance and low resistivity. Both types of films are with good adhesion and possess a transmittance over 90% in the visible region. Highly transparent bi-layer films (ZnO/ZnO:Al) were finally embedded in the solar cell structure: glass/Mo/CIGS/ZnO/ZnO:Al/Al.

References:

1. Empa takes thin film solar cells to a new level – A new world record for solar cell efficiency". Empa. https://www.empa.ch/web/s604/weltrekord
2. Dou Li et al. RSC Adv., 2017,7, 6040-6045, https://doi.org/10.1039/C6RA25177C
3. Ziyang Hu et al., Solar Energy Materials & Solar Cells 95 (2011) 2126–2130.
4. Tseng, Z., Chiang, C. & Wu, C. Surface Engineering of ZnO Thin Film for High Efficiency Planar Perovskite Solar Cells. Sci Rep 5, 13211 (2015). https://doi.org/10.1038/srep13211, https://www.nature.com/articles/srep13211

Acknowledgements:

Research is sponsored by the Bilateral programs between Bulgarian Academy of Sciences and Estonian Academy of Sciences – 2022 - 2024. The experiments were performed with equipment included in the National Infrastructure NI SEVE supported by the Ministry of Education and Science under grant agreement № DO1-160/28.08.18.

2.11. Optical and photocatalytic properties of ZnO thin films prepared by modified sol-gel method

R. Gegova-Dzhurkova[1,*], D. Nesheva[1], I. Stambolova[2], K. Zaharieva[3], P. Terziyska[1], I. Miloushev[1], V. Dzhurkov[1]

[1] G. Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, Tzarigradsko Chaussee, Blvd. 72, 1784 Sofia, Bulgaria
[2] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev St., Bldg. 11,1113 Sofia, Bulgaria
[3] Institute of Mineralogy and Crystallography "Akad. Ivan Kostov", Bulgarian Academy of Sciences, Acad. G. Bonchev St., Bl. 107, 1113 Sofia, Bulgaria

* radka.dzhurkova@issp.bas.bg

Photocatalysis is a clean technology for the degradation of various toxic organic materials used in many industries. During the last few decades, intense investigations have been addressed not only to improve photocatalytic activity under UV light, but also to obtain materials which are active under illumination with visible light. In this work two types of ZnO films are prepared on silicon wafers with oxidized surface by modified sol-gel "spin coating technique" with monoethanolamine (MEA) or diethanolamine (DEA) as stabilizers, and treated with warm air as first step in the drying procedure followed by furnace heat treatment at 140°C as second step. Annealing at 400°C is also applied to a part of the films. X-ray diffraction measurements reveal that both the films treated only at 140°C and those annealed at 400°C and 600°C, are crystalline with wurtzite structure. The obtained scanning electron microscopy images show presence of nanosized particles and some microcracks on the films surface. Spectroscopic ellipsometry results show that the film thickness is affected by both the type of the stabiliser used (MEA or DEA) and the annealing temperature. The observed thickness changes are related to effusion of organic molecules or parts of them which incorporate during the film deposition. Optical properties are investigated with UV-VIS transmission measurements and the calculated optical band gaps are in the range 3.2 to 3.4 eV. The effect of the MEA and DEA stabilizers on the photocatalytic activity of the films under UV and visible light is explored.

Acknowledgements:

RD, PT and IM acknowledge the financial support by the National Science Fund under the project KP-06-H57/5 (16.11.2021). DN and VD acknowledge the financial support provided by the European Regional Development Fund within the OP "Science and Education for Smart Growth 2014 - 2020", project No BG05M2OP001-1.001-0008.

2.12. Investigation of porous ZnSe thin films prepared by thermal evaporation

V. Dzhurkov[1,*], Z. Levi[1], D. Nesheva[1], T. Hristova-Vasileva[1,2], P. Terzyiska[1], I. Miloushev[1], T. Tenev[1]

[1] G. Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, Tzarigradsko chausse 72 Blvd, 1784, Sofia, Bulgaria
[2] Institute of Optical Materials and Technologies "Acad. Jordan Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev St., Bl. 109,1113 Sofia, Bulgaria

* valeri.dzhurkov@issp.bas.bg

Zinc selenide is an important material, which finds applications in various electronic and optoelectronic devices. The film porosity plays an important role for some application of ZnSe films such as chemical sensing, photocatalysis, etc. In this study ZnSe films with thickness of 50, 70 and 100 nm were prepared on Corning 7059 glass substrates at room temperature by applying continuous and periodically interrupted physical vapour deposition of ZnSe at very low deposition rates 0.2, 0.5 nm/s). Part of as-deposited films was annealed at 200^{o}C. Optical absorption spectra indicate direct allowed transitions, which show that the films are crystalline which is in agreement with the X-ray diffraction and atomic force microscopy results. Results from spectroscopic ellipsometry have shown that the porosity of the films depends on both manner of deposition and deposition rate. The film annealing temperature causes some porosity decrease which is greater for the films deposited at the lower deposition rate. The observed high porosity makes these films suitable for chemical sensing application.

Acknowledgements:

VD, PT, IM and TT acknowledge the financial support by the National Science Fund under the project KP-06-H57/5 (16.11.2021). DN acknowledge the financial support provided by the European Regional Development Fund within the OP "Science and Education for Smart Growth 2014 -2020", project No BG05M20P001-1.001-0008.

2.13. Surface plasmon-like properties of one dimensional photonic crystal and its application in surface-enhanced luminescence

Anna Atanasova*, Vesela Katrova, Rossen Todorov,
Temenuga Hristova-Vasileva, G. Milushev

Institute of Optical Materials and Technologies "Acad. J. Malinowski",
Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, 1113 Sofia, Bulgaria

* alalova@iomt.bas.bg

The present work reports on the plasmon-like properties of one dimensional photonic crystal (1DPC) as active material for surface-enhanced luminescence application. 1DPC in form of 9 layered stack was prepared through layer-by-layer deposition of spin coated Poly (methyl methacrylate) and vacuum deposited As_2S_3. The thicknesses of the alternating layers are tailored with Bragg's condition for a quarter wave stack ($nd = \lambda/4$, n - refractive index, d - physical thickness, λ - operating wavelength)[1]. The optical properties of the 1DPC were characterized by UV-Vis-NIR spectrophotometry. Efficiency of the surface-enhanced luminescence was investigated by using 0.1 % w/v of Cu (II)-phthalocyanine (CuPc) in Pluronic PE 6800 water solution with concentration 0.1 % w/v.

References:

1. Joanopoulus J D, Meade R D and Winn J N 1995*Photonic crystals: Molding the Flow of Light* (Princeton, N.J.: Princeton University Press,).

Acknowledgements:

This work is financially supported by contract KP-06-N38/8 - 05.12.2019 with the Bulgarian National Science Fund. Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

2.14. Structural and optical characterization of thin films from bimetallic Au-Sb system as tunable plasmonic material for UV spectral range

R. Todorov[1,*], V. Katrova[1], T. Hristova-Vasileva[1,2], A. Atanasova[1], G. Milushev[1]

[1] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, 1113 Sofia, Bulgaria
[2] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* rossen@iomt.bas.bg

The optical properties of silver and gold based bimetallic alloys make possible to adjust their plasma frequency. In the present work, the deposition, microstructure and phase composition of thin layers from the Au-Sb system are presented. The thin films were deposited by thermal co-evaporation of gold and antinomy. The chemical and phase composition, as well as the surface morphology of thin films, were analysed by energy dispersive X-ray microanalysis (EDAX), X-ray diffraction (XRD) and scanning electron microscopy, respectively. The results of the X-ray microanalysis show that the composition of the thin layers corresponds well to the predetermined. The X-ray diffraction patterns, depending on the envisaged compositions, show formation of gold-based solid solution, intermetallic compound $AuSb_2$ and binary alloys between the initial elements and the intermediate compound, which is in accordance with their phase diagram.

The dispersion of the complex permittivity was determined by spectroscopic ellipsometry. The results show that the increase of the antimony content leads to an increase of the values of the imaginary part of the complex permittivity in the visible spectral region at photon energies greater than 3 eV, and their decrease in the ultraviolet spectral region. Based on the obtained dispersions of the complex permittivity, extinction and scattering cross-sections, local field enhancement of spherical Au-Sb nanoparticles were determined and their plasmon activity was evaluated.

Acknowledgements:

This work is financially supported by contract KP-06-N38/8 - 05.12.2019 with the Bulgarian National Science Fund. Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

2.15. Thickness dependence of the optical properties of thin Ag-Bi films and their surface plasmon-enhanced photoluminescence capability

V. Katrova[1,*], A. Atanasova[1], R. Todorov[1], T. Hristova-Vasileva[1,2], V. Strijkova[1]

[1] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, 1113 Sofia, Bulgaria
[2] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* vlozanova@iomt.bas.bg

Preparation technology, optical properties and surface-enhanced photoluminescence features of thin Ag-Bi layers with different ratios of the chemical elements are subject of present work. The results show that the plasmon resonances can be tuned by controlling the coating thickness. Surface-enhanced Stokes and anti-Stokes emission has been achieved due to the surface plasmons activity.

A series of thin metallic Ag-Bi films with different thicknesses were obtained by layer-by-layer thermal evaporation of bismuth and silver substances at a residual pressure of ~ 1×10^{-3} Pa. The multilayer coatings were deposited on glass and Si substrates and the composition during evaporation was controlled by varying the thickness of the sublayers in one vacuum cycle. The chemical composition and the surface morphology of thin films were analyzed by X-ray microanalysis and atomic force microscopy, respectively. The optical properties were characterized from spectroscopic ellipsometry and UV-Vis-NIR spectrophotometry measurements.

Coatings with different numbers of stacks were tested in order to determine the minimum number of sublayers required to achieve epsilon-near-zero properties. The results for the complex permittivity showed the Ag-Bi films possess epsilon-near-zero properties in wide spectral range of 1.3 − 6 eV. With decreasing of the film thickness, the observed minimum in the reflectance spectra is redshifted with 0.3 eV. The films with a higher silver content have a reflection coefficient over 75% in the range of 0.6 to 2 eV.

The essential in protein biosynthesis α-amino acid tryptophan was used to analyze the enhanced properties of the Ag-Bi layers. The photoluminescence spectra were performed by using an Ocean Optics spectrometer in the range from 300 nm to 600 nm. Laser with λ = 514 nm was used for the excitation of electrons. The presence of localized surface plasmon in the thin layers causes increase in the luminescence signal of tryptophan with a maximum at ~ 350 and 580 nm.

Acknowledgements:

This work is financially supported by contract KP-06-N38/8 - 05.12.2019 with the Bulgarian National Science Fund. Research equipment of Distributed Research Infrastructure INFRAMAT, part of Bulgarian National Roadmap for Research Infrastructures, supported by Bulgarian Ministry of Education and Science was used in this investigation.

2.16. Interfaces in very thin ALD Al_2O_3/HfO_2 stacks studied by ellipsometry

Y. Karmakov[1,*], A. Paskaleva[2], D. Spassov[2]

[1] Department of Solid State Physics and Microelectronics, Faculty of Physics, Sofia University, 5 James Bourchier Blvd., 1164, Sofia, Bulgaria
[2] Institute of Solid State Physics, G. Nadjacov, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd., 1784, Sofia, Bulgaria

* karmakov@phys.uni-sofia.bg

Stacks and laminates of binary oxides HfO_2/Al_2O_3, deposited by Atomic Layer Deposition (ALD), are intensively investigated recently not only for optical applications and microelectronics/nanoelectronics devices such as non-volatile flash memories. The efforts are focused on low dimensional dielectric structures with advanced characteristics achieved by variation of the number HfO_2 and Al_2O_3 ALD deposition cycles and the way the sublayers alternate in the blocks. Although, both HfO_2 and Al_2O_3 offer fixed refractive index dispersions in combination whit a fixed optical band gap these parameters show some flexibility in regard to the thickness, in case of low dimensions (a few monolayers). The ternary mixtures as $(Al_2O_3)_x(HfO_2)_{1-x}$ demonstrate even more flexibility, still keeping the fundamental relations between the refraction index and band gaps. Ellipsometry is a known optical method with powerful algorithms for experimental data interpretations that may detect changes in the thickness of the layers with 0.01 monolayer dimension. Here the experimental ellipsometric data on very thin HfO_2/Al_2O_3 stacks were processed by suitable algorithms in order to determine the individual thickness of HfO_2 and Al_2O_3 sublayers, their variation in stack depth and deviations from the nominal thicknesses. Interface regions were determined to be clearly related with the initial growth of every block. Interfaces were identified as HfO_2-Al_2O_3 mixtures with a changeable composition and thickness within the stack. Quantitative estimations of some physical properties as refractive index, dielectric functions and dielectric constants, growth rates and their depth profiles (Figure 1) were also made.

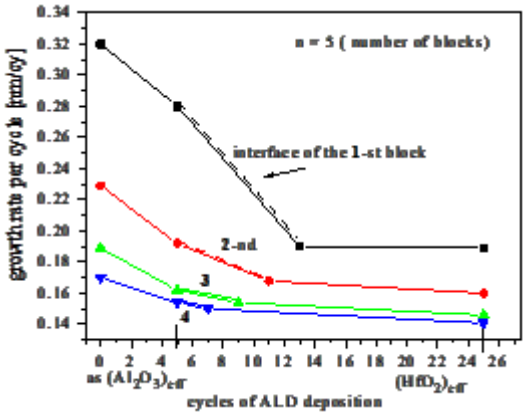


Figure 1. Ellipsometrically evaluated growth rate for a Al_2O_3/HfO_2 ALD stack build of 5× repeated block composed by 5cy Al_2O_3 and 20cy HfO_2.

Acknowledgements

The work is supported by Bulgarian National Science Fund under project KP-06-H37/32.

2.17. Investigation of optical constants of Al_2O_3 films in the spectral range 0.2 - 0.8 microns

E. N. Kotlikov[1], N. P. Lavrovskaya[1,*], I. K. Miloushev[2], T. K. Tenev[2]

[1] Saint-Petersburg State University of Aerospace Instrumentation, 67 Bolshaya Morskaya str., Saint-Petersburg, 190000, Russia
[2] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko chausse, 1784 Sofia, Bulgaria

* adele1993@mail.ru

Optical films of aluminum oxide Al_2O_3 have been known for a long time and are applied largely in the interference coatings for the ultraviolet, visible and near-infrared spectral ranges [1-3]. Practically, they have no competitors among film-forming materials with low absorption and high refractive index in the UV spectral range of 0.15 - 0.25 microns. Dispersion of the optical constants in this region should be known for modeling and fabrication of such interference coatings [4]. So far, the information about the refractive index $n(\lambda)$, the absorption coefficient $\alpha(\lambda)$ or the extinction coefficient $k(\lambda)$ in the UV region is practically absent.

The optical constants' dispersions of Al_2O_3 films on a quartz substrate in the spectral range 0.2-0.8 microns are investigated. They are calculated from the spectrophotometric measurements of the reflection and transmission spectra using the spectral analysis program based on the matrix methods [4]. New method for correction of the films' spectra was carried out taking into account the absorption [5,6]. The refractive indices are determined from absorption–free spectra and extinction coefficients are obtained from absorption spectra in the specified spectral region. The determined values of the optical constants of the Al_2O_3 films were successfully used at the Institute of Solid State Physics of Bulgarian Academy of Sciences for the synthesis and manufacture of highly reflective mirrors at wavelength of 0.22 microns with reflection of 94%.

References:

1. Krylova T N, Interference Coatings, Leningrad: Mashinostroenie, 1973.
2. Ritter E, Film Dielectric Materials for Optical Applications: Thin Film Physics, Moscow: Mir, vol. 8, 1978, p. 7.
3. Seredin V, Goloshchapov D L, ets.. Optical devices of ultrashort Al_2O_3 films on GaAs substrates (100). Condensed substances and interphase boundaries 16(2), 2014, p. 196.
4. Born M and Wolf E, Principles of Optics, Pergamon Press. Oxford-London-Edinburgh-New-York-Paris-Frankfurt, 1970.
5. Kotlikov E N, Kotlikov A N and Yurkovets E V 2018 Program for the analysis of optical spectra of films "FilmAnalysis" certificate of registration No. 2018611718 dated February 6 2018.
6. Kotlikov E N, Kovalenko I I, ets.. Program of the synthesis and analysis of interference coating FilmManager. Sci. journal: information management systems 3(76), 2015, p. 51.

Acknowledgements

This work was supported from the Bulgarian Ministry of Education and Science, National Science Fund, grant No KP-06-N57/5 (2021) and grant MNiV0 of the Russian Federation No. FSFR-2020-0004.

2.18. Charge trapping effects in nonvolatile memory cells with HfO_2/Al_2O_3 nanolaminated trapping layer

D. Spassov[1], A. Paskaleva[1], E. Guziewicz[2], T. Stanchev[1,*], Tz Ivanov[1]

[1] *Institute of Solid State Physics, Bulgarian Academy of Sciences, Tzarigradsko Chaussee 72, Sofia 1734, Bulgaria*
[2] *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, Warsaw 02-668, Poland*

* stanchev@issp.bas.bg

Nonvolatile flash memory cells based on charge trapping are widely regarded as the near future replacement of traditionally used floating gate memory cells. In this work a comparative investigation of the charge trapping in memory cells based on nanolaminated HfO_2-Al_2O_3 charge trapping layer, depending on the thickness of the tunnel SiO_2 layer are presented. The dielectric stack of memory cells except the tunnel oxide (TO) was fabricated by low temperature Atomic Layer Deposition in a frame of single deposition process. The SiO_2 layer employed as TO layer was obtained by thermal oxidation. Cells with TO of 2.4 and 3.5 nm were investigated. The structures were subjected to rapid thermal annealing in O_2 at 800° C for 1 min to enhance their charge trapping abilities. The thinner TO provides lower starting voltages for the charge trapping, but the amount of trapped electrons is lower. The amount of trapped positive charges does not depend on the thickness of TO. Charge trapping dynamics was studied at the range of voltage pulse duration (t_p) from 1ms to 10s. The electron trapping strongly depends on the amount of carriers in the silicon inversion layer. The hole trapping is slower than electron one – for t_p=1ms ~60% of the traps are filled with electrons, compared to about 7% for the holes.

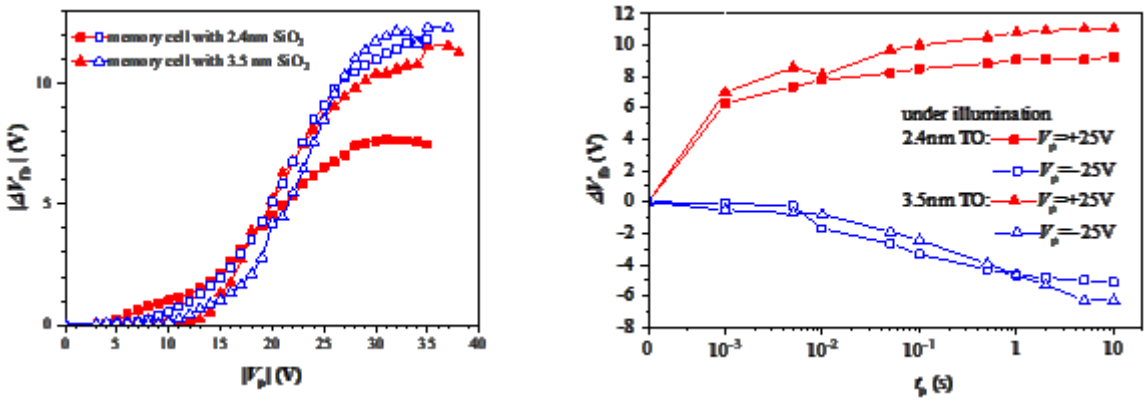


Figure 1. (a) Absolute values of the flat band voltage shifts due to the charge trapping in the memory capacitors under positive (red, closed symbols reprsenting negative charge buildup) and negative (open, blue symbols – corresponding to the accumulation of positive charge) voltage pulses. (b) Flat band voltage shifts vs. pulse duration for ±25 V pulse amplitudes.

Acknowledgements:

The work is supported by Bulgarian National Science Fund under project KP-06-H37/32.

2.19. Electric breakdown characteristics of ALD HfO_2/Al_2O_3-based memory capacitors

D. Spassov[1,*], A. Paskaleva[1], E. Guziewicz[2], Tz. Ivanov[1], T. Stanchev[1]

[1] Institute of Solid State Physics, Bulgarian Academy of Sciences, Tzarigradsko Chaussee 72, Sofia 1784 Bulgaria

[2] Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, Warsaw 02-668, Poland

* d.spassov@issp.bas.bg

HfO_2-Al_2O_3 based dielectric stacked structures have been extensively studied recently in connection with future applications in the non-volatile memories operating on the charge trapping effect. One of their characteristics that are not often targeted, is the reliability in terms of electrical breakdown. In this work, experimental results on the electrical breakdown of ALD deposited HfO_2/Al_2O_3 memory capacitors comprising Al_2O_3 blocking and SiO_2 tunnel oxides (with thickness of 2.4 and 3.5 nm) before and after O_2 annealing are presented. The breakdown voltages and the charge to breakdown were evaluated using the voltage ramp method [1] at negative gate voltages. It was obtained that breakdown voltage (V_{bd}) does not depend neither on the thickness of tunnel SiO_2, nor on annealing. The median V_{bd} is -31 V. For the capacitors with 3.4 nm SiO_2, O_2 treatment substantially increases the charge to breakdown (Q_{bd}) from 8.3×10^{-6} to 6.6×10^{-4} C/cm^2 due to the higher leakage current through the annealed samples at the same voltage. Q_{bd} for capacitors with the thinner tunnel SiO_2 does not change upon annealing (the median value is ~3×10^{-6} C/cm^2), although the annealing spreads the V_{bd} distribution to lower voltages (Figure 1). The results from the voltage ramp method were juxtaposed to time-to-breakdown data obtained from constant voltage stress.

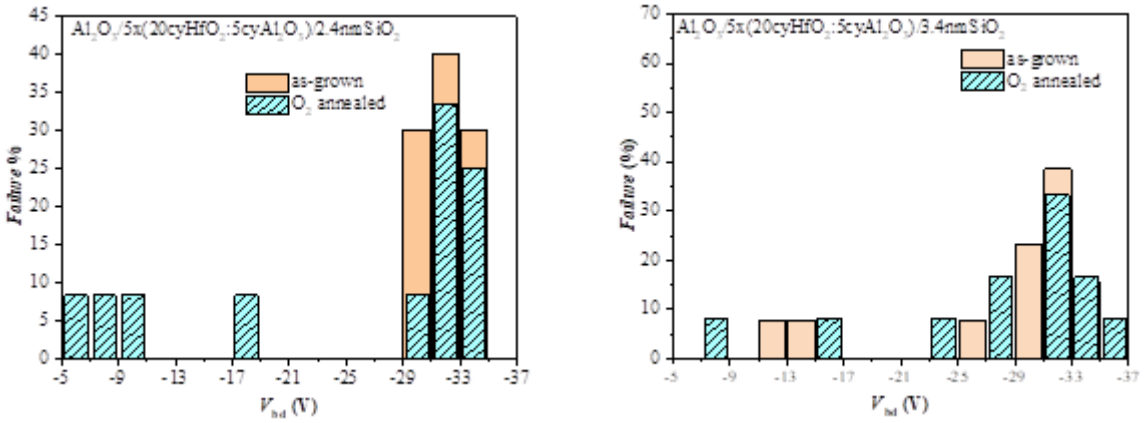


Figure 1. Breakdown voltage histograms for memory capacitors with: (a) 2.4 nm and (b) 3.5 nm tunnel SiO_2, before and after O_2 annealing.

References:

1. Procedure for the Wafer-Level Testing of Thin Dielectrics, JESD35-A, JEDEC Solid State Technology Association, Arlington, USA, p.4, 2001.

Acknowledgments:

The work is supported by Bulgarian National Science Fund under project KP-06-H37/32.

2.20. AlN films grown by plasma enhanced atomic layer deposition

M. Beshkova[1,*], B.S. Blagoev[2], V. Mehandzhiev[2], R. Yakimova[3], I. Avramova[4], P. Terziyska[2], V. Strijkova[5]

[1] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd, 1784 Sofia, Bulgaria
[2] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd, 1784 Sofia, Bulgaria
[3] Department of Physics, Chemistry and Biology, Linköping University, 58183 Linköping, Sweden
[4] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, bl. 11, 1113 Sofia, Bulgaria
[5] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev Str. bl. 109, 1113 Sofia, Bulgaria

* mbeshkova@yahoo.com

Aluminum nitride (AlN) combines a wide and direct band gap of 6.2 eV, high dielectric permittivity (6-18) and high sound velocity (up to 6000 m/s) which make it an excellent material for UV range light emitting diodes [1], high-k stacks [2] and surface acoustic wave devices (SAW) for harsh environments [3].

Due to the accurate thickness control, scale-up potential and excellent conformality atomic layer deposition (ALD) has been developed for AlN thin films using trimetylaluminum (TMA) and ammonia (NH_3) as aluminum and nitrogen sources, respectively.

However, the major disadvantage of ammonia is its low dissociation efficiency on the growth surface, which is due to the strength of the N-H bond 435 kJ/mol.

In this study AlN thin films were grown with a Beneq TFS-200 ALD reactor equipped with a capacitive plasma source. On axis 4H-SiC(0001) wafers (10 mm × 10 mm) were used as a substrate. TMA and NH_3 enhanced by nitrogen plasma were used as precursors while nitrogen (N_2) as a carrier gas. TMA pulse time was 180 ms. The effect of the plasma on the film growth was studied in the range 60-100W and plasma pulse time has been varied in the range 60-90 ms. The substrate temperature was 330°C, ALD cycles were 550.

AFM (atomic force microscopy) data demonstrate that RMS (root mean square) variations increased when the plasma power of 100 W is used.

Chemical composition and bonding states were investigated by X-ray photoelectron spectroscopy. High resolution Al 2p and N 1s spectra confirmed the presence of AlN with peaks located at 73.02 and 396.0eV, respectively for all layers. The atomic concentration of N is increased with increasing plasma power and Al/N ratio is close to the stoichiometric value (1:1) at 100 W plasma power, which is important when applying AlN films to SAW devices.

References:

1. H. Chang, Z. Liu, S. Yang, Y. Gao, J. Shan, B. Liu, J. Sun, Z. Chen, J.Yan, Z. Liu, J. Wang, P. Gao, J. Li, Z. Liu and T. Wei, Graphene-driving strain engineering to enable strain-free epitaxy of AlN film for deep ultraviolet light-emitting diode, Light: Sci. & Appl. (2022) 11:88.
2. K. G. Reid, A. Dip, S. Sasaki, D. Triyoso , S. Samavedam, D. Gilmer, C. F.H. Gondran, Electrical and materials properties of AlN/ HfO_2 high-k stack with a metal gate, Thin Solid Films 517 (2009) 2712–2718.
3. S. Xiong, X. Liu, J. Zhou, Y. Liu, Y. Shen, X. Yin, J. Wu, R. Tao, Y. Fu and H. Duan, Stability studies of ZnO and AlN thin film acoustic wave devices in acid and alkali harsh environments, RSC Adv. 10 (2020) 19178-19184.

Acknowledgements:

The work was supported by the Bulgarian National Science Fund under contract DN 18/6.

2.21. Effect of Ag on the glass formation ability and luminescence properties of Eu^{3+} doped $ZnO-B_2O_3-WO_3-Nb_2O_5$ glasses

Nikolay Nedyalkov[1], Rosen Nikov[1], Rumen Nikov[1], Lyubomir Aleksandrov[2], Margarita Milanova[2], Aneliya Yordanova[2], Reni Iordanova[2]

[1] Institute of Electronics, Bulgarian Academy of Sciences, Tzarigradsko shousse 72, Sofia 1784, Bulgaria
[2] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, blvd. Akad. G. Bonchev bl.11, Sofia 1113, Bulgaria

The effect of silver ions on the glass ability and luminescence properties of $50ZnO:40B_2O_3:10\text{-}xWO_3:xNb_2O_5:1Eu^{3+}$ (x=0 and 5 mol%) glasses ware investigated in this work. The synthesized glasses characterize with good transmittance and homogeneity. The amorphous state of the glasses was demonstrated X-ray diffraction analysis (XRD). The thermal parameters such as glass transition temperature, glass crystallization temperature and thermal stability of the glasses were determined by differential thermal analysis. Physical parameters of synthesized glasses such as density, molar volume, oxygen molar volume, oxygen and packing density were determined.

Irradiation by nanosecond laser pulses at wavelength of 266 nm was applied in order to induce composition changes of the studied glass. Photoluminescence emissions due to the 4f transitions $^5D_0 \rightarrow {}^7F_j$ (j=0-4) of Eu^{3+} ions were observed. Influence of Ag content on the emission intensity of the prepared glasses was established.

Acknowledgements:

This work is supported by Bulgarian National Science Fund under project КП-06-Н29/7.

2.22. X-ray photoelectron spectroscopy investigation on thermally treated iron-rich oxide glasses

Ivalina Avramova[1,*], Irena Mihailova[2], Ruzha Harizanova[2], Georgi Avdeev[3]

[1] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Akad. G. Bonchev Str., bl. 11, Sofia 1113, Bulgaria
[2] University of Chemical Technology and Metallurgy, 8 Kliment Ohridski Blvd., Sofia 1756, Bulgaria
[3] Institute of Physical Chemistry, Bulgarian Academy of Sciences, Akad. G. Bonchev Str., bl. 11, Sofia 1113, Bulgaria

* iva@svr.igic.bas.bg

Iron oxide glass-ceramics exhibit useful mechanical, thermal and bioactive properties. Additionally, these glasses and glass-ceramics have shown magnetic properties which arise from the magnetite crystallizing in the glasses. Thus, these materials can find application in various biomedical applications like magnetic resonance imaging, hyperthermia, drug delivery, etc.

Soda-lime silicate glasses with high iron concentration and formula $16Na_2O$-$10CaO$-$(74-x)SiO_2$-xFe_2O_3, x= 20 , 25, 30 mol % have been prepared by melt quenching. The glass samples are subjected to controlled heat-treatment at 580 °C for 1, 3 and 7 h to obtain crystallized samples. The phase composition investigation by means of X-ray diffraction reveals presence of magnetite, Fe_3O_4 and hematite, α-Fe_2O_3 in the as quenched samples with x = 20, 25 and 30 mol % Fe_2O_3. The applied thermal treatment results in growth of the magnetite and hematite crystals with increasing volume fraction and average size. The scanning electron microscopy imaging of the obtained glass-ceramics supports the results from the X-ray diffraction that a Fe-rich phase is precipitated and further grows after the applied thermal treatment. The elemental composition and oxidation states of the constituents of the as quenches glasses and the samples prepared after the applied thermal treatment are studied by the X-ray photoelectron spectroscopy method. All elements, except Fe, in the composition are present in their oxidized states, i.e. Na^+, Ca^{2+} and Si^{4+} while Fe is present both as Fe^{2+} and Fe^{3+}. The O1s, Fe2p and Fe3p photoelectron spectra provide information on the valence state of iron and the corresponding oxygen bonds in the glass network. The number of non-bridging and bridging oxygen ions is calculated and its dependence on the iron concentration and the thermal treatment program applied is traced.

Acknowledgements:

The authors acknowledge the financial support of the Bulgarian National Science Fund under contract KP-06-N48/4.

2.23. Physicochemical and structural characterization of silicate glasses and glass-ceramics containing iron oxides

Irena Mihailova*, Ruzha Harizanova, Nikoleta Shtapleva, Tina Tasheva

University of Chemical Technology and Metallurgy, 8 Kliment Ohridski Blvd., Sofia 1756, Bulgaria

* irena@uctm.edu

The interest in glasses containing iron oxides is determined by the possibility to obtain from them ferrimagnetic glass-ceramics for biomedical applications such as anticancer therapy by means of magnetic induction hyperthermia.

Subject of the present investigation is the compositional series of glasses and glass-ceramics in the system $16Na_2O/10CaO/(74-x)SiO_2/xFe_2O_3$, x = 5, 10, 15, 20, 25, 30 mol%. The samples are prepared by soaking the melt at 1400 °C for 2 h on air and then melt quenching. X-ray diffraction analysis proves that the materials containing up to 15 mol% Fe_2O_3 are amorphous. Increasing the concentration of Fe_2O_3 above 15 mol% results in the occurrence of crystalline phases during melt quenching – magnetite and hematite. The degree of crystallinity increases with the increasing iron oxide concentration. The sample morphology and the elemental composition of the precipitated crystalline phase have been studied by Scanning Electron Microscopy and Energy Dispersive X-ray Spectrometry, respectively. For the physicochemical characterization of the synthesized glasses the density, molar volume and oxygen packing density have been estimated. The Becke line method has been utilized for the refractive indices measurement. The structural evolution in dependence of the Fe_2O_3 concentration in the samples has been studied by means of Fourier Transformed Infrared Spectroscopy. The data obtained from the different methods well correlates and reveals depolymerization tendency of the silicate network with the increasing Fe_2O_3 concentration, i.e. increase in the number of SiO_4 tetrahedra with more non-bridging oxygens as a result of the occurrence of Fe-containing polyhedra in the glass structure.

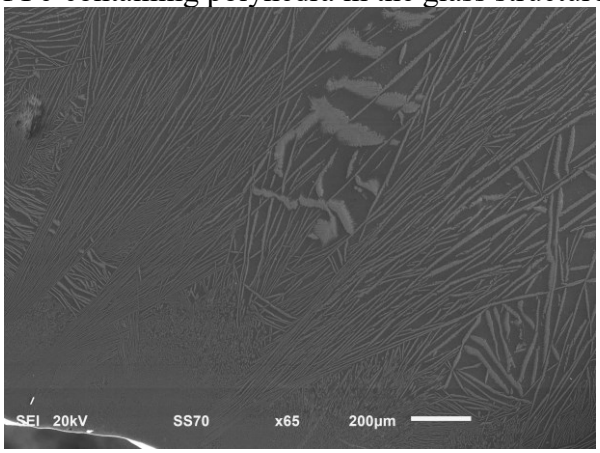


Figure 1. Microphotograph of a glass-ceramic sample with 30 mol% Fe_2O_3.

Acknowledgements:

The authors acknowledge the financial support of the Bulgarian National Science Fund under contract KP-06-N48/4.

2.24. Phase composition and microstructure characterization of strontium-modified barium titanate glass-ceramics

Ruzha Harizanova[1,*], Martin Pernikov[1], Irena Mihailova[1], Dragomir Tatchev[2], Georgi Avdeev[2], Ivalina Avramova[3], Christian Rüssel[4]

[1] *University of Chemical Technology and Metallurgy, 8 Kliment Ohridski Blvd., Sofia 1756, Bulgaria*
[2] *Institute of Physical Chemistry, Bulgarian Academy of Sciences, Akad. G. Bonchev Str., bl. 11, Sofia 1113, Bulgaria*
[3] *Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Akad. G. Bonchev Str., bl. 11, Sofia 1113, Bulgaria*
[4] *Otto Schott Institute of Materials Research, University of Jena, Fraunhoferstr. 6, 07743 Jena, Germany*

* rharizanova@uctm.edu

Dielectric glass-ceramic materials find various applications as parts of sensors, electronic components and even in biomedicine. The present work reports on the synthesis of glass-ceramic materials in the complex oxide system (23.1-x)Na_2O/17.1BaO/6SrO/23TiO_2/17.4SiO_2/7.6B_2O_3/ 5.8Fe_2O_3/xAl_2O_3, x = 0 and 3 mol%. The melts show spontaneous crystallization during quenching. The phase composition is studied using X-ray Diffraction and reveals crystallization of $Ba_{1-x}Sr_xTiO_3$ solid solution with varying Ba/Sr ratio. The valence states and the local environments of the Ba, Ti and Fe ions of the prepared materials are investigated by utilizing X-ray photoelectron spectroscopy. It is shown that all the elements in the composition are present in their oxidized states (Ti^{4+} and Fe^{3+}) and the formation of barium titanate based compounds is as well possible. The microstructure of the obtained samples is imaged by scanning electron microscopy and shows occurrence of bright platelet-like crystalline structures embedded in a dark amorphous matrix. The further evaluation of the microstructure as average crystal size and volume fraction of the precipitated crystals is done by using microcomputed tomography. A relatively high crystalline volume fraction is observed for the samples without alumina while the samples with alumina possess smaller crystals and smaller volume fraction of the crystalline phase.

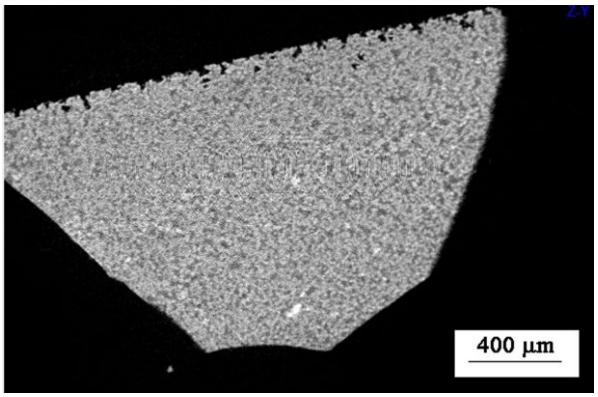


Figure 1. Microtomography image of a glass-ceramic sample with 3 mol% Al_2O_3.

Acknowledgements:

The authors acknowledge the financial support of the Bulgarian National Science Fund under contract KP-06-N28/1.

2.25. Influence of Al-substitution on the Structure and Magnetic Properties of $BaFe_{12}O_{19}$ Obtained by Modified Co-precipitation Methods

Ch. Ghelev[1,*], B. Georgieva[1], S. Kolev[1,2], P. Peneva[1], K. Krezhov[1], D. Kovacheva[3], B. Vertruyen[4], R. Closset[4], L. M. Tran[5], M. Babij[5], A. Zaleski[5], T. Koutzarova[1]

[1] *Institute of Electronics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria*
[2] *Neofit Rilski South-Western University, 66 Ivan Mihailov Str., 2700 Blagoevgrad, Bulgaria*
[3] *Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. Georgi Bonchev Str., bld. 11, 1113 Sofia, Bulgaria*
[4] *Greenmat, Chemistry Department, University of Liege, 11 allée du 6 août, 4000 Liège, Belgium*
[5] *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okólna 2, 50-422 Wroclaw, Poland*

* chavdarghelev@yahoo.com

We report studies on the influence of Al substitution on the microstructure, the magneto-crystalline structure and the magnetic properties of barium hexaferrite nanopowders. The role is also discussed of the synthesis procedure on the properties of the resulting powders. These were synthesized using single microemulsion and sonochemical co-precipitation methods.

The average particle size of the $BaFe_{12}O_{19}$ powders was in the range from 50 nm to 150 nm depending on the method and conditions of synthesis. They had irregular shapes between spherical and plate-hexagonal. The microscopy studies showed that the Al-substituted $BaFe_{12}O_{19}$ particles in the sample synthesized by single microemulsion had a size below 100 nm and a very thin flat shape, in contrast with those of the unsubstituted barium hexaferrite. The powders prepared by sonochemical synthesis had the same irregular shapes as the unsubstituted $BaFe_{12}O_{19}$.

The magnetic properties of the powder were investigated at 4.2 K and at room temperature. The saturation magnetization values (M_s) were obtained from the magnetization curves in high magnetic fields up to 130 kOe. The Al-substitution does not change significantly the saturation magnetization M_s of the powders. The coercivity field (H_c) values for the Al-substituted samples were much lower than those of the unsubstituted ones. The H_c values for samples with a similar particle size are 400 Oe and 4.34 kOe for substituted and unsubstituted samples, respectively.

Acknowledgements:

The work was supported by the Bulgarian National Science Fund under contract KP-06-N48/5 "Multifunctional composite structures based on ferrites (including magneto-electrics) and carbon materials". This work was also supported by a joint research project between the Bulgarian Academy of Sciences and WBI, Belgium, and by a joint research project between the Bulgarian Academy of Sciences and the Institute of Low Temperature and Structure Research, Polish Academy of Sciences.

2.26. Growth of Fe Oxide Nanofilms by Atomic Layer Deposition

B.S. Blagoev[1,*], V.B. Mehandzhiev[1], P. Terziyska[1], I. Avramova[2], P. Tzvetkov[2], D. Kovacheva[2], A. Paskaleva[1]

[1] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd, 1784 Sofia, Bulgaria
[2] Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, bl. 10, 1113 Sofia, Bulgaria

* blago_sb@yahoo.com, blago@issp.bas.bg

Transition metal oxides (TMO) are a large group of oxide compounds of metals with partially filled d-shell. In spite of extensive research the interest toward them increased because of their exciting properties like Colossal Magnetoresistance (CMR), High Temperature Superconductivity (HTSC), Magnetic properties, Multiferroism, etc. The existence of multiple oxidation states and strong catalytic activity in TMO lead to various applications like batteries, memristors and photon-induced water splitting. Furthermore the transition metals could be used as dopants in semiconductors and thus to enrich their properties. Thus obtained materials are of great interest for the practice because of their potential low consumming energy and their multifunctionality. The high-quality TMO nanofilms for all these applications are a challenge for deposition technology. Atomic Layer Deposition (ALD) turns out to be one of the most suitable techniques for obtaining uniform ultra thin films on large areas.

In this work Fe oxide nanofilms were obtained by ALD using ferrocene and ozone precursors. Nanofilms of Fe oxides on different substrates and at different deposition temperatures were obtained on a Beneq TFS-200 ALD apparatus. Ferrocene (FeCp2) was used as first precursor and ozone (O_3) as oxidant. The films are characterized by Ellipsometry, XRD and XPS analaisys.

Acknowledgements:

The work is supported by Bulgarian National Science Fund under project KP-06-H28/9.

2.27. Variation of UV-A/UV-B daily profiles depending on location and altitude

Christo Angelov[1,*], Nikolay Tyutyundzhiev[2], Todor Arsov[1], Hristo Nitchev[2], Konstantin Lovchinov[3]

[1] Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria;
[2] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria
[3] Acad. J. Malinowski Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., bl. 109, 1113 Sofia, Bulgaria.

* hangelov@inrne.bas.bg

In this work, the variation was studied of the daily profiles of the UV radiation component (UV-B/UV-A) depending on the location and the altitude. The measurement locations have been selected to satisfy two criteria: 1 - Specific type of climate conditions (high-mountain, sea level, residential, urban, hot valley); 2 - Good internet infrastructure suitable for long-time remote data logging. The as selected location points are: the Basic Environmental Observatory (BEO) – Moussala Peak (2925 m a.s.l.), the National Astronomic Observatory (AO) – Rozhen (1720 m a.s.l.), the Astronomic Observatory (AO) – Belogradchik (Danube River valley), a Bulgarian Academy of Sciences (BAS) laboratory building – Sofia City (612 m a.s.l.), the BAS Rest House, Varna (51 m a.s.l.), the Hydro-Meteorological Station (HMS) – Ahtopol (Black Sea shore), and Hotovo village Melnik (196 m a.s.l.). For the purpose of the measurements, cost-efficient, easy-to-use UV sensor equipment was developed based on integrated digital sensors (VEML 6075, TSL 2591) and an Wi-Fi ESP 32 microcontroller, an ODROID microcomputer and open–source software (InfluxDB and Grafana visualization tool). In this paper, we present the first UV measurements with the UV-B/UV-A/Visible/near-IR sensor system. The UV sensor station thus developed is a flexible solution capable of operating under severe atmospheric conditions. An additional advantage is the possibility for parallel measurements and direct comparison of the diurnal variations at different wavelengths. We thus expect that it should attract the attention of many researchers looking for new technical solutions and wider applications.

Acknowledgements:

This research was funded by the Bulgarian Science Fund through the IntegraUV project KP-06-24/1-2018. We also acknowledge the support given by the BEO-Moussala team of INRNE-BAS in preparing the UV measurements at Moussala Peak.

2.28. Remote datalogging of solar UV irradiation using open-source ESP32 platform and MQTT protocol

Christo Angelov[1,*], Nikolay Tyutyundzhiev[2], Todor Arsov[1], Konstantin Lovchinov[3], A. Mitafov[4]

[1] Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 72 Tzarigradsko chausse, Blvd. 1784 Sofia, Bulgaria;
[2] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tzarigradsko chausse, Blvd. 1784 Sofia, Bulgaria
[3] Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Acad. G. Bonchev str., bl. 109, 1113 Sofia, Bulgaria.
[4] Institute of Astronomy, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria

* hangelov@inrne.bas.bg

Recent data loggers are computer peripheral devices or stand-alone smart instruments which can collect local databases and are able to transfer data to remote servers. Therefore, an appropriate communication protocol is required to facilitate the integration to existing computer infrastructure. This study proposes the utilization of MQTT as a communication protocol between scientific instrumentation: UV sensors, open-source data processing controllers and SoC computers. Datalogging of sensor measurement of solar UV irradiation informs the user of variations in UV fluxes over certain location which can be dangerous for humans or which can influence over plants, animals, machine equipment, human behavior, etc... Measured parameters are UVA (315-400nm), UVB (280-315nm), and visible (400-780 nm) + NIR (700-1100nm) radiation and calculated UV-index (UVI). The architecture of modern IoT distributed sensor monitoring system consists of numerous remote sensors connected by wireless or wired to internet. In order to ensure the reliable data logging the data is stored locally on small machines and transferred later to central servers. Local storage is important for speed optimization of fast sensors and to ensure reliable datalogging if short interval are selected. Data acquisition was done in real-time, stored in InfluxDB database and graphically presented by Grafana visualization tool.

Acknowledgements:

This research paper is funded by the Bulgarian Research Fund through the IntegraUV project КП-06-24/1-2018.

2.29. Laser-Induced Periodic Surface Structuring of Wide Bandgap Transparent Materials

Stefan Karatodorov[1,*], Mariam Shehadi[1], Lyubomir Stoychev[1], Docho Tsankov[2], Boris Shivachev[3], Todor Petrov[1,2]

[1] Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784, Sofia, Bulgaria
[2] Technical University of Sofia, 8, Kliment Ohridski St. Sofia-1000, Bulgaria
[3] Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

* skarat@issp.bas.bg

Semiconductors materials from group III- nitrides have exceptional set of properties, i.e. wide energy bandgap, hardness, high thermal conductivity, lower energy consumption, and high breakdown voltage [1], due to which they have found significant applications in the field of microelectronic devices [2,3]. For many optoelectronic applications of these materials, a specially designed surface structuring is required in order to facilitate the application itself or/and to optimize the material performance. Among the many methods for surface modifications, Laser-Induced Periodic Surface Structures (LIPSS) [5] has proven one of the most used in recent years, mainly due to its simple experimental setup, availability of short-pulse laser sources and applicability to wide range of solid materials (metals, semiconductors and isolators).

In this work, we present results on the formation of LIPSS on the surface of wide band gap materials – fused silica, Aluminum nitride (AlN) and Gallium nitride (GaN). The LIPPS are formed under irradiation with tens of pulses from a diode pumped femtosecond laser (Pharos PH2-SP-HP) with pulse energies in the range of 0.5-10 μJ with two separate wavelengths 515 nm (140 fs) and 1030 nm (180 fs). The created surface ripples are characterized by a confocal scanning optical microscope Zeiss LSM 900. The results are discussed in view of potential applications for the formed surface structures.

References:

1. Q. Hua, B. Ma and W. Hu., Aluminum, Gallium, and Indium Nitrides". Encyclopedia of Materials: Technical Ceramics and Glasses 3, 2021, 74-83.
2. F. Roccaforte, P. Fiorenza, G. Greco, R. L. Nigro, F. Giannazzo, F. Iucolaano and M. Saggio, Microelectronic Engineering 187-188, 2018, 66-67.
3. M. Shur, Solid State Electronics 155, 2019, 65-75.
4. J. Bonse, S. Höhm, S. V. Kirner, A. Rosenfeld, and J. Krüger, Laser-induced periodic surface structures—A scientific evergreen. IEEE Journal of selected topics in quantum electronics, 23(3), 2016.

Acknowledgments:

The research is funded by projects: Bulgarian Science Fund DN – 18/7 -10.12.2017, BG05M2OP001-1.001-0008 National center of Mechatronics and Clean Technologies Operational Program: Science and Education for Smart Growth 2014-2020 and ELI "Extreme Light" (Extreme Light Infrastructure BG) D01– 401/18.12.2020.

LIST OF PARTICIPANTS

Alexieva, Gergana	Faculty of Physics, Sofia University	Sofia, Bulgaria	gerry@phys.uni-sofia.bg
Angelov, Christo	Institute for Nuclear Research and Nuclear Energy - BAS	Sofia, Bulgaria	hangelov@inrne.bas.bg
Angelova, Elena	Institute of Solid State Physics - BAS	Sofia, Bulgaria	angelova@issp.bas.bg
Atanasova, Anna	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	alalova@iomt.bas.bg
Avramova, Ivalina	Institute of General and Inorganic Chemistry - BAS	Sofia, Bulgaria	iva@svr.igic.bas.bg
Balestra, Francis	CNRS, IMEP-LAHC	Grenoble, France	balestra@minatec.grenoble-inp.fr
Banerjee, Sarbajit	Department of Chemistry; Department of Materials Science & Engineering, Texas A&M University	Texas, USA	banerjee@chem.tamu.edu
Baranovskii, Sergei	Faculty of Physics, Philipps University Marburg	Marburg, Germany	sergei.baranovski@physik.uni-marburg.de
Baranovskii, Svetlana	Faculty of Physics, Philipps University Marburg	Marburg, Germany	svetlana.baranovski@physik.uni-marburg.de
Beshkova, Milena	Institute of Electronics - BAS	Sofia, Bulgaria	mbeshkova@yahoo.com
Bineva, Irina	Institute of Solid State Physics - BAS	Sofia, Bulgaria	irka@issp.bas.bg
Blagoev, Blagoy	Institute of Solid State Physics - BAS	Sofia, Bulgaria	blago@issp.bas.bg
Buchkov, Krastyo	Institute of Solid State Physics - BAS	Sofia, Bulgaria	buchkov@issp.bas.bg
Čelebonović, Vladan	Institute of Physics	Belgrade, Serbia	vladan@ipb.ac.rs
Chamati, Hassan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	chamati@issp.bas.bg

Christova, Darinka	Institute of Polymers - BAS	Sofia, Bulgaria	dchristo@polymer.bas.bg
Danel, Zoriana	Faculty of Materials Engineering and Physics, Cracow University of Technology	Cracow, Poland	zoriana.danel@pk.edu.pl
Danev, Mario	Institute of Solid State Physics - BAS	Sofia, Bulgaria	mariodanev89@gmail.com
Dedinska, Liubomila	Institute of Solid State Physics - BAS	Sofia, Bulgaria	buba@issp.bas.bg
Dencheva-Zarkova, Maria	Institute of Solid State Physics - BAS	Sofia, Bulgaria	biolayer@issp.bas.bg
Dimitrova, Yana	Faculty of Chemistry and Pharmacy, Sofia University	Sofia, Bulgaria	yanadim123@gmail.com
Donchev, Vesselin	Faculty of Physics, Sofia University	Sofia, Bulgaria	vtd@phys.uni-sofia.bg
Dzhurkov, Valeri	Institute of Solid State Physics - BAS	Sofia, Bulgaria	valeri.dzhurkov@issp.bas.bg
Esmeryan, Karekin	Institute of Solid State Physics - BAS	Sofia, Bulgaria	karekin_esmerian@abv.bg
Exner, Ginka	Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski"	Plovdiv, Bulgaria	ginka.exner@gmail.com
Fabian, Margit	Centre for Energy Research	Budapest, Hunagry	fabian.margit@ek-cer.hu
Gegova-Dzhurkova, Radka	Institute of Solid State Physics - BAS	Sofia, Bulgaria	radka.dzhurkova@issp.bas.bg
Georgiev, Miroslav	Institute of Solid State Physics - BAS	Sofia, Bulgaria	mgeorgiev@issp.bas.bg
Georgiev, Stefan	Faculty of Physics, Sofia University	Sofia, Bulgaria	stefangg1@gmail.com
Georgieva, Borislava	Institute of Electronics - BAS	Sofia, Bulgaria	b.georgiewa@abv.bg
Georgieva, Desislava	Faculty of Physics, Sofia University	Sofia, Bulgaria	dnikolaevg@phys.uni-sofia.bg
Gergova, Rositsa	Central Laboratory of Solar Energy and New Energy Sources - BAS	Sofia, Bulgaria	rgergova@phys.bas.bg
Ghelev, Chavdar	Institute of Electronics - BAS	Sofia, Bulgaria	chavdarghelev@yahoo.com

Grigorov, Aleksandar	Department of Physics, University of Plovdiv "Paisii Hilendarski"	Plovdiv, Bulgaria	aleksandar.grigorov@abv.bg
Guziewicz, Elżbieta	Institute of Physics, Polish Academy of Sciences	Warsaw, Poland	guzel@ifpan.edu.pl
Hadjichristov, Georgi	Institute of Solid State Physics - BAS	Sofia, Bulgaria	georgibh@issp.bas.bg
Halun, Joanna	Institute of Nuclear Physics, Polish Academy of Sciences	Kraków, Poland	joanna.halun@ifj.edu.pl
Harizanova, Ruzha	University of Chemical Technology and Metallurgy	Sofia, Bulgaria	rharizanova@uctm.edu
Hristova-Vasileva, Temenuga	Institute of Solid State Physics - BAS	Sofia, Bulgaria	teddie@issp.bas.bg
Iglič, Aleš	University of Ljubljana, Slovenia	Ljubljana, Slovenia	ales.iglic@fe.uni-lj.si
Iordanova, Ekaterina	Institute of Solid State Physics - BAS	Sofia, Bulgaria	eiordanova@issp.bas.bg
Ivanov, George R.	University Laboratory "Nanoscience and Nanotechnology", University of Architecture, Civil Engineering and Geodesy	Sofia, Bulgaria	george@at-equipment.com
Ivanov, Nedko	Institute of Solid State Physics - BAS	Sofia, Bulgaria	ivanov@issp.bas.bg
Ivanov, Petar	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	petar@iomt.bas.bg
Ivanov, Tsvetan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	tsvn@issp.bas.bg
Ivanova, Dobrina	Faculty of Chemistry and Pharmacy, Sofia University	Sofia, Bulgaria	dobrina.k.ivanova@gmail.com
Ivanova, Nikoleta	Institute of Solid State Physics - BAS; University of Chemical Technology and Metallurgy	Sofia, Bulgaria	n.ivanova@uctm.edu
Kamburova, Radostina	Institute of Solid State Physics - BAS	Sofia, Bulgaria	krad@issp.bas.bg

Karakashkova, Petya	Institute of Catalysis - BAS	Sofia, Bulgaria	petia.karakashkova@gmail.com
Karatodorov, Stefan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	skarat@issp.bas.bg
Katranchev, Boyko	Institute of Solid State Physics - BAS	Sofia, Bulgaria	boykopk@issp.bas.bg
Katrova, Vesela	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	vlozanova@iomt.bas.bg
Kodru, Hari Krishna	Institute of Solid State Physics - BAS	Sofia, Bulgaria	koduru@issp.bas.bg
Kolev, Petar	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	p.kolev@iomt.bas.bg
Korutcheva, Elka	Universidad Nacional de Educación a Distancia	Madrid, Spain	elka@fisfun.uned.es
Koutzarova, Tatyana	Institute of Electronics - BAS	Sofia, Bulgaria	tanya@ie.bas.bg
Kralj, Samo	Jožef Stefan Institute, University of Maribor	Ljubljana, Slovenia	samo.kralj@um.si
Kuterba, Piotr	Institute of Theoretical Physics, Jagiellonian University	Kraków, Poland	piotr.kuterba@uj.edu.pl
Lazarova, Madlena	Institute of Chemical Engineering - BAS	Sofia, Bulgaria	m.lazarova@iche.bas.bg
Lovchinov, Konstantin	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	lovchinov@iomt.bas.bg
Malka, Dror	Faculty of Engineering, Holon Institute of Technology (HIT)	Holon, Israel	drorm@hit.ac.il
Marinov, Yordan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	ymarinov@issp.bas.bg
Marudova, Maria	Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski"	Plovdiv, Bulgaria	marudova@uni-plovdiv.net
Mihailescu, Ion N.	National Institute for Laser, Plasma and Radiation Physics (INFLPR)	Ilfov-Magurele, Romania	ion.mihailescu@inflpr.ro

Mihailova, Irena	University of Chemical Technology and Metallurgy	Sofia, Bulgaria	irena@uctm.edu
Mihova, Gergana	Faculty of Physics, Sofia University	Sofia, Bulgaria	gerganamm@uni-sofia.bg
Milenkova, Sofia	Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski"	Plovdiv, Bulgaria	sophiamilenkowa@gmail.com
Miloushev, Ilko	Institute of Solid State Physics - BAS	Sofia, Bulgaria	miloushev@issp.bas.bg
Minkovska, Stela	Institute of Catalysis - BAS	Sofia, Bulgaria	stelamin@ic.bas.bg
Montgomery, Paul	Université de Strasbourg - CNRS	Strasbourg, France	paul.montgomery@unistra.fr
Nedyalkov, Nikolay	Institute of Electronics - BAS	Sofia, Bulgaria	nned@ie.bas.bg
Paskaleva, Albena	Institute of Solid State Physics - BAS	Sofia, Bulgaria	paskaleva@issp.bas.bg
Petrik, Peter	Centre for Energy Research, Budapest	Budapest, Hungary	petrik.peter@ek-cer.hu
Petrov, Miroslav	Institute of Electronics - BAS	Sofia, Bulgaria	petrov_80@ie.bas.bg
Petrova, Petia	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	petia@iomt.bas.bg
Petrov, Todor	Institute of Solid State Physics - BAS	Sofia, Bulgaria	petrovts@gmail.com
Pisanova, Ekaterina	Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski"	Plovdiv, Bulgaria	katia_pisanova@abv.bg
Poklar, Ulrih Nataša	Biotechnical Faculty, University of Ljubljana	Ljubljana, Slovenia	natasa.poklar@bf.uni-lj.si
Reynolds, Steve	School of Science and Engineering, University of Dundee	Dundee, UK	s.z.reynolds@dundee.ac.uk
Reznik, Alla	Physics Department, Lakehead University; Advanced Detector Devices, Thunder Bay Regional Health Research Institute	Thunder Bay, ON Canada	areznik@lakeheadu.ca
Santosh, Poornima	Institute of Solid State Physics - BAS	Sofia, Bulgaria	poorni@issp.bas.bg

Shehadi, Mariam	Institute of Solid State Physics - BAS	Sofia, Bulgaria	mshehadi@issp.bas.bg
Slavov, Lyubomir	Institute of Electronics - BAS	Sofia, Bulgaria	l_slavov@yahoo.co.uk
Soares, Dinesh	ACS Publications, American Chemical Society	Oxford, UK	DSoares@acs-i.org
Solunov, Hristo	Department of Physics and Technology, University of Plovdiv "Paisii Hilendarski"	Plovdiv, Bulgaria	solunov@uni-plovdiv.bg
Spassov, Dencho	Institute of Solid State Physics - BAS	Sofia, Bulgaria	d.spassov@issp.bas.bg
Stanchev, Todor	Institute of Solid State Physics - BAS	Sofia, Bulgaria	stanchev@issp.bas.bg
Stankova, Stanka	Central Laboratory of Solar Energy and New Energy Sources - Bulgarian Academy of Sciences	Sofia, Bulgaria	perovskite.psc@gmail.com
Stoyanova, Elena	Institute of Solid State Physics - BAS	Sofia, Bulgaria	e.stoyanova@issp.bas.bg
Todorov, Rosen	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	rossen@iomt.bas.bg
Tolnai, Istvan	Centre for Energy Research	Budapest, Hungary	tolnai.istvan@ek-cer.hu
Vanderbemden, Philippe	University of Liege, Institut Montefiore	Liege, Belgium	Philippe.Vanderbemden@uliege.be
Varonov, Albert	Institute of Solid State Physics - BAS	Sofia, Bulgaria	varonov@issp.bas.bg
Vaseashta, Ashok	Office of Applied Research, International Clean Water Institute	Manassas, USA	prof.vaseashta@nanoknowledge.info
Velkova, Irina	Institute of Solid State Physics - BAS	Sofia, Bulgaria	velkova@issp.bas.bg
Vlakhov, Todor	Institute of Solid State Physics - BAS	Sofia, Bulgaria	todor_vlakhov@issp.bas.bg
Yankov, Georgi	Institute of Solid State Physics - BAS	Sofia, Bulgaria	gjankov@issp.bas.bg
Zsivanovits, Gabor	Institute of Food Preservation and Quality	Plovdiv, Bulgaria	g.zsivanovits@canri.org