GEORGI NADJAKOV INSTITUTE OF SOLID STATE PHYSICS

23rd INTERNATIONAL SCHOOL ON CONDENSED MATTER PHYSICS

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

"Recent Progress in Advanced Materials and Applications"

August 26th - 30th, 2024

Varna, Bulgaria

Papers will be published in:

ACS OMEGA

JOURNAL OF PHYSICS: CONFERENCE SERIES
IOP Publishing

Supported by:

ZEISS Seeing beyond

АКВАХИМ AQUACHIM

TECPORT

PLANT FOR OPTICS PURE FINE OPTICS

dh DEMAX HOLOGRAMS

БЪЛГАРСКА АКАДЕМИЯ НА НАУКИТЕ 155 BULGARIAN ACADEMY OF SCIENCES

Organising Committee

Chairpersons

Assoc. Prof. E. Iordanova & Prof. H. Chamati
Georgi Nadjakov Institute of Solid State Physics,
Bulgarian Academy of Sciences, Sofia, Bulgaria

Local Organising Committee

Viktoria Atanassova, Temenuga Hristova-Vasileva, Elena Stoyanova

International Programme Committee

Sergei Baranovskii (Philipps-University Marburg, Germany)
Sarbajit Banerjee (Texas A&M University, Texas, USA)
Hassan Chamati (ISSP-BAS, Sofia, Bulgaria)
Adrian Dinescu (IMT Bucharest, Romania)
Doriana Dimova-Malinovska (CLSENES-BAS, Sofia)
Elżbieta Guziewicz (Polish Academy of Sciences, Poland)
Aleš Iglič (University of Ljubljana, Slovenia)
Ekaterina Iordanova (ISSP-BAS, Sofia, Bulgaria)
Samo Kralj (University of Maribor, Slovenia)
Paul Montgomery (Unistra-CNRS, Strasbourg, France)
Diana Nesheva (ISSP-BAS, Sofia, Bulgaria)
Albena Paskaleva (ISSP-BAS, Sofia, Bulgaria)
Stephen Reynolds (School of Science and Engineering, University of Dundee)
Imre Miklós Szilágyi (Budapest University of Technology and Economics)
Philippe Vanderbemden (Institut Montefiore, Liège, Belgium)
Marian Zamfirescu (CETAL, INFLPR-Bucharest, Romania)

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, E. Iordanova, A. Paskaleva

TABLE OF CONTENTS

PROGRAM ……..…… 4

POSTER PRESENTATIONS …… 7

ABSTRACTS OF INVITED LECTURES ……..…….. 9

ABSTRACTS OF ORAL PRESENTATIONS ……... 30

ABSTRACTS OF FIRST POSTER SESSION ……... 42

ABSTRACTS OF SECOND POSTER SESSION …….. 63

LIST OF PARTICIPANTS …….. 83

PROGRAM

August 25th (Sunday)

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

August 26th (Monday)

08:30-09:00 *Registration*

09:10-09:30 **Opening Ceremony**

09:30-11:00 **Chair: E. Iordanova**
09:30-10:15 S. REYNOLDS, "Carrier transport and electronic defects in gallium oxide studied by photoconductivity techniques"
Georgi Nadjakov Memorial Lecture
10:15-11:00 P. MONTGOMERY, "From Rolls Royce engines to butterfly wings, or using photonics for seeing the invisible in advanced materials"
Milko Borisov Memorial Lecture

11:00-11:30 *Coffee break / Collective photo*

11:30-12:30 **Chair: E. Reznik**
11:30-12:10 Ph.VANDERBEMDEN, "Simultaneous partial discharge and current measurements in a needle-plane configuration at different pressures"
12:10-12:30 D. MUKHERJEE, "Finite element simulations for the optical sensing performance of gold gratings"

12:30-16:00 *Lunch break*

16:00-18:00 **Chair: H. Chamati**
16:00-16:40 S. BARANOVSKII, "Fundamental spatial scales for charge transport and recombination in disordered semiconductors"
16:40:17:00 N. GEORGIEVA, "Characterization of unsaturated lipid bilayer properties under different conditions with a Slipids force field"
17:00-18:30 Five minutes' presentations of posters

August 27th (Tuesday)

08:30-09:00 *Registration*

09:10-10:30 **Chair: Ph.Vanderbemden**
09:10-09:50 H. CHAMATI, "Novel insights into the physics of molecular magnets"
09:50-10:30 M. FABIAN, "Interactions within an advanced glass/copper/bentonite system under simulated geological disposal conditions"

10:30-11:00 *Coffee break*

11:00-12:20 **Chair: T. Koutzarova**
11:00-11:40 P. PETRIK, "Recent progress in ellipsometry at solid-liquid interfaces"
11:40-12:20 A. DINESCU, "Wireless temperature and pressure sensors based on surface acoustic wave resonators – fabrication processes"

12:20-16:00 *Lunch break*

16:00-17:00 **Chair: Z. Danel**
16:00-16:20 M. ZID, "Criticality controlling mechanisms in nematic liquid crystals"
16:20-16:40 G. IVANOV, "Langmuir and Langmuir-Blodgett Nanocomposite Films from Adsorbed Glucose Oxidase Enzymes"
16:40-17:00 K. ESMERYAN, "Effect of commercial cryoprotectants and hybrid "instant" freezing on the outcome of soot-assisted human sperm cryopreservation"

17:00-18:30 **First poster session** / *Coffee break*

August 28th (Wednesday)

08:30-09:00 *Registration*

09:10-10:30 **Chair: A. Dinescu**
09:10-09:50 R. TODOROV, "Engineering of the interband transitions of silver- and gold-based alloys and post-transition metals for preparation of effective substrates for surface-enhanced spectroscopic techniques"
09:50-10:30 A. REZNIK, "Advances in Lead Oxide X-ray technology for application in direct conversion medical imaging detectors"

10:30-11:00 *Coffee break*

11:00-12:20 **Chair: S. Baranovskii**
11:00-11:40 E. ANGELOVA, "Spin-lattice interaction in magnetic materials"
11:40-12:20 T. KOUTZAROVA, "The hexaferrites – structure, magnetic properties, electromagnetic shielding"

12:20-16:00 *Lunch break*

16:00-17:00 **Chair: P. Petrik**
16:00-16:20 V. DONCHEV, "Investigation of GaSb micro-islands deposited on Si substrates"
16:20-16:40 K. KREZHOV, "Characterization of Ni- and Co-based bifunctional electrocatalysts for application in carbon-free air electrodes for rechargeable Zinc-air batteries"
16:40-17:00 L. MIHAYLOVA & A. TONCHEV, "ZEISS Innovative Research Solutions in Material Science" (Sponsor Presentation)

17:00-18:30 **Second poster session** / *Coffee break*

August 29th (Thursday)

08:30-09:00 *Registration*

09:10-10:30 **Chair: M. Zamfirescu**
09:10-09:50 S. BANERJEE, "Modulating the Energy Positioning of Lone-Pair-Derived States for the Design of Photocatalytic Architectures"
09:50-10:30 V. GUERRA, "CO_2 plasmas for sustainable chemistry"

10:30-11:00 *Coffee break*

11:00-12:20 **Chair: S. Banerjee**
11:00-11:40 E. IORDANOVA, "New methods for acceleration of neutral atoms and nuclei of light elements"

11:40-12:20	Ts. BABEVA, "Soft and hard templated Nb_2O_5 thin films and multilayered structures for sensing applications"
12:20-16:00	*Lunch break*
16:00-17:20	**Chair: A. Iglič**
16:00-16:40	Z. DANEL, "The analytical investigation of star polymers and copolymers in confined geometries"
16:40-17:20	S. KRALJ, "Topologically stable localized distortions in axial fields"
17:20-17:40	*Coffee break*
17:40-18:20	**Chair: M. Fabian**
17:40-18:00	V. GEORGIEVA, "Engineering the mechanical and X-ray attenuation properties of gelatine composite hydrogels with a potential for tissue mimicking materials"
18:00-18:20	S. BOYADJIEV, "ALD and sol-gel grown ZnO, Ni- and Li/Ni-doped ZnO thin films for gas sensors"
20:00	***Farewell Dinner***

August 30th (Friday)

09:10-10:30	**Chair: S. Kralj**
09:10-09:50	M. ZAMFIRESCU, "Optical microcavities and their applications as quantum sources"
09:50-10:30	A. IGLIČ, "On the role of orientational and lateral distribution of membrane attached proteins and cytoskeleton forces in shape and migration of cells"
10:30-11:00	*Coffee break*
11:00-12:00	**Chair: H. Chamati**
11:00-11:20	V. CHITANOV, "Ti/TiN/AlTiCrN hard coating investigated by Close Field Unbalanced Magnetron Sputtering"
11:20-11:40	L. MAKEDONSKI, "Application of RBF ANN in NIR Spectroscopy for improving the efficiency in Citalopram production"
11:40	**Closing Ceremony**

POSTER PRESENTATIONS

1. FIRST POSTER SESSION, August 27th (Tuesday)

1.1. S. BARANOVSKI, "Mechanism of photoinduced nucleation in supersaturated metallic vapors"

1.2. M. DANEV, "Dynamics of soliton excitations in an inhomogeneous a magnetic chain"

1.3. N. GEORGIEVA, "Adsorption of ammonia and hydrazine on a metal oxide layer"

1.4. N. ZAHARIEV, "Zener-Kondo interaction in layered perovskites and the emergence of zero sound"

1.5. V. STRIJKOVA, "Nanomechanical properties of lymphocytes in chronic lymphocytic leukemia: assessment of response to Venetoclax and Obinutuzumab therapy. Case report"

1.6. A. VIRANEVA, "Physicochemical properties of sesame oil blending with sunflower and soybean oil"

1.7. M. LAZAROVA, "Concentration of red wine phenolic compounds applying nanofiltration with Alfa Laval NF99HF membrane"

1.8. E. KORUTCHEVA, "Relationship between routes and population within city structures"

1.9. M. DUDEK, "Investigation of the elastic properties of star polymers in semi-infinite space"

1.10. V. GEORGIEV, "Effects of Temporin A analogs on lipid membrane models"

1.11. V. GEORGIEVA, "Effect of different fillers on hydrogels for application as tissue-substitute materials in Computed tomography"

1.12. A. GRIGOROV, "Composite porous biopolymer multilayer films as potential controlled delivery systems for tolfenamic acid"

1.13. S. MILENKOVA, "Poly(Lactic Acid)-based active packages loaded with polyphenolic compounds"

1.14. S. MINKOVSKA, "Photoswitchable molecular systems based on spironaphthoxazines for detection of metal ions"

1.15. Y. MARINOV, "Combining gravimetric with electrical transduction methods for the detection of volatile organic compounds (VOCs) by Langmuir-Blodgett films from metal-organic framework (MOF) MIL-101(Cr)"

1.16. Y. MARINOV, "Ion-conducting nematic nanocomposites from nematic liquid crystals and single-walled carbon nanotubes: enhancement by nanodoping"

1.17. Y. FEDCHENKO, "Studying the impact of physicochemical profile of metal-phenolic films on the sensitivity and selectivity of QCM-based alcohol sensors"

1.18. B. GEORGIEVA, "Petroleum vapors sensor with polyvinyl trimethylsilane sensitive coating"

1.19. B. GEORGIEVA, "Investigation of partial Al^{3+} substitution on the properties of Y-type $Ba_{0.5}Sr_{1.5}MgNiFe_{12-x}Al_xO_{22}$ hexaferrites"

1.20. P. NEDYALKOVA, "Inertial sensor to determine the ballistic resistance state and traumatic effect of multilayer lightweight armor made of (UHMWPE), polyvinyl botyral and nanoparticles SiC"

2. SECOND POSTER SESSION, August 28th (Wednesday)

2.1. A. BENKOVSKI, "Titanium dioxide thin films prepared on different substrates by sol-gel process: optical and morphological properties"

2.2. E. ZLATAREVA, "Development and research of a graded AlTiN hard coating"

2.3. V. DULEV, "Chemical bath deposition of tin sulphide thin films"

2.4. G. YANKOV, "Study of the nonlinear optical properties of glasses doped with gold nano-particles using the z-scan method"

2.5. Ch. GHELEV, "Low temperature investigation of nanosized $BaFe_{12}O_{19}$ powders"

2.6. M. GORANOVA, "Optical materials for the electronic industry from fluorite"

2.7. M. GORANOVA, "Optical spectra in SWIR based on data from Icelandic spar measurements in Bulgaria"

2.8. A. PAL, "Spin-induced strongly correlated magnetodielectricity, magnetostriction effect and spin-phonon coupling in helical magnet $Fe_3(PO_4)O_3$"

2.9. H. SOLUNOV, "Metallic glass from the point of view of the molecular entropy theory"

2.10. I. AVRAMOVA, "Preparation and spectroscopic characterization of nano-sized glass-ceramics obtained from a sodium silicate glass with high Fe and Mn concentrations"

2.11. A. PASKALEVA, "XPS study of ALD HfO_2/Al_2O_3 stacks on Si"

2.12. T. STANCHEV, "Evaluation of write/erase operations performance in HfO_2/Al_2O_3 based flash memory stacks"

2.13. T. TENEV, "A study to determine the optical constants of PVD ZrO_2 layers"

2.14. E. STOYANOVA, "Ion irradiation assistance alters the microstructure and optical constants of vacuum deposited ZrO_2 thin layers"

2.15. P. KUTERBA, "Physical properties of fermions obeying exclusion and superexclusion principles"

2.16. T. HRISTOVA-VASILEVA, "Functionalization of metallic polycrystalline thin films with tryptophan for surface enhanced Raman spectroscopy (SERS) applications"

2.17. Ch. ANGELOV, "On-ground observations of solar over-irradiance effects and their influence on low-voltage electric power grid"

2.18. T. ARSOV, "Comparative gamma background measurements, spectrum horizontal mapping and vertical profile in Sofia, Beli Iskar and at high mountain station BEO Moussala"

2.19. V. ATANASSOVA, "Femtosecond laser modification of optical thin films"

ABSTRACTS OF INVITED LECTURES

GEORGI NADJAKOV MEMORIAL LECTURE

Carrier transport and electronic defects in gallium oxide studied by photo-conductivity techniques

Steve Reynolds[1,*], David Nicol[2] and Fabien Massabuau[2]
[1] – University of Dundee, UK
[2] – University of Strathclyde, UK
* – s.z.reynolds@dundee.ac.uk

Gallium oxide Ga_2O_3 is a wide-bandgap compound semiconductor (E_G ~ 5 eV) with applications in power electronics, solar-blind UVC detectors, photocatalysis and gas sensing [1]. n-type doping may be achieved by addition of Si, Ge or Sn donors, and there have been recent reports of successful p-type doping [2]. However, due to the self-trapping nature of the holes, electrons are the dominant charge carrier in the material. We will briefly review the properties and applications of Ga_2O_3 before focusing on the use of photoconductivity techniques for energy mapping of the localised density of states (DOS) in the bandgap.
Dark-current thermal activation measurements indicate the equilibrium Fermi energy E_F in unintentionally-doped samples lies around 1 eV below the conduction band edge, suggesting that transport is mediated by both electron and hole traps. Following low-temperature optical charging of states above E_F, thermally-stimulated currents (TSC) due to an applied temperature ramp reveal several electron trap species [3], and the constant-photocurrent method (CPM) indicates a broad DOS distribution below E_F with a few sharper features [4]. We seek to correlate these observations with the literature to identify corresponding structural assignments. The slow, non-linear photo-response of Ga_2O_3 appears to distort the DOS obtained from 'traditional' transient and modulated photoconductivity [5], possibly due to hole self-trapping.

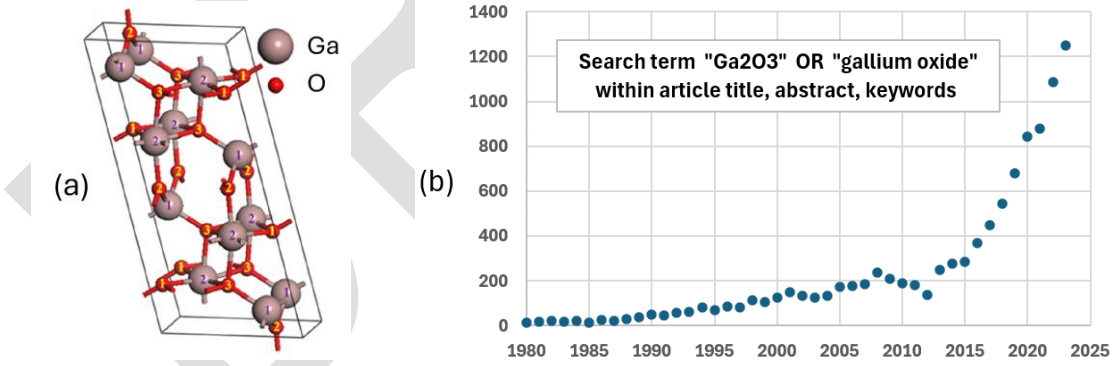

Figure 1: (a) β-phase Ga_2O_3 [1]; (b) Upward trend in Ga_2O_3 publications/year (Scopus)

References:

[1] S J Pearton, J Yang, P H Cary IV, F Ren, J Kim, M J Tadjer, M A Mastro, *Appl. Phys. Rev.* **5** (2018) 011301.
[2] C Ma, Z Wu, Z Jiang, Y Chen, W Ruan, H Zhang, H Zhu, G Zhang J Kang, T-Y Zhang, J Chu and Z Fang, *J. Mater. Chem. C* **10** (2022) 6673.
[3] B R Tak, M-M Yang, M Alexe and R Singh, *Crystals* **11** (2021) 1046.
[4] D Nicol, S Reynolds, K Barr, J W Roberts, J J Jarman, P R Chalker and F C-P Massabuau, *Phys. Status Solidi B* **261** (2024) 2300470.
[5] S Reynolds, C Main, D P Webb and M J Rose, *Phil. Mag B* **80** (2000) 547.

MILKO BORISOV MEMORIAL LECTURE

From Rolls Royce engines to butterfly wings, or using photonics for seeing the invisible in advanced materials

P.C. Montgomery
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
* paul.montgomery@unistra.fr

In this presentation, I will give an overview of some of the photonics techniques I have helped develop during my career for the characterization of advanced materials. At Loughborough University (UK) during my PhD, I worked on the early laser speckle techniques for the study of mechanical structures, such as Electronic Speckle Interferometry (ESPI) for studying vibration modes in engines (Figure 1) [1]. During my post-doc work in Montpellier, we used near IR transmission microscopy for studying defects inside semi-conductors, such as the pinned screw dislocation in InP using phase contrast microscopy in Figure 2 [2]. I then applied the newly developed Phase Shifting Microscopy (PSM) technique at the end of the 1980's for measuring nanometric surface roughness. The need to measure deeper surface structures led to white light scanning interferometry (WLSI) which I then spent the rest of my career developing, mainly in Strasbourg, such as in real time 4D microscopy, tomography, microsphere-assisted microscopy (Figure 3) [3], local spectroscopy and the use of environmental chambers. I will finish with a few thoughts on lessons learnt from the scientific method, management, the beauty and success of science and the importance of passing on good scientific values to the younger generation.

Figure 1: ESPI vibration fringes on a Rolls Royce engine [1].

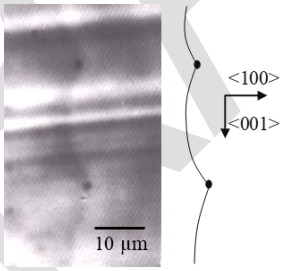

Figure 2: Pinned dislocations in InP using phase contrast microscopy [2].

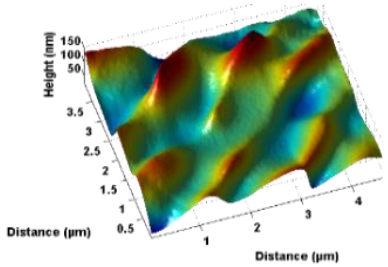

Figure 3: Nanoripples on stainless steel measured with microsphere-assisted WLSI [3].

References:

1. Montgomery P.C., Bergquist B.D., Contrast enhancement of ESPI vibration patterns by speckle averaging in a video frame store, Proc. SPIE 599, 1986, p. 201.
2. Montgomery P.C., Fillard J.P., High-resolution imaging of defects in III-V compound wafers by near-infra-red phase contrast microscopy, Electronic Letters, 25, 2, 1989, p. 89.
3. Leong-Hoï A., Hairaye C., Perrin S., Lecler S., Pfeiffer P., Montgomery P. High resolution microsphere-assisted interference microscopy for 3D characterization of nanomaterials, Phys. Status Solidi A, 215, 2017, 1700858.

Acknowledgements:

Thanks are extended to the colleagues in the Laser Group at Loughborough University (UK), the LINCS group at Montpellier university (France) and the IPP team at ICube, Strasbourg (France).

Simultaneous partial discharge and current measurements in a needle-plane configuration at different pressures

T. Gillis, J.-F. Fagnard and P. Vanderbemden*
Electrical measurements and instrumentation, Department of Electrical Engineering and Computer Science Montefiore Institute, University of Liege, 4000 Liège, Belgium
* – Philippe.Vanderbemden@uliege.be

Phase-resolved partial discharge (PRPD) measurement has been used for decades as a method of monitoring defects in electrically insulating materials. More recently, it has seen a renewed interest in the context of flash sintering [1]. Flash sintering is carried out through the application of an electric field in addition to the classical heating procedure, and is mainly characterised by its rapid densification time of the order of the minute. In the context of flash sintering, partial discharge activity has been shown to increase when approaching the onset of the thermal runaway phenomenon leading to the quick densification of the material [2]. The partial discharge activity is also influenced by relative humidity [3]. While PDRD measurement is traditionally carried out by only measuring the partial discharges and voltage applied to the material to be densified, we show in this work that carrying out simultaneous measurement of the current going through the material using a bespoke partial discharge measurement system [4] allows for the collection of data related to the electrical power transferred to the material during the process. In this talk we first recall the concept of PRPD measurements. We will then investigate how the discharge characteristics are affected by reducing the ambient pressure. Examples of PRPD patterns will be given for a simple needle-plane configuration. As pressure decreases down from atmospheric levels, the threshold voltage leading up to the apparition of discharges decreases following a trend similar to the classical Paschen curve. Additionally, the nature of the discharge activity transitions from low-amplitude, rapid-firing tightly packed trains of pulses to high-amplitude, longer-lasting and more spread out pulses. Simultaneous measurement of discharges, applied voltage and current going through the material show that this second type of discharge activity can be synchronous with high-amplitude current pulses that are in phase with the applied voltage, therefore suggesting a transfer of active electrical power into the device under test.

References:

[1] M. Cologna, B. Rashkova, and R. Raj, "Flash Sintering of Nanograin Zirconia in < 5 s at 850°C," J. Am. Ceram Soc., vol. 93, no. 11, pp. 3556-3559 (2010).
[2] J.-F. Fagnard, C. Gajdowski, L. Boilet, F. Henrotte, C. Geuzaine, B. Vertruyen and P. Vanderbemden, "Use of partial discharge patterns to assess the quality of sample/electrode contacts in flash sintering," J. Eur. Ceram. Soc, vol. 41, no. 1, pp. 669-683 (2021).
[3] J.-F. Fagnard, L. Boilet, J. P. Erauw, F. Henrotte, C. Geuzaine, B. Vertruyen and P. Vanderbemden, "Use of partial discharges measurements and video recordings to investigate the influence of relative humidity on zinc oxide subjected to high electric fields," J. Phys. D, vol. 561, 465305 (2023).
[4] T. Gillis, J.-F. Fagnard, and P. Vanderbemden, "Development of a Microcontroller-Based Phase-Resolved Partial Discharge Measurement System With Application to the Monitoring of Flash Sintering Discharge Patterns," IEEE Sens. J., vol. 23, no. 19, pp. 22704-22712 (2023).

Fundamental spatial scales for charge transport and recombination in disordered semiconductors

Sergei Baranovskii [1,2*]
[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

In order to describe charge carrier transport and recombination in disordered semiconductors, it is of vital importance to reveal the relevant spatial and energy parameters responsible for such phenomena [1].
In the presentation, such parameters are revealed for the combined effects of the electric field and temperature on charge transport and recombination. We consider disordered organic semiconductors, as an example of materials with the hopping transport mechanism [2], and amorphous inorganic semiconductors, as an example of materials with the multiple-trapping transport mechanism [3].

References:

1. B.I. Shklovskii, H. Fritzsche, S.D. Baranovskii "Electronic Transport and Recombination in Amorphous Semiconductors at Low Temperatures" Phys. Rev. Lett. 62, 2989 (1989).
2. A. V. Nenashev, J. O. Oelerich, A. V. Dvurechenskii, F. Gebhard, and S. D. Baranovskii, "Fundamental characteristic length scale for the field dependence of hopping charge transport in disordered organic semiconductors", Phys. Rev. B 96, 035204 (2017).
3. A. V. Nenashev, J. O. Oelerich, K. Jandieri, V.V. Valkovskii, O. Semeniuk, A. V. Dvurechenskii, F. Gebhard, G. Juska, A. Reznik, and S. D. Baranovskii, "Field-enhanced mobility in the multiple-trapping regime", Phys. Rev. B 98, 035201 (2018).

Novel insights into the physics of molecular magnets

Miroslav Georgiev and Hassan Chamati *
Institute of Solid State Physics, Bulgarian Academy of Sciences
Tsarigradsko Chaussee 72, 1784 Sofia, Bulgaria
* – chamati@issp.bas.bg

Molecule magnets are a class of nanomagnetic materials capable of displaying complex magnetic phenomena on the molecular level including magnetic ordering. For instance, some types of molecule magnets exhibit an energy barrier to the reversal of magnetization and a suppressed magnetic tunnelling effect. Molecule magnets possessing a high energy barrier are viable candidates to be used as high density information storage devices. The knowledge of their intrinsic electronic structure and the interplay of the crystal field, spin exchange, spin-orbit and effective spin-spin interactions have attracted the interest of researchers in chemistry, physics, nanotechnology and material engineering. In this lecture, we present our recent research in the field and provide details on our approach based on the multi-configurational self-consistent field method and the direct diagonalization one. The used approach advances the conventional methods by imposing constraints on the electrons' orbital dynamics. That allowed us to shed light on the contribution of all relevant interaction terms into the occurrence of the fine structure in the resulting energy spectrum and trace back the origin of anisotropic magnetic behaviour. In particular, we unveil the mechanism underlying the emergence of the unexpected large and huge splitting in the fine structure related to the ground state of $3d^8$ compounds with trigonal (bi-)pyramidal crystal field.

References:

1. M. Georgiev and H. Chamati, Fine structure and the huge zero-field splitting in Ni^{2+} complexes, *ASC Omega*, **7** (2022).
2. M. Georgiev and H. Chamati, Fine structure and the huge zero-field splitting in Ni^{2+} complexes, Molecules **27** (2022) 8887.
3. M. Georgiev and H. Chamati, The magnetic behavior of trigonal (bi-)pyramidal $3d^8$ mononuclear nanomagnets: The case of $[Ni(MDABCO)_2Cl_3]ClO_4$ complexes, *ACS Omega*, **8** (2023)

Acknowledgements:

This work was supported by the Bulgarian National Science Fund under grant No КП-06-Н78/6.

Interactions within an advanced glass/copper/bentonite system under simulated geological disposal conditions

Margit Fabian*, Istvan Tolnai, Janos Osan
HUN-REN Centre for Energy Research, 1121 Budapest, Konkoly Thege st 29-33, Hungary
* – fabian.margit@ek.hun-ren.hu

All states engaged in nuclear applications must consider the management of radioactive waste and must secure safe handling based on the level of radioactivity and the national/international regulations. There is a broad consensus that the accepted 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 copper canister is specifically designed for long-term durability during storage and disposal [1,2]. The requirements for container lifetime and integrity depend on the DGR concept and the chosen geological medium.

The purpose of this research was to study the corrosion behavior of glass and copper in a bentonite environment. We focused on the interface of two materials in contact with B75 bentonite to obtain information on the chemical evolution in terms of alteration in solid phase composition at a detailed small scale (micron and sub-micron).

A glass/copper/bentonite scale model system was built in triplicate and kept under conditions close to those expected for the real repository (temperature: 80°C, porewater chemistry) [3,4]. The main goal was to understand the system's characteristics, applicability, and stability, spanning from the physical/chemical properties of the glass and copper to the bentonite response in the repository. The corrosion potential was continuously measured (Cu wire vs Pt electrode). After 30/60/90-day exposure, one of the model systems was opened for post-mortem characterization. The corresponding porewater solutions were analyzed by ICP-OES/IC. With SEM/EDX investigations we focused on the composition and nature of alteration products formed on the glass/copper and within the bentonite. Slight corrosion appeared on the Cu-plate but no S species were detected in the corrosion product layer. No alteration layer has been found on the borosilicate glass samples, rather small changes were detected in the elemental composition of the investigated material. The B, Ca, K and Na concentrations of the porewater increased, while those of Mg and Si decreased with time. Concentrations of Cl^- and SO_4^{2-} ions in the final porewater are close to the starting ones, 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 discussed.

References:

[1] F. King, Integrity Corrosion Consulting Ltd.; Posiva-Working Report 2021-11, pp. 84.
[2] F. King et al. Integrity Corrosion Consulting Ltd. and Swedish Nuclear Fuel and Waste Management Co.; Posiva-Working Report 2021-10, pp. 56.
[3] M. M. Fernandes at al. Applied Geochemistry 59 (2015) 189-199.
[4] D. Breitner et al. Environmental Earth Sciences 73(1) (2015) 209-219.

Acknowledgements:

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

Recent progress in ellipsometry at solid-liquid interfaces

Peter Petrik[1,2*]
[1] – Hungarian Research Network, Centre for Energy Research,
Institute of Technical Physics and Materials Science, Budapest, Hungary
[2] – Department of Electrical and Electronic Engineering, Institute of Physics,
Faculty of Science and Technology, University of Debrecen, Hungary
* – petrik.peter@ek.hun-ren.hu

The application areas of ellipsometry are broadening rapidly, especially in the field of in-situ characterizations [1]. These investigations utilize the combination of high-sensitivity, high speed and non-destructive nature. Vacuum processes have traditionally been studied by ellipsometry for many decades, but the investigation of solid-liquid interfaces is a field that started to increase later. This review attempts to give an overview of the major results and trends in in-situ ellipsometry of solid-liquid interface characterizations, as a continuation of the review [1] on the previous ISCMP conference.

References:
1. D. Mukherjee, P. Petrik, Real-Time Ellipsometry at High and Low Temperatures, ACS Omega 8 (2023) 3684–3697. https://doi.org/10.1021/acsomega.2c07438.

Acknowledgements:
Support from OTKA K-146181, H2020 20FUN02 ‘‘POLight’’ and TKP2021-EGA04 projects are gratefully acknowledged.

Wireless temperature and pressure sensors based on surface acoustic wave resonators – fabrication processes

Adrian Dinescu*, Alexandra Stefanescu, Ioana Zdru, Claudia Nastase, George Boldeiu, Dan Vasilache and Alexandru Muller
IMT Bucharest, Romania
* adrian.dinescu@imt.ro

Surface Acoustic Wave (SAW) resonators are based on Interdigital Transducers (IDT) placed on piezoelectric substrate, featuring the period of digits bellow 200nm for high frequency applications, up to 20 GHz [1]. They are most frequently used for signal processing, but because their resonant frequency, is influenced by temperature or pressure (among other physical parameters) the SAW resonators proved to be valuable temperature [2] or pressure [3] sensors. A great advantage offered by the SAW sensors is the wireless functionality, important for sensing in difficult to reach locations or harsh environment.
The fabrication process of SAW resonators for higher than 5GHz frequencies is quite challenging. The sumicron pitch of the metalic lines deposited on the piezoelectric substrate and acting as a transducer requires high resolution lithography (such lectron beam or nano-imprint) instead of classic optical lithography and also refined lift-off techniques employing deposition tools with high directionality of the vapors and/or uising a bilayer electronresist. Simultaneously, in order to limit conductive losses, the pads, coplanar waveguide lines and the inductive components must be much thicker.
This talk is focused on the fabrication of SAW resonators on different piezoelectric layers such as GaN, AlN and AlScN, placed on various substrates (Si, sapphire and SiC). The role of electron beam lithography in patterning lines with sub-200nm pitch is described in detail with emphasis on patterning parameters and methods to achieve an undistorted pattern when working on unconductive substrates.

References:

[1] Muller A., Neculoiu D., Konstantinidis G., Deligeorgis G., Dinescu A., Stavrinidis A., Cismaru A., Dragoman M. and Stefanescu A., "*SAW Devices Manufactured on GaN/Si for Frequencies Beyond 5 GHz*", in IEEE Electron Device Letters, 31(12), pp. 1398–1400, 2010.
[2] Muller A., Giangu I., Stavrinidis A., Stefanescu A.,., Dinescu A., and Konstantinidis G., "*Sezawa Propagation Mode in GaN on Si Surface Acoustic Wave Type Temperature Sensor Structures Operating at GHz Frequencies*", IEEE Electron Device Letters, 36(12), pp. 1299–1302, 2015
[3] A. Muller, G. Konstantinidis, I. Giangu, G. C. Adam, A. Stefanescu, A. Stavrinidis, G. Boldeiu, A.Dinescu, "*GaN Membrane Supported SAW Pressure Sensors with Embedded Temperature Sensing Capability*", IEEE Sensors Journal, vol. 17, no. 22, Nov. 15, 2017, pp. 7383 – 7393

Engineering of the interband transitions of silver- and gold-based alloys and post-transition metals for preparation of effective substrates for surface-enhanced spectroscopic techniques

Rosen Todorov[1*], Temenuga Hristova-Vasileva[1,2]
[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

Surface-enhanced Raman spectroscopy (SERS) and fluorescence spectroscopy (SEF) are analytical techniques that are increasingly being used in various fields of biological diagnostics, environmental monitoring and food safety control. The principle of signal amplification for both spectroscopic methods is based on a dramatic increase of the intensity of the local electromagnetic field on and near the metal nanostructures at the plasmon resonance wavelength, which allows identification and characterization of molecules at very low concentrations and even single molecules can be analyzed.
A critical factor in achieving high sensitivity is the quality of the metal nanostructures, as well as the material from which they are made. By changing nanostructure's size, shape and composition, the optical response can be tuned to match the excitation fluorescence and/or the Raman signal radiation. On the other hand, the material of the nanostructures determines the interaction with the registered molecules, which can result in amplification of the registered signal.
The addition of post-transition metals to noble metals (such as Ag and Au) allows changing their electronic structure. These changes affect their complex dielectric function and determine the frequency domain for excitation of surface plasmon resonance and its efficiency.
In this work, we present a study of the changes in the electronic structure of alloys of silver with post-transition metals (Cd, In, Sn and Sb) by X-ray photoelectron spectroscopy (XPS), density functional theory (DFT) calculations and spectroscopic ellipsometry. The obtained results show that the addition of *p*-block metals leads to an increase in the energy required for interband electron transitions from the 4*d* and 5*d* levels of silver and gold to the Fermi level. The most significant *d*-band shift occurs in the case of cadmium and decreases with increasing the atomic number of the post-transition metal, as the smallest changes occur in the case of antimony. The possibility for control of the interband transitions allows to achieve frequency variation of localized surface plasmon resonance in a wide spectral region from the near-infrared region to the ultraviolet region, as well as to improve the efficiency of LSPR excitation in the spectral interval 4-7 eV.
The performance of silver alloys and *p*-block metals to for preparation of signal enhancing substrates was validated by SERS measurements and SEF analysis at 350 nm emission line of tryptophan aqueous solution. The results show that the used nanostructured substrates make possible to register very low concentrations of 10^{-10} wt.% tryptophan. It illustrates that the bonding of tryptophan with metal structures leads to a red-shift of the emission band. These results suggest that tryptophan interacts with the surface of metal nanostructures.

Advances in Lead Oxide X-ray technology for application in direct conversion medical imaging detectors

A. Reznik*
Physics department, Lakehead University, Thunder Bay, Ontario, Canada
* areznik@lakeheadu.ca

Large-area amorphous and polycrystalline x-ray photoconductors are of great significance to the field of x-ray image sensor applications, as they are used as x-ray-to-charge transducers in direct conversion flat panel x-ray imagers (FPXIs). In the direct conversion detection method, x-ray quanta are absorbed in a photoconductor that directly creates electron-hole pairs. These electrons and holes are then separated by a bias electric field to generate an electrical signal in the imaging array. With the appropriate 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.

Lead oxide (PbO) x-ray photoconductor is one of the most promising materials for applications as x-ray-to-charge transducers. It exists as two disordered polymorphs: polycrystalline lead oxide (poly-PbO) and amorphous lead oxide (a-PbO). Both polymorphs can be deposited over large-area imaging substrates kept at comparatively low temperatures by thermal deposition, with the peculiar requirement that the deposition of a-PbO occurs in an atmosphere of ionized oxygen, as opposed to molecular oxygen for poly-PbO. Oxygen ion bombardment, delivered by a specialized ion source with either a hot filament or a hollow-cathode electron emitter, causes the amorphization of the grown layers [1,2].

Here, we present our approach to optimizing PbO detectors in terms of temporal performance and efficiency in the collection of x-ray generated signals. In our approach, a thin layer of a-PbO is combined with a thick layer of poly-PbO in an a-PbO/poly-PbO bilayer structure. The poly-PbO layer serves as an x-ray-to-charge transducer, while the a-PbO layer acts as a barrier to prevent signal lag—a residual current after exposure termination. The hole mobility in the a-PbO/poly-PbO bilayer structure was measured using the photo-Charge Extraction by Linearly Increasing Voltage technique [3] at different temperatures and electric fields to investigate charge transport properties. It was found that the hole mobility is similar to that in a-Se, currently the only commercially viable photoconductor for direct conversion x-ray detectors. Evaluation of the x-ray temporal performance demonstrated complete suppression of signal lag, allowing the a-PbO/poly-PbO detector to operate in real-time imaging.

References:

1. O. Grynko, A. Reznik, Progress in Lead Oxide X-ray Photoconductive Layers, S. O. Kasap, Photoconductivity and Photoconductive Materials, 2 Volume Set, pp.643-688, 2022
2. E. Pineau, O. Grynko, T. Thibault, A. Alexandrov, A. Csík, S. Kökényesi, A. Reznik, Comparative Analysis of Multilayer Lead Oxide-Based X-ray Detector Prototypes, Sensors 2022, 22(16), 5998
3. O. Grynko, G. Juska, A. Reznik, Charge Extraction by Linearly Increasing Voltage (CELIV) method for investigation of charge carrier transport and recombination in disordered materials, Safa O. Kasap, Photoconductivity and Photoconductive Materials, 2 Volume Set (2): pp.339-368, 2022

Acknowledgements:

Author gratefully acknowledge financial support from Natural Sciences and Engineering Research Council of Canada Discovery and Alliance programs, MITACS IT30395, Ontario Research Fund: Research Excellence, Terry Fox Foundation and Research Institute, Ontario Institute for Cancer Research, Canadian Research Chairs 2018-00015

Spin-lattice interaction in magnetic materials

Elena Angelova* and Hassan Chamati
Institute of Solid State Physics, Bulgarian Academy of Sciences,
Tsarigradsko Chaussee 72, 1784 Sofia, Bulgaria
* – angelova@issp.bas.bg

Magnetic materials, except lattice motion, possess a very special atomic scale degree of freedom called spin as an intrinsic form of angular momentum carried by atoms or molecules. Because these particles demonstrate classical and spin movement at the same time, physicists expect their interplay. Then, in physics of 20th century the theme of spin-lattice (SL) interaction describing the coupling between the magnetic and lattice subsystems in magnetic materials arose. The first paper devoted on this subject was published by Waller [1] in 1932. His pioneer article contains idea to couple the spins to the phonons starting from the dipolar spin-spin interaction. This item, appearing before any measurements, was an early impact on investigations of SL relaxation in theoretical and applied physics. Since then, the theory of SL interaction in ionic solids was quite well substantiated by experiments of Gorter [2] and his co-workers.
The idea for SL mutual influence which goes back to Waller nowadays is primary for understanding phase transitions and transport behaviors in magnetic solids. Moreover, it plays a leading role in various advanced research areas, including antiferromagnetic and terahertz spintronics, spin-caloritronics, curvilinear magnetism and quantum criticality. Given significance of the topic, there is a big need in methods descripting the SL coupling in adequate manner. Moreover, to study processes of the propagation of particles and quasi – particles in magnetic materials effectively, it is essential to precisely predict firstly the potential and then the driving forces that influence the evolution of atoms positions and their magnetic moments [3]. We propose and develop a new method aiming to couple molecular dynamics with spin dynamics at the atomic scale that combines simulation in LAMMPS with an auxiliary postprocessing code to compute the phonon and magnon dispersion in magnetic crystals [4,5].

References:

1. I. Waller. Über die Magnetisierung von paramagnetischen Kristallen in Wechselfeldern. Zeitschrift für Physik, Tome 79, N 5-6, 1932, P. 370–388.
2. C.J. Gorter. Paramagnetic Relaxation. Elsevier Publishing Co. Inc., 1947, 127 pages.
3. H. Chamati, N.I. Papanicolaou, Y. Mishin, D.A. Papaconstantopoulos. Embedded-atom potential for Fe and its application to self-diffusion on Fe(100). Surface Science, Tome 600, N 9, 2006, P. 1793 - 1803.
4. 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.
5. E. Angelova, H. Chamati. Dynamic simulation of the quasiparticle excitations spectra in the magnetic bcc iron. Journal of Physics: Conference Series, Tome 2436, 2023, P. 012011.

Acknowledgements:

This work was supported by the Grant No KP-06-N78/2 of 05.12.2023 from the Ministry of Education and Science of Bulgaria.

The hexaferrites – structure, magnetic properties, electromagnetic shielding

T. Koutzarova[1*], S. Kolev[1,2], B. Georgieva[1], Ch. Ghelev[1], K. Krezhov[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

Although hexaferrites were discovered in the middle of the last century, research on their properties still continues to be attractive due to their wide application; in recent years, the interest has been linked to their potential applications as magnetoelectric materials. They are one of the most widely used magnetic materials in communication and high-frequency technologies as well. The progress in the microwave (MW) technologies and the consequent use of high-frequency ranges in the everyday life of the modern society resulted in a drastic rise in the electromagnetic interference (EMI) (frequently referred to as "pollution") that "jams" the modern sensitive electronics devices. The past decade saw increasing efforts focused on the research and development of materials that absorb (screen) microwaves with high efficiency aimed at alleviating the problems arising from EMI and EM pollution; at the same time, the massive use of the GHz frequency range brought about a huge demand for devising novel functional materials (such as composites) that possess qualitatively novel properties. The hexaferrites form a group of complex oxides in the system $AO\text{-}Fe_2O_3\text{-}MeO$, where A is a large divalent cation, e.g., Ba, Sr, Ca, and Me is a small divalent cation, e.g., Mn, Fe, Co, Ni, Cu, Zn. They can be classified on the basis of the chemical composition by varying the A – Me combination and, respectively, on the crystal structure. This gives us a wide opportunity to influence the crystal and magnetic structure by varying the composition leading to a change in the magnetic properties. On the other hand, this allows hexaferrites to be used as magnetic materials in composite structures for electromagnetic shielding. Here we will present the recent progress on the structure changes (including magnetic one) on the magnetic and magnetoelectric properties in M-, Y- and Z- hexaferrites and their electromagnetic shielding properties in novel composite structures.

Acknowledgements:
The work was supported by the Bulgarian National Science Fund under contract KP-06-N48/5, 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.

Modulating the Energy Positioning of Lone-Pair-Derived States for the Design of Photocatalytic Architectures

Sarbajit Banerjee[1,2]
[1] –Department of Chemistry
[2] –Department of Materials Science & Engineering, Texas A&M University, College Station, TX (USA)
* banerjee@chem.tamu.edu

Harnessing solar irradiance, through photocatalytic generation of solar fuels has emerged as an urgent imperative for the energy transition. Functional photocatalysts must be capable of efficiently absorbing sunlight, separating electron—hole pairs, and ensuring they are delivered at appropriate potentials to catalytic sites to mediate redox reactions. Such photocatalytic architectures must further direct redox events down specific reaction trajectories to yield desired products, and ensure the transport of reactants between catalytic sites. I will describe collaborative work to design a palette of heterostructures that promote robust and efficient direct solar-driven water splitting. The heterostructures comprise $M_xV_2O_5$ or $M_xM'_yV_2O_5$ (where M is a p-block cation, M′ is an s-, p-, or d- block cation) and V_2O_5 represents one of multiple polymorphs of this composition interfaced with semiconductor quantum dots (QDs). The stereochemically active $5/6s^2$ electron lone pairs of p-block cations in $M_xV_2O_5$ give rise to filled mid-gap electronic states. Within heterostructures, the photoexcitation of QDs results in the transfer of holes to such mid-gap states at <1 ps time scales. Ultrafast charge separation minimizes the photoanodic corrosion of QDs, which has been a major impediment to their use in photocatalysis, and enables charge transport and the subsequent redox reactions underpinning photocatalysis to compete with electron-hole recombination. Design principles for understanding the nature of lone pair states will be discussed (**Fig. 1**). The dimensions and composition of QDs along with interfacial structure afford additional levers for heterostructure integration, enabling tuning of thermodynamic energy offsets and charge transfer dynamics, which have been systematically modulated across several generations of heterostructures to improve photocatalytic performance.

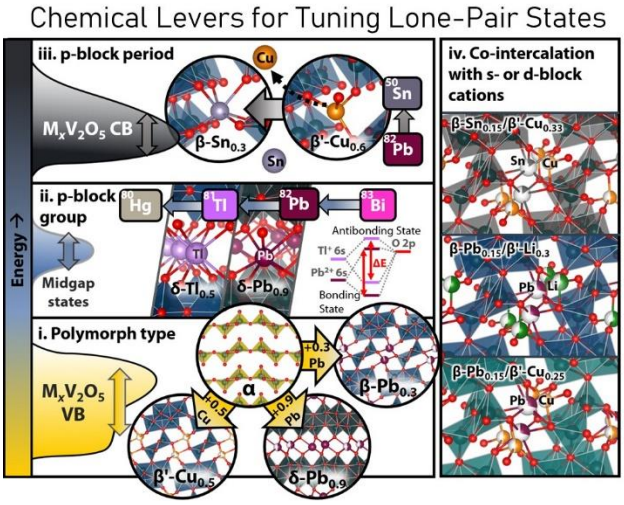

Figure 1: An illustration of site-selective modification strategies to tune the energy positioning of lone-pair-derived midgap states.

References: [1] J. V. Handy, et al. Lone but not alone: Precise positioning of lone pairs for the design of photocatalytic architectures. Chemistry of Materials 2022, 34, 1439-1458. [2] Andrews et al. Hole extraction by design in photocatalytic architectures interfacing CdSe quantum dots with topochemically stabilized tin vanadium oxide. Journal of the American Chemical Society 2018, 140, 17163-17174.

Acknowledgements:
We are grateful to the National Science Foundation and Welch Foundation for support.

CO_2 plasmas for sustainable chemistry

Vasco Guerra[1*], Tiago Silva[1] and Olivier Guaitella[2]
[1] Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal
[2] Laboratoire de Physique des Plasmas, École Polytechnique, France
* vguerra@tecnico.ulisboa.pt

CO_2 plasmas are currently a major focus of research due to their potential in various carbon dioxide valorisation strategies, where CO_2 is treated as a valuable resource instead of waste. A key application is the production of solar fuels, which involves converting renewable electricity into fuels, necessitating the reduction of CO_2 into CO [1]. Additionally, there has been growing interest in using CO_2 plasmas for in-situ resource utilisation (ISRU) on Mars [2].
This contribution reports a systematic modelling effort carried out at IST Lisbon to unveil the energy transfer pathways and establish a reaction mechanism – *i.e.* a set of reactions and rate coefficients validated against benchmark experiments – for plasmas of CO_2 and mixtures of CO_2 with other gases. The model couples the electron Boltzmann equation, in the usual two-term expansion in spherical harmonics, with a 0D system of rate balance equations describing the creation and destruction of the most important neutral and charged heavy-particles, and with the gas thermal balance equation. The simulations are performed with the LoKI (LisbOn Kinetics) simulation tool [3]. The system under study is a DC glow discharge, operated either in a continuum or a pulsed regime, at pressures ~ 1 Torr and discharge currents of 10s of mA, in a Pyrex tube of radius 1 cm. This system is very homogeneous and ideally suited for fundamental studies, as it is accessible to a variety of diagnostics. The modelling effort is complemented with a series of experiments carried out at LPP, measuring the concentration of different molecules, the gas temperature and the vibrational temperatures of CO and of the three CO_2 vibrational modes, the electric field, and the O-atom concentration.
The results allow to validate the vibration-vibration (V-V) and vibration-translation (V-T) rate coefficients involving different collision partners, the electron impact excitation rate coefficients by electron impact, the electron impact dissociation cross section, as well as comprehensive reaction mechanisms for O_2, CO_2, CO_2-CO, CO_2-N_2 and CO_2-CH_4 plasmas. The knowledge acquired constitutes an essential step for the design and optimisation of a future plasma reactor.

References:
1. A. Goede and R. van de Sanden, *EPN* **47**(3) (2016) 22.
2. V. Guerra *et al*, *Plasma Sources Sci. Technol.* **26** (2017) 11LT01.
3. http://nprime.tecnico.ulisboa.pt/loki/
4. A. Tejero-Del-Caz *et al*, *Plasma Sources Sci. Technol*. **28** (2019) 043001.

Acknowledgements:
IPFN activities were supported by the Portuguese FCT - Fundação para a Ciência e Tecnologia, under projects UIDB/50010/2020 (https://doi.org/10.54499/UIDB/50010/2020), UIDP/50010/2020 (https://doi.org/10.54499/UIDP/50010/2020), LA/P/0061/2020 (https://doi.org/10.54499/LA/P/0061/2020), and PTDC/FIS-PLA/1616/2021 (PARADiSE, https://doi.org/10.54499/PTDC/FIS-PLA/1616/2021).

New methods for acceleration of neutral atoms and nuclei of light elements

L. M. Kovachev[1], E. Iordanova[2], G. Yankov[2], I. P. Angelov[1]
[1] – Institute of Electronics, Bulgarian Academy of Sciences,
72 Tzarigradsco shoussee, 1784 Sofia, Bulgaria
[2] – Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsco shoussee, 1784 Sofia, Bulgaria

Our recent studies have proposed a novel physical mechanism for trapping neutral atoms, molecules, and particles within the envelopes of femtosecond laser pulses [1-2]. This mechanism enables the acceleration of light atoms, such as hydrogen and helium, to the group velocity of the pulse, resulting in energies ranging from 200 MeV to 1-2 GeV. In this presentation, we will demonstrate how the nuclei of these accelerated light atoms can be captured by an external electric field on the cathode of a cylindrical condenser. Given that the kinetic energy of the nuclei impact on the cathode (approximately 1 GeV) significantly exceeds the nucleon binding energy in an alpha particle (28 MeV), two primary decay channels emerge: the production of He^3 nuclei with neutron emission or the formation of two deuterium nuclei accompanied by intense gamma radiation. Furthermore, the Coulomb repulsion among the trapped He^3 or deuterium nuclei on the cathode is considerably reduced, facilitating the possibility of secondary fusion reactions through multiple fusion pathways.
In this investigation, we demonstrate that femtosecond laser pulses can be utilized in devices to accelerate neutral particles and light nuclei to energies of several GeV. The combination of these high energies and the reduced Coulomb repulsion between nuclei on the cathode presents a viable application for nuclear fusion in future laser-based nuclear reactors.

References:

1. L.M. Kovachev, "Radiation forces and confinement of neutral particles into the pulse envelope. New regime of collision ionization", Optik, 269, 169943 (2022).
2. G. Yankov, E. Iordanova, L.M. Kovachev, "Radiation forces and compression of neutral particles by an optical lens," Optik, 273, 170452 (2023).

Acknowledgements:

The present work is funded by Bulgarian National Science Fund by Grant no. KP-06-H78/3-2023 and The National Roadmap for Research Infrastructure, Bulgaria "Extreme Light" ELI-ERIC Consortium under contract D01-351/13.12.2023.

Soft and hard templated Nb_2O_5 thin films and multilayered structures for sensing applications

Venelin Pavlov[1], Georgi Zlatinov[1], Biliana Georgieva[1], Rosen Georgiev[1] and Tsvetanka Babeva[1]*
[1] – Institute of Optical Materials and Technologies "Acad. J. Malinowski", Bulgarian Academy of Sciences, Akad. G. Bonchev Str., Bl. 109, 1113 Sofia, Bulgaria
* babeva@iomt.bas.bg

Porous Nb_2O_5 thin films with tailored structure and properties were obtained utilizing two different processing approaches. In the first one, an aqueous solution of commercially available triblock copolymers Pluronic with optimized concentration and composition were added in Nb sol and thin Nb_2O_5 films were prepared by spin coating. The removal of polymer and generation of mesoporosity (pores with size of 4 – 6 nm) were achieved through proper annealing at moderate temperatures. In the second approach commercially available colloidal SiO_2 (Ludox®) with nominal diameter of 12 nm were used as hard template. Thin Nb_2O_5 / SiO_2 composite films were obtained by post deposition annealing of spin-coated mixtures of Nb sol and Ludox at different volume fractions. For generating a porosity a selective removal of silica nanoparticles was utilized through wet-etching in a very diluted aqueous solution of nitric and hydrofluoric acids. The process of selective etching was controlled by calculating the volume fractions of two constituents and the free volume in the film using Bruggemann effective medium approximation.
The sensing properties of films and multilayered structures comprising porous films with different levels of porosity were studied and the influence of the type of template was discussed.

Acknowledgements:
T.B. acknowledges the financial support of CoE "National center of mechatronics and clean technologies supported by the European Regional Development Fund within the Operational Programme "Science and Education for Smart Growth 2014 - 2020". Research equipment of INFRAMAT (part of Bulgarian National roadmap for research infrastructures) supported by Bulgarian Ministry of Education and Science was used in this investigation.

The analytical investigation of star polymers and copolymers in confined geometries

Zoriana Danel[1*], Joanna Halun[2]
[1] – Faculty of Materials Engineering and Physics, Cracow University of Technology, Cracow
[2] – Institute of Nuclear Physics, Polish Academy of Sciences, Cracow
* – zoriana.danel@pk.edu.pl

The analysis of the influence of star polymer and copolymer topology on the depletion interaction potentials and the depletion forces was carried out analytically. The method of calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star polymers with f=3, 5 legs and copolymer star constituted by two different species of polymers with f_1+f_2 legs in a Θ - solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the case of one repulsive and the other inert surface was proposed. We performed the investigation of following cases of copolymers: $f_1=2, f_2=1$ and $f_1=2$, $f_2=3$. Furthermore, the dimensionless depletion interaction potentials and the dimensionless depletion forces for ideal star polymers and copolymers with different number of legs immersed in a dilute solution of big colloidal particles with different adsorbing or repelling properties in respect to polymers were calculated, bearing in mind the Derjaguin approximation. The obtained analytical results for star polymers and copolymers are compared with the results for linear polymers in confined geometries. The acquired results show that a dilute solution of star polymers and copolymers can be applied for the production of new functional materials because the behavior of these solutions is strictly correlated with the topology of polymers, and also with the nature and geometry of confined surfaces. The above mentioned properties can find practical application in nano - technology, as well as in biotechnology and medicine for drug and gene transmission.

Topologically stable localized distortions in axial fields

Samo Kralj[1,2*], Damjan Dovnik[2], Maha Zid[1]
[1] Solid State Department, Jozef Stefan Institute, Ljubljana, Slovenia
[2] Faculty of Natural Sciences and Mathematics, University of Maribor, Maribor, Slovenia
* samo.kralj@um.si

There is strong evidence that many natural phenomena could be described using geometrical approaches Furthermore, the discovery of the Higgs boson proved the existence of the entire Universe pervaded by the Higgs field, suggesting that *physical fields* represent the fundamental natural entity. Consequently, it is of interest to identify experimentally accessible systems in which universality of geometry-based approaches could be tested or/and investigated in detail. Testbed laboratory systems could serve as gateways toward a deeper understanding of phenomena in other ways hardlyor even experimentally inaccessible systems that are mathematically related to such analogs.
Diverse liquid crystalline (LC) phases and configurations are ideal candidates for such purposes. These optically anisotropic soft matter representatives combine properties of ordered crystals and liquids, and exhibit rich diversity of different symmetries. Their states could be well described by mesoscopic molecular fields, which could be easily manipulated by diverse external stimuli, and the resulting field-configurations could be probed using relatively simple and inexpensive optical methods (e.g., optical polarizing microscopy).
In our presentation we intend to illustrate how phenomena studied in LCs could be exploited to get insight into open problems of particle physics and cosmology. In particular, we address (i) the Kibble-Zurek mechanism describing coarsening dynamics of the Higgs field in the early universe, (ii) the stabilization and manipulation of skyrmion-family structures (these quasiparticle configurations were originally proposed to describe hadrons and mesons), (iii) the stabilization and manipulation of fermionic Weyl-type excitations, and (iv) illustrate analogs of "virtual particles".

Acknowledgements:
S.K. acknowledges the financial support of Projects P1-0099 and J2-4447 from the Slovene Research Agency.

Optical microcavities and their applications as quantum sources

Marian Zamfirescu, Nicu Scarișoreanu, Raluca Ivan,
Eliseia Petre, Luiza Stingescu
INFLPR, Atomistilor 409, Magurele, RO-077125, ROMANIA
* marian.zamfirescu@inflpr.ro

Optical microcavities (MC) are possible candidates for entangled photon pair sources that can be integrated in optical chips [1,2]. In this work, we introduce the physics of optical MC hetero-structure, the recent progress, and their applications in the field of quantum sources. We discuss a particular design of MC based on ZnO. Due to its high excitonic binding energy of 60 MeV, the ZnO excitons can survive at room temperature. The excitons coupled with the cavity resonance allow for polaritonic scattering in the semiconductor microstructure and emission of entangled photons [4,5]. The strong coupling between the cavity's photons and ZnO excitons gives rise to the polaritonic states in the microcavity. The dispersion curve of the polaritons in the cavity is numerically studied from angle resolved reflectance, for different detuning parameters between the cavity and exciton resonance. Experimentally, a ZnO cavity have been produce by Pulse Laser Deposition (PLD). The reflectance and photoluminescence spectra of the sample were measured at room temperature. The parametric polaritonic scattering mechanisms in such structures and possible configuration for generation of entangled photon pair sources from ZnO microcavities are discussed. Also, the application of MC in quantum technologies are presented, as well as some designs for their integration with optical chips and fibre optical systems.

References:

1. Wei-Jian Chen, Fang-Wen Sun, Chang-Ling Zou, and Guang-Can Guo, "Integrated entangled photons source from microcavity parametric down conversion," J. Opt. Soc. Am. B 29, 1884-1888 (2012).
2. Hisaki Oka; Goro Oohata; Hajime Ishihara Efficient generation of energy-tunable entangled photons in a semiconductor microcavity Appl. Phys. Lett. 94, 111113 (2009).
3. Joanna M. Zajac et al. Parametric scattering of microcavity polaritons into ghost branches, Phys. Rev. B 92, 165305 (2015).
4. Ravyn Malatesta et al. Optical microcavities as platforms for entangled photon spectroscopy, arXiv:2309.04751v1 (2023) https://arxiv.org/pdf/2309.04751.pdf.

Acknowledgements:

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P4-PCE-2021-1710, within PNCDI III.

On the role of orientational and lateral distribution of membrane attached proteins and cytoskeleton forces in shape and migration of cells

Raj Kumar Sadhu[1], Samo Penič[2], Mitja Drab[2], Luka Mesarec[2], Veronika Kralj-Iglič[3], Nir S. Gov[4], Aleš Iglič[2]*

[1] Institut Curie, PSL Research University, CNRS, UMR 168 Paris, France
[2] Laboratory of Physics, Faculty of Electrical Engineering, University of Ljubljana, Ljubljana, Slovenia
[3] Laboratory of Clinical Biophysics, Faculty of Health Sciences, University of Ljubljana, Ljubljana, Slovenia
[4] Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel
* ales.iglic@fe.uni-lj.si

Protrusions at the leading-edge of a cell play an important role in cellular spreading and motility. However, the physics of the cell motility is still not well understood. We present a combined theoretical study of the cell movement on the surface of different geometry as well as the mechanism of efficient phagocytosis and the mechanism of coiling of cellular protrusions around fibers. Our theoretical model describes the membrane leading-edge that are produced by curved membrane proteins that recruit the protrusive forces of actin polymerization, and identifies the role of bending and adhesion energies. Among other our model recovers the observed cell migration on the sinusoidal substrate, where cells move along the grooves, while avoiding motion along the ridges. Further we predicted in accordance with experimental results that the cell's leading-edge may coil on fibers with circular cross-section (above some critical radius), but the coiling ceases for flattened fibers of highly elliptical cross-section. We also considered the phagocytosis of spherical (Fig. 1) and non-spherical particles and found that non-spherical particles are more difficult to engulf in comparison to the spherical particles of the same surface area. For non-spherical particles, the engulfment time depends on the initial orientation of the particles with respect to the vesicle.

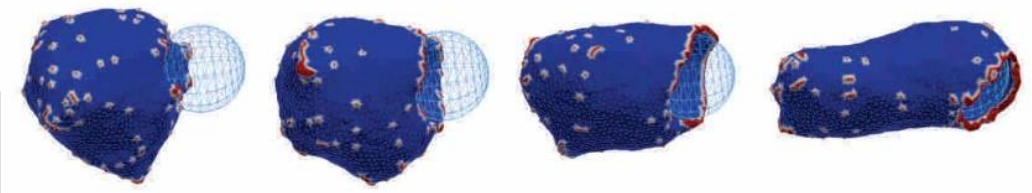

Figure 1: MC simulation of membrane engulfment of spherical particle (adapted from ref. 3).

References:

1.R.K. Sadhu, M. Luciano, W. Xi, C. Martinez-Torres, M. Schröder, C. Blum, M. Tarantola, S. Villa, S. Penič, A. Iglič, C. Beta, O. Steinbock, E. Bodenschatz, B. Ladoux, S. Gabriele, Nir Gov: A minimal physical model for curvotaxis driven by curved protein complexes at the cell's leading edge. *PNAS* 121 (12): e2306818121, 2024.
2. R.K. Kumar Sadhu, C. Hernandez-Padilla, Y.E. Eisenbach, S. Penič, L. Zhang, H.D. Vishwasrao, B. Behkam, K. Konstantopoulos, H. Shroff, A. Iglič, E. Peles, A. S. Nain, N. Gov: Experimental and theoretical model for the origin of coiling of cellular protrusions around fibers. *Nature Communications* 14: 5612, 2023.
3. R.K. Sadhu, S. Barger, S. Penič, A. Iglič, M. Krendel, N.C. Gauthiere, N. Gov: A theoretical model of efficient phagocytosis driven by curved membrane proteins and active cytoskeleton forces. *Soft Matter* 19, 31-43, 2023.
4. Mesarec, W. Góźdź, V. Kralj-Iglič, S. Kralj, A. Iglič: Coupling of nematic in-plane orientational ordering and equilibrium shapes of closed flexible nematic shells. *Scientific Reports* 13:10663, 2023.

ABSTRACTS OF ORAL PRESENTATIONS

Finite element simulations for the optical sensing performance of gold gratings

Deshabrato Mukherjee[1,2]*, Sven Burger[3,4], Thomas Siefke[5], Jeetendra Gour[5], Bernd Bodermann[6], Peter Petrik[1,7]

[1] – Hungarian Research Network, Centre for Energy Research, Institute of Technical Physics and Materials Science, Budapest, Hungary
[2] – Doctoral School of Materials Sciences and Technologies, Óbuda University, Budapest, Hungary
[3] – Zuse Institute Berlin, Takustraße 7, 14195 Berlin, Germany
[4] – JCMwave GmbH, Bolivarallee 22, 14050 Berlin, Germany
[5] – Institute of Applied Physics, Friedrich Schiller University, Jena, Germany
[6] – Physikalisch-Technische Bundesanstalt, Bundesallee 100 38116, Braunschweig, Germany
[7] – Department of Electrical and Electronic Engineering, Institute of Physics, Faculty of Science and Technology, University of Debrecen, Hungary
* – mukherjee.deshabrato@ek.hun-ren.hu

Optical methods can be used to measure the dimensions of sub-wavelength structures utilizing diffraction [1-4]. It has been demonstrated on silicon and oxide-based structures using a range of optical modeling approaches including rigorous coupled wave analysis and finite element methods [1, 2]. Standard ellipsometry uses the effective medium theory to determine the volume fractions of components in multi-component materials, however, the sizes of the domains cannot be determined. In this work we demonstrate the finite element method using the JCMwave solver to calculate the far-field optical response of gold gratings to estimate the parameter-dependent limit of detection values for different periods, line widths, thicknesses, angles of incidence and wavelengths in both traditional and Kretchmann reflection geometries.

References:

1. W.H Weber, S.L McCarthy. Surface-plasmon resonance as a sensitive optical probe of metal-film properties. Physical Review B, 12, 1975, 5643-5650.
2. N. Kumar, P. Petrik, G.K.P. Ramanandan, O. El Gawhary, S. Roy, S.F. Pereira, W.M.J. Coene, H.P. Urbach. Reconstruction of sub-wavelength features and nano-positioning of gratings using coherent Fourier scatterometry. Opt. Express 22, 2014, 24678.
3. P. Petrik, N. Kumar, M. Fried, B. Fodor, G. Juhasz, S.F. Pereira, S. Burger, H.P. Urbach, Fourier ellipsometry – an ellipsometric approach to Fourier scatterometry. JEOS:RP 10, 2015, 15002.
4. B. Liedberg, I. Lundström, E. Stenberg. Principles of biosensing with an extended coupling matrix and surface plasmon resonance. Sensors and Actuators B: Chemical, 1, 1993, 63-72.

Acknowledgements:

Support by OTKA grant Nr. K-146181 is gratefully acknowledged. The work in the frame of the 20FUN02 "PO-Light" project has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme. On behalf of the 'MFA-Fotonika-1'project we are grateful for the possibility to use HUN-REN Cloud Project no. C1792954.

Characterization of unsaturated lipid bilayer properties under different conditions with a Slipids force field

N. Ivanova[1,2*], 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,
72 Tzarigradsko Chaussée, 1784 Sofia, Bulgaria;
* – n.ivanova@uctm.edu

We use molecular dynamics to check the ability of the Slpids force field [1] to correctly describe the main characteristics of SOPC (1-stearoyl-2-oleoyl-sn-glycero-3-phosphocholine) – an unsaturated lipid – under different physical conditions. The behavior of SOPC lipid bilayers with different amounts of cholesterol (ranging from 10% mol to 50% mol) in atomistic model systems at a temperature of 273 K was examined [2,3]. It was found that at 30% mol cholesterol some of the properties of the bilayer saturate and there is significant ordering of the lipid molecules. In addition, three degrees of hydration (25, 40 and 50 water molecules per lipid) at 50% mol concentrations of cholesterol content with two water models (TIP3P and TIP4P) were considered at the same temperature [4]. It is found that the system involving TIP3P water model and a hydration number of 40 reproduces well the experimental data. Based on these results, the phase behavior of the lipid layer with three concentrations of cholesterol (0%, 10% and 30%) was investigated in a temperature range (271 K to 283 K) in the vicinity of the experimental melting temperature T_m = 279. The cooling properties of the systems from high temperature (400 K) to those in the discussed interval are probed. To conclude Slipids force field, with few exceptions, was found to do well in describing the parameters of the model bilayer systems and provides useful information on phase behavior of unsaturated lipids.

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, H Chamati, The effect of cholesterol in SOPC lipid bilayers at low temperatures, Membranes 13 (3), 2023, 275.
3. N Ivanova, H Chamati, Physical properties of phospholipids at low temperatures through Slipid force field, J. Phys.: Conf. Ser. 2436, 2023, 012025.
4. N Ivanova, The influence of the hydration number in a mixed lipid bilayer with cholesterol, J. Chem. Tech. Metall. 59 (2), 2024, 279-286.

Acknowledgements:

This work was supported by Grant No BG05M2OP001-1.001-0008 funded by the Operational Programme Science and Education for Smart Growth, co-financed by the European Union through the European Regional Development Fund.

Criticality controlling mechanisms in nematic liquid crystals

Maha Zid[1,2,*], George Cordoyiannis[1], Zdravko Kutnjak[1], and Samo Kralj[1]
[1] – Condensed Matter Physics Department, Jožef Stefan Institute, 1000 Ljubljana, Slovenia
[2] – Jožef Stefan International Postgraduate School, Jamova cesta 39, 1000 Ljubljana, Slovenia
* – maha.zid@ijs.si

We theoretically study [1] the generic mechanisms that could establish a critical behavior in nematic liquid crystals (NLCs). Our analysis focuses on the free energy density terms that exhibit a linear coupling with the nematic order parameter and consequently enhance the nematic order. We consider both temperature- and pressure-driven, order-disorder phase transitions. By deriving an expression for the scaled effective free energy, we provide a detailed description of how various mechanisms can enforce critical behavior in NLCs. This expression allows us to qualitatively and quantitatively analyze the differences between the effects of temperature and pressure on the phase transitions.
A significant part of our study focusses on the impact of nanoparticles (NPs) in homogeneous NP-NLC mixtures. We illustrate that in the case of pressure-driven phase changes, lower concentrations are needed to impose critical point conditions in comparison with pure temperature variations.

References:
1. Zid, M.; Cordoyiannis, G.; Kutnjak, Z.; Kralj, S. Criticality Controlling Mechanisms in Nematic Liquid Crystals. Nanomaterials 14 (3), 2024, 320.

Acknowledgements:
M.Z. acknowledges the financial support of Project PR-12878

Langmuir and Langmuir-Blodgett Nanocomposite Films from Adsorbed Glucose Oxidase Enzymes

George R. Ivanov[1], Evgenia Bogdanova[1]
[1] University Laboratory "Nanoscience and Nanotechnology", University of Architecture, Civil Engineering and Geodesy, blvd. H. Smirnenski 1, 1064 Sofia, Bulgaria
* george@at-equipment.com

The human body's blood glucose (BG) concentration serves as an important index for diagnosing diabetes, and its detection methods need to be more efficient due to high mortality rates for diabetes. Glucose Oxidase enzyme (GOx) was frequently used for developing electrochemical BG sensors with several generations of sensors being developed. Here we propose a new method for preparing a sensing layer from GOx. The water-soluble GOx molecules are dissolved in the water subphase in a Langmuir-Blodgett (LB) film deposition system. They are surface-active molecules and create some surface pressure. Then, on top of the prepared in this way subphase is formed an insoluble monolayer from different molecules at the air-water interface (Langmuir film). Due to electrical or steric interactions GOx is adsorbed to this layer. Afterward, this nanosized composite structure is deposited following the LB method on a solid substrate layer after layer. This approach can provide at least two advantages to alternative deposition methods: a nano-thin uniform layer, a prerequisite for fast sensing, and protection of the enzyme molecule from environmental degradation. This work presents results from such adsorbed GOx monolayers to different Langmuir films. For the Langmuir film, we focus our work on two distinct classes of compounds: a fluorescently labeled phospholipid DP-NBD-PE, which was previously shown to produce high sensitivity layers [1], and Metal Organic Framework (MOF) MIL-101(Cr), which was used for the first gravimetric detection of small-sized molecules dissolved in water [2].

References:

1. Avramov, I.D.; Ivanov, G.R. Layer by Layer Optimization of Langmuir–Blodgett Films for Surface Acoustic Wave (SAW) Based Sensors for Volatile Organic Compounds (VOC) Detection. *Coatings* **2022**, 12, 669.
2. Ivanov, G.R.; Venelinov, T.; Marinov, Y.G.; Hadjichristov, G.B.; Terfort, A.; David, M.; Florescu, M.; Karakuş, S. First Direct Gravimetric Detection of Perfluorooctane Sulfonic Acid (PFOS) Water Contaminants, Combination with Electrical Measurements on the Same Device - Proof of Concepts. *Chemosensors*, **2024**, 12, 116.

Acknowledgements:
This work is supported by the Bulgarian National Science Foundation contract No. KP-06-N68/3/2023.

Effect of commercial cryoprotectants and hybrid "instant" freezing on the outcome of soot-assisted human sperm cryopreservation

Karekin D. Esmeryan[1*], Yulian Fedchenko[1], Todor Angelov Chaushev[2]
[1] – Acoustoelectronics Laboratory, Georgi Nadjakov Institute of Solid State Physics,
Bulgarian Academy of Sciences, 72, Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria
[2] – Specialized Surgical Hospital "Doctor Malinov", 46, Gotse Delchev blvd., 1860 Sofia, Bulgaria
* – karekin_esmerian@abv.bg

Nowadays, the cryopreservation of human and animal spermatozoa is necessary in cases of impaired spermatogenesis, fertility treatment with donor sperm, autologous use, upcoming dangerous surgical interventions, gender transition or for enhancing the breeding of livestock and poultry.

Upon freezing of cellular suspensions, however, the extracellular region transforms into ice, relocating the solutes in the gradually narrowing unfrozen liquid channels and creating osmotic elimination of the cell water. When the rate of external crystallization of the solution is comparable to the rate of cellular dehydration (defined by the membrane permeability), the freezing is harmless, but any loss in such a subtle balance may lead to either hypertonic damage or lethal intracellular icing – the famous theory of two-factor freezing injury, first introduced by Peter Mazur in 1960s.

It is possible to alleviate or entirely avoid the cryoinjury by making the solid-liquid contact interface non-wettable. For instance, the deposition of rapeseed oil soot nanoparticles on the solid surface accommodating the biological matter leads to inherently impeded heterogeneous nucleation, so the growing ice crystals are small enough to keep most of the cells intact, maintaining the solution composition in equilibrium with the increasing ice fraction and in certain circumstances, enabling full (100 %) recovery of the original motility of human spermatozoa, even at slow warming rates (previously shown to be detrimental to the cells' survival). Nevertheless, reaching repeatable 100 % success rate regardless of the sperm parameters (i.e., initial concentration, motility, as well as biochemistry of the seminal plasma) would not be accomplishable if the effect of different cryoprotective agents and cooling velocity on the outcome of soot-assisted sperm cryopreservation is still elusive.

In this proceeding, we represent a pioneering study concerning the impact of three types of commercial cryoprotectants, in combination with "hybrid" instant freezing (a novel approach explained in the lecture), on the kinematics of post-thaw human semen. Our newest experimental results show that increasing the cooling velocity fiftyfold, by partially immersing a soot fabric-coated sheet metal cryobox in liquid nitrogen, hinders the formation of intracellular and extracellular ice crystals, while the subsequent slower freezing over the vapor of liquid nitrogen balancedly removes the water from cytoplasm, ending up with sperm survival rates ~74-100 % independently of the used cryoprotectant and thawing time. This previously unseen freezing approach moves the Society for cryobiology forward by opening opportunities to overcome the deleterious effects of cryoprotectants and devitrification phenomena.

Acknowledgements:
This research was performed thanks to the financial support of Bulgarian National Science Fund under grant No. KP-06-H57/1/15.11.2021

Investigation of GaSb micro-islands deposited on Si substrates

Vesselin Donchev[1]*, Kiril Kirilov[1], Malina Milanova[2], Petko Vitanov[3], Hristosko Dikov[3], Pavlina Ralova[2]
[1] – Faculty of Physics, Sofia University, 5, blvd. J.Bourchier, BG-1164, Sofia, Bulgaria
[2] – Central Laboratory of Applied Physics, Bulgarian Academy of Sciences, 61 Sanct Petersburg Blvd, 4000, Plovdiv, Bulgaria
[3] – Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee Blvd, 1784 Sofia, Bulgaria
* – vtd@phys.uni-sofia.bg

In this paper, we report our investigations of the properties of GaSb islands grown on a Si substrate by a thermal evaporation method using Ag nanoparticles as catalysts. The size and shape of the grown structures have been determined by atomic force microscopy and scanning electron microscopy measurements. GaSb islands varying in size from 0.5 to 1.5 μm are formed at an evaporation temperature of 800°C. The X-ray diffraction curves reveal that the islands are monocrystalline with a (111) crystallographic orientation. The Raman spectra exhibit a slight red shift in the Ga-Sb peaks, compared to bulk GaSb, as a result of the compressive strain of the islands. SPV spectroscopy combined with Kelvin probe force microscopy provides information about the energy band alignment between Si and GaSb.

Characterization of Ni- and Co-based bifunctional electrocatalysts for application in carbon-free air electrodes for rechargeable Zinc-air batteries

K. Krezhov[1*], G. Raikova[2], E. Mihaylova-Dimitrova[2], E. Mladenova[2], T. Malakova[1], P. Tzvetkov[3], T. Koutzarova[1]

[1] – Institute of Electronics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria

[2] – Institute of Electrochemistry and Energy Systems, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

[3] – Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria

* – kiril.krezhov@gmail.com

Spinel-structured oxides continue to be intensively investigated due to their high efficiency for both the oxygen reduction reaction (ORR) during discharge and the oxygen evolution reaction (OER) during charge of secondary metal-air batteries with alkaline media. Most papers report their reduction activities, as the ORR is the kinetically slower process than OER and it governs the practical application of these materials. We present here additional results on the performance of the recently developed carbon-free gas-diffusion electrode (GDE) - a mixture of catalyst (Co_3O_4, $NiCo_2O_4$) and polytetrafluoroethylene (PTFE) hot-pressed onto a stainless-steel mesh that works as a current collector. To enhance the ORR efficiency 70 wt.% Ni powder was incorporated to the catalyst. Electrochemical characteristics were investigated, including volt-ampere characteristics, charge/discharge tests and specific electrochemical techniques including impedance spectroscopy were applied. Sensitive techniques such as neutron and X-ray diffraction combined with scanning electron microscopy and EDX-analysis were applied to improve the understanding of structural stability and recharge-related properties as an important step in the development of an innovative design of rechargeable zinc-air cells with high performance carbon-free reversible GDEs. $NiCo_2O_4$ oxide showed better bifunctional behaviour and was tested as a GDE component in a secondary tri-electrode Zn–air cell. Acceptable coulombic and energy efficiencies were obtained. The results show that prepared in this way carbon-free gas-diffusion electrode is enough competitive to those prepared by classical technology using carbon black, which stability is the limiting factor for the cycle life of bifunctional air electrodes.

Acknowledgements:
The study was partially supported by the Bulgarian National Science Fund under contract KP-06-N48/5.

Engineering the mechanical and X-ray attenuation properties of gelatine composite hydrogels with a potential for tissue mimicking materials

Georgi Tankovski[1], Veselina Georgieva[1,2*], Nikoleta Traikova[2], Ginka Exner[1]
[1]Faculty of Physics and Technology, Plovdiv University Paisii Hilendarski, 4000-Plovdiv, Bulgaria
[2]UMBAL "St. Georgi", 4000-Plovdiv, Bulgaria
* veselina_ngeorgieva@abv.bg

In the present study, modification and engineering of the properties of gelatine composite hydrogels, *GH*, are studied. The composites differ in their distilled water/glycerol ratio, *DW*/*Gly*, and the filler type (8 g, collagen, *Coll*, and eggshells, *ES*). The gelatine, *G*, content was fixed (0.08 g/ml). Computed tomography (CT Somatom Definition AS64, Siemens, Germany) tests were performed (tube voltage, *TV*, 70 – 120 kVp). As a practical measure of the X-ray attenuation, the Hounsfield units, *HU*, were obtained. The mechanical performance was also investigated (Lloyds universal instrument LS), as a prerequisite for the practical implementation and for the possibility to couple the composite properties for a multimodal phantom material. Cylindrical samples with a diameter and a height of 30 mm were used. Loading-unloading cycles were performed at a rate of 0.2 mm/s. Young's modulus, *E*, the force at maximum deformation, F_{max}, and the work of deformation, W_d were derived.

Table 1. The maximum values of Young's modulus, *E*, force at the maximum deformation, F_{max}, and work of deformation, W_d. The corresponding *DW*/*Gly* ratio is given in parentheses.

	HU, at 80 kVp	*E*, kPa	F_{max}, N	W_d, N.mm
GH	156 (100:0)	43 (70:30)	18 (70:30)	113 (70:30)
Coll GH	176 (30:70)	29 (70:30)	18 (50:50)	78 (50:50)
ES GH	275 (30:70)	51 (50:50)	26 (50:50)	107 (50:50)

According to our results, the *HU*s for the neat *GH*, increase with the *Gly* content but they are almost independent of the *TV*. The *HU*s for both composites are higher but the *ES GH* showed a more significant increase. The *ES GH* voltage dependence is opposite to that of the neat *GH* but it is in agreement with our experiments using porcine bones. The maximum *HU* values, together with the corresponding *DW*/*Gly* are shown in Table 1. The results show that the composites can be used to adjust some soft tissue and trabecular bone *HU*s in CT. The mechanical performance of the investigated samples, within the experimental limits, corresponds to almost entirely elastic behaviour. The *E*, F_{max}, and W_d dependences on the *Gly* content pass through a maximum. In some cases, the maximum shifts to higher *Gly* content, as seen in Table 1. The *E* values correspond to breast and prostate tissues [1].

References:

1. C. K. McGarry, L. J. Grattan, A. M. Ivory, F. Leek, G. P Liney, Y. Liu, P. Milor, R. Rai, A. P. Robinson, A. J. Shih, B. Zeqiri, C. H. Clark, "Tissue mimicking materials for imaging and therapy phantoms: a review", Phys. Med. Biol. 65 (2020) 23TR01.

Acknowledgements:

Work supported by the Ministry of Education and Science of Bulgaria (MESB), through the National Research Fund of Bulgaria (research project "Liquid crystal nanocomposites for applications in photonics, sensors and biomedicine", No. KP-06-N58/6/2021).

ALD and sol-gel grown ZnO, Ni- and Li/Ni-doped ZnO thin films for gas sensors

S.I. Boyadjiev[1*], S. Mihaiu[2], I. Atkinson[2], V. Georgieva[1], P. Rafailov[1], L. Vergov[1], I.M. Szilágyi[3]

[1] "Georgi Nadjakov" Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee blvd., 1784 Sofia, Bulgaria

[2] "Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, 202 Splaiul Independenţei, 060021 Bucharest, Romania

[3] Budapest University of Technology and Economics, Department of Inorganic and Analytical Chemistry, Szent Gellért tér 4, Budapest, H-1111, Hungary

* boiajiev@gmail.com

The study presents the preparation and characterization of zinc oxide (ZnO), as well Ni- and Li/Ni-doped ZnO thin films studied for gas sensors. For preparing the samples the methods of atomic layer deposition (ALD) and sol-gel, combined with dip coating, were used. Hence, bare, Ni- and Li/Ni-doped ZnO layers were deposited on quartz resonators and their properties were studied and compared.

The surface analysis was performed using scanning electron microscopy (SEM), coupled with energy dispersive X-ray (EDX) analysis. As the surface properties are the most important for the gas sensing of the films, X-ray photoelectron spectroscopy (XPS) was also applied. The structure of the films was studied by X-ray diffraction (XRD), Raman and FTIR spectroscopy, while their thickness was determined by ellipsometry.

Both the ZnO and doped ZnO films of various thicknesses were deposited on quartz resonators and the quartz crystal microbalance (QCM) method was used for gas sensing. Prototype QCM sensors with pristine and doped ZnO gas-sensitive films were tested for sensing NO_2 in the range between 10 ppm and 5000 ppm. On the basis of registered frequency change, the adsorbed mass for each concentration was calculated. The films showed good gas sensitivity and fast reaction at room temperature. According to the results, the described fast, simple and cost-effective technology could be implemented for producing ZnO-based gas sensors working at room temperature and capable to register low concentrations NO_2. The Li/Ni co-doped ZnO films showed superior sensitivity to NO_2 compared with the bare or Ni-doped ZnO films.

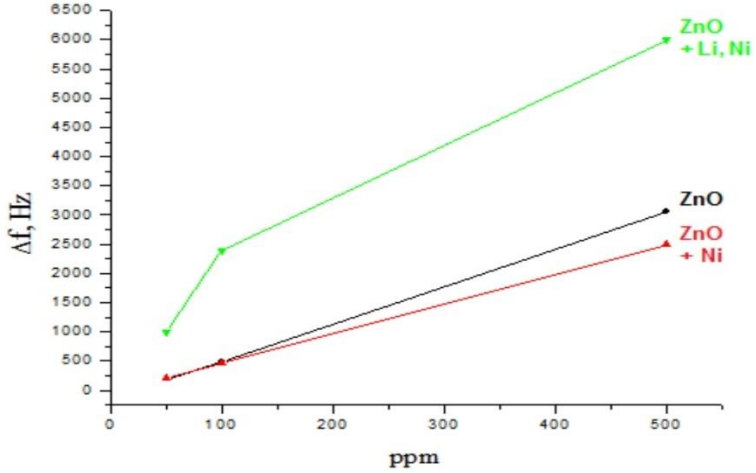

Figure 1: Frequency shift at various NO_2 concentrations for sol-gel grown bare, Ni, and Li/Ni-doped ZnO gas sensor

Ti/TiN/AlTiCrN hard coating investigated by Close Field Unbalanced Magnetron Sputtering

Vasiliy Chitanov[1*], Ekaterina Zlatareva[1], Stefan Kolchev[1], Lilyana Kolaklieva[1], Roumen Kakanakov[1], Tetiana Cholakova[1], Chavdar Pashinski[1,2]
[1] – Central Laboratory of Applied Physics, Bulgarian Academy of Sciences,
61 Sankt Peterburg Blvd., 61, 4000 Plovdiv, Bulgaria
[2] – Department of Mechanics, Technical University-Sofia, Bt. Plovdiv,
25 Tsanko Dyustabanov St., 4000 Plovdiv, Bulgaria
* – vchitanov@gmail.com

A Ti/TiN/AlTiCrN hard coating was developed and deposited with Close Field Unbalanced Magnetron Sputtering. Technological experiments were performed to optimize the ratio between the composed metals Al, Ti, and Cr, and the ratio metals/nitrogen. Nanoindentation measurements obtained nanohardnes of 32 GPa. A scratch test with a normal load up to 30 N indicated good adhesion to the substrate. A tribological test with a rotational drive (ball on plate) was made with a load of 3N and a path length of 50 m. The measured coefficient of friction was 0.34. It should be noted that the reported results are obtained at temperatures as low as 270 ^{o}C, which determines the coating as universal. The obtained results are compatible with ones obtained on the same coating deposited by high-temperature techniques as Cathodic Arc Deposition and HIPIMS. The investigated coating is aimed to improve the performance of tools made of materials with different thermal stability.

Acknowledgements:
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.

Application of RBF ANN in NIR Spectroscopy for improving the efficiency in Citalopram production

G. Gergov[1], J. Cruz[2], O. Kostadinova[3], A. Gerasimova[4*]
L. Makedonski[4+]and K. Nikolova[5]
[1] Bulgarian Academy of Sciences, Institute of Chemical Engineering,
Acad. Georgi Bontchev Str., Bl. 103, Sofia 1113, Bulgaria
[2] Escola Universitària Salesiana de Sarrià (EUSS), Passeig de Sant Joan Bosco, 74, 08017 Barcelona, Spain
[3] Bulgarian Academy of Sciences, Institute of Electrochemistry and Energy Systems "Acad. E. Budevski",
"Acad. Georgi Bonchev" Str. Bl.10, 1113 Sofia, Bulgaria
[4] Department of Chemistry, Medical University of Varna, Faculty of pharmacy,
84 Tzar Osvoboditel Blvd, 9002 Varna, Bulgaria
[5] Department of Physics and Biophysics, Medical University of Varna, Faculty of pharmacy,
84 Tzar Osvoboditel Blvd, 9002 Varna, Bulgaria
* – Anelia.Gerasimova@mu-varna.bg

The pharmaceutical industry faces significant challenges in processing increasingly large spectral datasets. This study presents a solution using spectroscopic techniques for efficient production process management. The critical point for this purpose lies in selecting an optimal machine learning method tested using an open-source dataset.
A dataset made with real samples from the industry and registered with Near-Infrared (NIR) spectroscopy was used to illustrate our approach. This open-source tablet dataset, available at http://www.models.life.ku.dk/Tablets, encompasses a wide range of variables, including different dosages, tablet shapes, and sizes, manufacturing scales (lab, pilot, full), and coating variations (coated vs uncoated).
This study proposes a sensor based on NIR spectroscopy to monitor the production process of citalopram, a widely used antidepressant. We established calibration models of citalopram concentrations using an Artificial Neural Network (ANN). The Radial Basis Function Artificial Neural Network (RBF-ANN) was found to have the best prediction in internal validation with full scale.
Different RBF ANN architectures were tested, and their parameters were optimized. When combined with different pre-processing techniques, the standard normal variate (SNV) emerged as the optimal choice. Compared to standard Partial Least Squares (PLS) regression techniques, the RBF ANN demonstrated a reduction in both the Root Mean Square Error of Prediction (RMSEP) and Residual Prediction Deviation (RPD).
These improvements, coupled with the ease of implementing NIR technology in process engineering, make this approach highly beneficial for the pharmaceutical industry. This study thus provides a robust framework for enhancing production efficiency and accuracy in pharmaceutical manufacturing.

Acknowledgements:
This study is financed by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project No. BG-RRP-2.004-0009-C02.

ABSTRACTS OF FIRST POSTER SESSION

1.1. Mechanism of Photoinduced Nucleation in Supersaturated Metallic Vapors

Svetlana Baranovski
Faculty of Physics, Philipps-Universität Marburg, Marburg 35032, Germany
* svetlana.baranovski@physik.uni-marburg.de

In this presentation, we focus on the effect of photoinduced condensation in supersaturated vapours. Experimental studies of this effect in an upward thermal diffusion cloud chamber show drastic effects of the light absorption on the nucleation rate [1, 2]. In Figure 1, the spectral dependence of the nucleation rate is compared with the absorption and ionization spectra for cesium vapour [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.

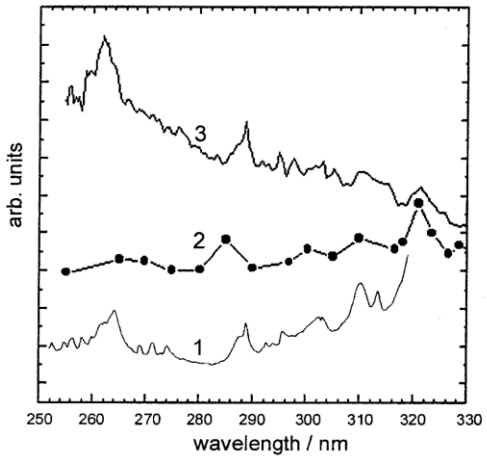

Figure 1: 1- Absorption cross-section of saturated cesium vapor at T=767 K; 2 – photoionization cross-section of cesium dimers from Ref. 3; 3 – the nucleation rate spectrum.

Also mercury vapours show in an upward thermal diffusion cloud chamber the drastic effect of the light absorption on the nucleation rate [2]. The rate of nucleation is greatly enhanced when the supersaturated vapour is illuminated with the light absorbed by gas molecules.
This effect can be described theoretically in close analogy to the well-known mechanism of the nucleation caused by ions [1 - 4]. In both effects, it is favourable for the particles to form growing clusters of vapour atoms and thus diminish the excess energy stored either by ionization or by optical excitation. This reduction of the excess energy is the driving force of the nucleation process.

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.
4. M. Volmer „Kinetik der Phasenbildung", (Theodor Steinkopff, Dresden, 1939).

1.2. Dynamics of soliton excitations in an inhomogeneous a magnetic chain

R. S. Kamburova*, M. T. Primatarowa and M. M. Danev
Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria
* krad@issp.bas.bg

The interaction of magnetic excitations with extended inhomogeneities modeled by the change in an anisotropy constant of a set of spins in an on-side anisotropic Heisenberg spin chain is studied numerically. The inhomogeneities lead to linear and nonlinear additional terms in the nonlinear Schrödinger (NLS) equation for the spin amplitude derived by consistently applying quasiclassical approximation and continuum limit (classical spin vectors and wide excitations). The spin set with distinct anisotropy constant consists of equal consecutive spins with modified coefficients of the linear and nonlinear interaction. For a homogeneous chain and easy axis NLS equation possesses a bright-type soliton excitation solution. When the anisotropy constant increases the spin set acts as a complex linear and nonlinear potential well with a dominant linear character and for a given range of initial velocities of the incoming bright soliton and the mismatch anisotropy the scattering pattern exhibits periodically repeating regions of trapping and transmission as a function of the length of the inhomogeneity. It is shown that the runaway of the soliton is due to a resonance between the period of the shape oscillations of the soliton inside the inhomogeneity and the length of the latter.

Acknowledgements:
This work was supported by the Grant No KP-06-N78/2 of 05.12.2023 from the Ministry of Education and Science of Bulgaria.

1.3. Adsorption of ammonia and hydrazine on a metal oxide layer

N. Ivanova[1,2*], 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,
72 Tzarigradsko Chaussée, 1784 Sofia, Bulgaria;
* – n.ivanova@uctm.edu

Metal oxides, in particular magnetite, are complex systems that are not well understood via computer modelling. Here we use molecular dynamics to gain insights in the adsorption of molecules on the surface. The initial coordinates of Fe_3O_4 in the {111} plane were generated with the aid of CrystalMaker [1]. By replicating the unit cell of the crystal, a monolayer of width 3.39 nm and height of 2.50 nm is built up. Further, ten molecules of ammonia and hydrazine each are placed at the vicinity of the surface of the metal oxide. Water molecules are added to the constructed systems so that overlapping of atoms was avoided. The size of the periodic box is 6 nm and the total number of atoms is over 6000. Atomistic molecular dynamics simulations are performed in conjunction with Clay force field [2] with an imposed charge modification for the iron atoms. The NPT ensemble is used at a temperature of 298 K and a pressure of 1 bar along with TIP3P water model, with a trajectory duration of 100 ns. The interaction of ammonia and hydrazine is considered and their initial molecular motion is recorded. The root mean square deviation (RMSD) and radial distribution functions (RDF) of both molecules were calculated. Adsorption of some of the ammonia and hydrazine molecules is reported.

References:
1. Y. W. Yin, CrystalMaker 6.3 CrystalMaker Software, Begbroke Science Park, Building 5, Sandy Lane, Yarnton OX5 1P5, Journal of the American Chemical Societ., 126, 45, 2004, 14996 -15007.
2. Molecular Models of Hydroxide, Oxyhydroxide, and Clay Phases and the Development of a General Force Field, Journal of Physical Chemistry B, 108, 2004, 1255-1266.

Acknowledgements:
Bulgarian National Science Fund under Grant No КП-06-Н78/2 (2023).

1.4. Zener-Kondo interaction in layered perovskites and the emergence of zero sound

Nedeltcho I. Zahariev*, Albert M. Varonov, Hassan Chamati
Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria
* – zahariev@issp.bas.bg

We identify the conditions for emergence of zero sound propagation in layered perovskites composed of transition metal ion and chalcogenide oxides. We find that the emergence of zero sound is achievable in the case of a ferromagnetic sign of the Zener-Kondo interaction. While for an antiferromagnetic sign, such as layered cuprates, the zero sound is a thermally activated dissipative mode that is observed in Angle Resolved Photoemission Spectroscopy (ARPES) as "hot spots" along the Fermi contour. Moreover, we show that the zero sound is possible when the 4*s* and 3*d* energy levels of the transition metal ion are sufficiently close to the 2*p* energy levels of the chalcogenide. Propagation of zero sound is possible only for ferromagnetic sign of the Zener-Kondo *s-d* exchange interaction.

References:
[1] T. M. Mishonov, N. I. Zahariev, H. Chamati and A. M. Varonov, "Possible zero sound in layered perovskites with ferromagnetic *s-d* exchange interaction", SN Appl. Sci. **4** (2022) 228.
[2] T. M. Mishonov, N. I. Zahariev, H. Chamati and A. M. Varonov, Hot spots along the Fermi contour of high-T_c cuprates analyzed by *s-d* exchange interaction, SN Appl. Sci. **4** (2022) 242.

Acknowledgements:
This research is supported by the Bulgarian National Science Fund under Grant No КП-06-Н78/2 (2023).

1.5. Nanomechanical Properties of Lymphocytes in Chronic Lymphocytic Leukemia: assessment of response to Venetoclax and Obinutuzumab therapy. Case Report.

Velichka Strijkova[1*], Vesela Katrova[1], Lidia Gartcheva[2], Anika Alexandrova[3], Ariana Langari[4], Miroslava Ivanova[4], Sashka Krumova[4], Svetla Todinova[4]
[1]Institute of Optical Materials and Technologies "Acad. Yordan Malinovski",
Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria;
[2]National Specialized Hospital for Active Treating of Haematological Diseases, 1756 Sofia, Bulgaria;
[3]Institute of Mechanics, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria;
[4]Institute of Biophysics and Biomedical Engineering,
Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria
* vily@iomt.bas.bg

Chronic lymphocytic leukemia (CLL) is yet incurable disease characterized by the accumulation of monoclonal B cells in secondary lymphoid organs, bone marrow, and peripheral blood. The introduction of more effective targeted therapies, such as Bruton tyrosine kinase inhibitors, Venetoclax (attacking the apoptosis regulator Bcl-2 protein), and Obinutuzumab (next-generation anti-CD20 monoclonal antibody) have significantly improved the outcomes in the treatment of CLL patients.

There is increasing evidence that CLL progression significantly alters the biophysical properties of peripheral cells, but the nature of those effects is still unclear. In this respect, atomic force microscopy offers the unique possibility to probe the structural and mechanical features of individual cells on the nanoscopic scale and therefore is expected to yield important details on CLL-related cell properties as well as on the efficacy of anti-leukemic treatments.

This case study reports on the morphological and nanomechanical properties of lymphocytes isolated from a 53-year-old male CLL patient and evaluates the impact of the application of two courses of treatment with Venetoclax and Obinutuzumab. The results reveal that lymphocytes from the CLL patient have a higher stiffness, i.e., a lower deformability, as compared to those from healthy individuals. The administration of Obinutuzumab+Venetoclax combination restores to a large extent the mechanical properties of CLL cells towards those of healthy lymphocytes. Furthermore, two types of CLL lymphocytes are observed which differ in their elastic properties after the applied treatment: (i) cells with elasticity similar to the one determined for healthy cells (ca. 73% of the population) and (ii) cells with higher elasticity (ca. 27% of the population).

In summary, our data demonstrate that Obinutuzumab/Venetoclax administration contributes to the restoration of lymphocytes' cell elasticity to normal levels and suggests that the mechanical features of CLL cells might be related to their malignant degeneration.

Acknowledgements:
This work was conducted with the financial support of Grant KP-06-H73/3, Competition for financial support for basic research projects—2023, 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.

1.6. Physicochemical properties of sesame oil blending with sunflower and soybean oil

Asya Viraneva[1*], Maria Marudova[1], Ginka Antova[2], Maria Romova[2]
[1] – Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski",
24 Tsar Asen Str.,4000 Plovdiv, Bulgaria
[2] – Faculty of Chemistry, University of Plovdiv "Paisii Hilendarski",
24 Tsar Asen Str.,4000 Plovdiv, Bulgaria
* – asia83@abv.bg

Vegetable oils can be adjusted by different methods to enhance their commercial applications. One of the easiest ways of creating new innovative products with desirable textured and oxidative properties is the mixing of vegetable oils of various concentrations. Vegetable oil blends are gaining popularity worldwide due to their advantages. Some oils have limited applications in their original form due to their chemical composition. Blending is one way to widen their commercial use. In the present paper blends (5:95, 10:90, 30:70, 50:50 70:30 and 90:10 w/w) of sesame oil with less stable edible oils like sunflower and soybean oil were investigated. Thus, the objective was to exploit the effect of the more potent antioxidant properties of oil blends to achieve longer shelf-life. The physicochemical properties of the blends as the fatty acid composition, thermal behavior (DSC), refractive indices and UV Vis spectroscopy were investigated. The blending of sesame oils with other vegetable oils would enable the initial properties of the oils to be modified or altered and provide functional and nutritional attributes for usage in various food applications, increasing the possibilities for the commercial use of these oils.

Acknowledgements:
The authors gratefully acknowledge the support of the project FP23-FTF-012/25.04.2023, Department of Scientific Research at the University of Plovdiv.

1.7. Concentration of Red Wine Phenolic Compounds Applying Nanofiltration with Alfa Laval NF99HF Membrane

M. Lazarova[1]*, M. Dencheva-Zarkova[2], J. Genova[2], D. Yankov[1]
[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 represents a rich source of polyphenols which strongly affect its quality. These bioactive compounds are also associated with a wide range of health benefits which is consistent with modern trends towards healthy lifestyles. However, polyphenolic content in red wine can vary extensively. It differs between wine varieties and is determined by viticulture and vinification practices, specific to different countries. Technologies based on membranes can be applied to increase the amount of these wholesome compounds in wine. Membrane processes are superior to the traditional methods used for polyphenol extraction in terms of high recovery efficiency, no phase transition, and mild operating conditions.
Nanofiltration for polyphenol concentration in native Mavrud red wine (wine cellar Harmanli, vintage 2020) was investigated. For this purpose, a MaxiMem membrane filtration system with a cross-flow rectangular flat-sheet cell was used. The effects of the operating parameters (transmembrane pressure and flow rate) on the retention of bioactive compounds in wine were examined. The phenolic amount of the obtained wine after nanofiltration was evaluated and compared with the data of the original wine. In our previous study, the membrane Microdyn Nadir™ NP030 P was employed to perform the process of wine nanofiltration. Maximum phenolic concentration of 29 % was achieved. In the present study, the nanofiltration membrane Alfa Laval NF99HF was used and an even much better result was realized. A maximum phenolic concentration of more than 67 % was reached with this membrane. This result was achieved with a set of transmembrane pressure and flow rate of 50 bar and 1.2 L/min, respectively. However, we recommend a set of 40 bar pressure and 2 L/min flow rate for optimal process performance, which results in a phenolic concentration of more than 56 %.

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

1.8. Relationship between routes and population within city structures

Diego Ortega[1] and Elka Korutcheva[1,2]
[1] – Department of Fundamental Physics, National University of Distance Education (UNED), 28040, Madrid, Spain
[2] – G. Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria

Urban development has progressed alongside the evolution of civilization, aiming at efficient travel and cost reduction. Numerous studies have investigated the unique characteristics of urban road networks, including their length, efficiency and connection to population density as well as other properties, often using mobile phone data for analysis.
In our research, we used the center of mass for each city tract, as defined by the US Census, as the starting and ending points for our itineraries. We measured travel time, and both Euclidean and travel distances for sixty cities with populations over 105,000. We found that the total sum of all routes follows an urban law. The distribution of these routes fits Weibull functions, indicating that city centers are crucial for optimizing routes across various cities. Additionally, we created a simple model of population point patterns, consistent with the commonly known decreasing exponential density expression. Our results demonstrate that the interaction between population and route optimization shapes city structures through their centers.
This study provides new insights into the fundamental principles that influence urban design.

References:

1. Barthelemy, M. Spatial Networks: *A Complete Introduction: From Graph Theory and Statistical Physics to Real-World Applications*. (Springer International Publishing, 2022).
2. Bettencourt, L. M. A. *Introduction to Urban Science: Evidence and Theory of Cities as Complex Systems*. (John Wiley & Sons, Ltd, 2021).

1.9. Investigation of the elastic properties of star polymers in semi-infinite space

Maciej Dudek[1*], Zoriana Danel[2]
[1] – Academy WSB, Cracow
[2] – Faculty of Materials Engineering and Physics, Cracow University of Technology, Cracow
* – macmatematyka@gmail.com

We performed the investigation of the elastic properties of four-armed and three-armed star polymers in a semi-infinite space confined by single wall with different boundary conditions and calculated Pincus force in the above mentioned cases. Calculations were carried out for four and three armed star polymers attached to the substrate with one or two arms. Besides, the case of freely placed star polymers with different number of arms in semi-infinite space also was analyzed. These showed that the Pincus force is affected by the number of arms attached to the surface. For star polymer with center near the surface, the Pincus force is almost twice higher for the case of two attached arms as it is for one attached arm. This difference increases as the distance of the star center from the wall increases. The results for the Pincus force agree with those obtained for the linear polymer chain in work [1], but have a larger value. Besides, we observe that the polymer topology have influence on the Pincus force value.
The obtained results are interesting from scientific and industrial point of view, because of their potential use in the production of paints, varnishes and functional materials. Star polymers, due to their structure and shape, provide higher performance compared to linear polymers. They can be used as viscosity modifiers, e.g. in engine oils, in cosmetics, and to increase the flexibility of the functional materials. Star polymers can be used as drug or gene transporters and to block RNA/DNA expression.

References:
1. Z. Usatenko, Stretching of a polymer chain anchored to a surface: the massive field theory approach, J.Stat.Mech.-Theory Exp., P09015 (2014).

1.10. Effects of Temporin A analogs on lipid membrane models

Victoria Vitkova[1], Angelina Stoyanova-Ivanova[1], Krassimira Antonova[1], Ognyan Petkov[1], Velizar Georgiev[1,*], Tihomir Tenev[1], Diliana Dimitrova, Nelly Georgieva, Dancho Danalev[2]
[1] – G. Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tzarigradsko Chaussee, 1784 Sofia, Bulgaria
[2] – University of Chemical Technology and Metallurgy, Biotechnology Department, 8 Kliment Ohridski blvd., 1756 Sofia, Bulgaria;
* – velizar@issp.bas.bg

Antibiotic resistance of microorganisms is a growing issue, which boosts the investigation of antibiotic alternatives. In this respect, the antimicrobial peptides Temporin A and F exhibit promising features such as antiproliferative properties against microorganisms and/or tumor cells [1,2], which reinforces their importance. Studies also show that some antimicrobial peptides are able to interact with model cell membranes, causing membrane softening, further underlining their antiproliferative properties [3]. Biological membranes are responsible not only for the integrity of the cell and its compartmentalization but also for many cellular processes where deformations and physicochemical properties of the membrane play an important role. In the present study we investigate the interaction of biomembrane models with Temporin A analogs, which have been shown to exhibit antiproliferative properties [1,2]. Fourier-transform infrared spectroscopy and electrochemical impedance spectroscopy were applied to infer about specific molecular sites of interaction as well as for alterations of important physicicochemical parameters of the bilayer such as electrical capacitance and resistivity. The modified peptides were synthesized by replacing the amino acid at the seventh position in the amino acid sequence with the unnatural amino acid ornithine (DTOrn), citrulline (DTCit), 2,4-diaminobutyric acid (DTDab) or 2,3-diaminopropionic acid (DTDap). The acquired knowledge on the interaction of the studied peptides with lipid bilayers provides insight into the effects of Temporins on the molecular organization and dielectric properties of biomimetic membranes as well as the possible mechanism of their penetration in the cells.

References:

1. Dimitrova, D.; Nemska, V; Foteva, T; Iliev, I; Georgieva, N; Danalev, D, Synthesis and Biological Studies of New Temporin A Analogs Containing Unnatural Amino Acids in Position 7. Pharmaceutics, 16, 2024, 716
2. Danalev, D.; Borisova, D; Yaneva, S; Georgieva, M; Balacheva, A; Dzimbova, T; Iliev, I; Pajpanova, T; Zaharieva, Z; Givechev, I; Naydenova, E. Synthesis, in Vitro Biological Activity, Hydrolytic Stability and Docking of New Analogs of BIM-23052 Containing Halogenated Amino Acids. Amino Acids, 52, 2020, 1581–1592
3. Vitkova, V.; Antonova, K; Petkov, O; Stoyanova-Ivanova, A; Jaber, S; Ivanova, V; Naydenova, E; Danalev, D, Interaction of KLAKLAK-NH_2 and Analogs with Biomimetic Membrane Models. Pharmaceutics, 16, 2024, 340

Acknowledgements:

We acknowledge funding from the National Science Fund of Bulgaria (KP-06-N58/6/2021). Synthesis of the targeted peptides is financed by the project BG-RRP-2.004-0002, "BiOrgaMCT".

1.11. Effect of different fillers on hydrogels for application as tissue-substitute materials in Computed tomography

Veselina Georgieva[1,2*], Georgi Tankovski[1], Nikoleta Traikova[2], Ginka Exner[1]
[1]Faculty of physics and technology, Plovdiv University Paisii Hilendarski, 4000-Plovdiv, Bulgaria
[2]UMBAL„St. Georgi", Plovdiv, Bulgaria
* veselina_ngeorgieva@abv.bg

ALARA (as low as reasonable achievable) is a basic concept in diagnostic radiology, where phantom materials replace the real patients when optimizing the protocol parameters. The primary requirement in the design of such materials is to match the attenuation coefficients of the real tissues, at the large variation of the employed diagnostic photon energies from 30 kVp to 150 kVp [1]. Gelatine is derived from biological tissues. It is nontoxic, ecofriendly, easy to be processed and inexpensive polymer, which finds numerous biomedical applications [2]. Due to its properties, it is a good candidate for diagnostic radiology tissue replacing material.
In the present study, composite hydrogels of gelatin (bovine, food grade, 250/260 Bloom) were prepared. The variation in the X-ray attenuation was achieved by adding several low-budget fillers (eggshells, microbubbles, baking soda, psyllium husks, zeolite, collagen) with a concentration of 0.08 g/ml. Initially, the gelatin was left to swell in a distilled water (DW), followed by dissolving it at 63°C by magnetic stirrer mixing. Finally the filler and glycerol (Gly) were added. Each step was taking 10 min. Composites with DW only and 70:30 DW to Gly ratio were prepared. The composites were poured into small vessels, left to cool down to room temperature and stored at 4°C minimum for 24 hours prior to the experiments. The ability to mimic different body tissues was tested by means of Computed tomography, CT, (CT Somatom Definition AS64, Siemens, Germany) at varying tube voltage 70 – 120 kVp, and 30 mAs current. For each composite Hounsfield's units (HU) were obtained: $HU = 1000(\mu_{sample} - \mu_{water})/(\mu_{water} - \mu_{air})$, where μ_{sample}, μ_{water} , and μ_{air} are the linear X-ray attenuation coefficients of the sample, water and air, respectively, so that $HU_{water} = 0$ and $HU_{air} = -1000$ HU.
In addition, the mechanical performance of the composite was investigated. Cylindrical samples with diameter and height of 3 cm were used. Loading-unloading cycles were performed (Lloids universal instrument LS, Ametek), with a loading of 40 % and an unloading of 1 % with respect to the initial height. Young's modulus, the work of deformation and the force at the maximum deformation were derived.
Our results show that the HU units of the composites, depending on the type of the filler, cover the range of the soft tissues. The mechanical properties show that all composites represent almost elastic behaviour in the used load limits, with neglible plastic deformations.

References:

1. P. Homolka, A. Gahleitner, M. Prokop, R. Nowotny, Optimization of the composition of phantom materials for computed tomography, Phys. Med. Biol. 47 (2002) 2907–2916
2. J. Sarwan, J. Narang, A. Kumari, M. Devi, N. Uddin, S. Sharma, K J. C. Bosee. Chaper 11: Biomedical Applications of Collagen/Gelatin, in: Biopolymers for Biomedical Applications, Ed. Annu, Wiley (2024), pp. 287-313. https://doi.org/10.1002/9781119865452.ch11

1.12. Composite porous biopolymer multilayer films as potential controlled delivery systems for tolfenamic acid

A Grigorov*, A Viraneva, M Marudova, T Yovcheva
Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski",
24 Tzar Assen str., 4000 Plovdiv, Bulgaria
* – aleksandar.grigorov@uni-plovdiv.bg

The aim of this paper is to investigate the potential of composite porous biopolymer films, created by lyoplilization of solutions of two different biopolymers (Poly-D-lactic acid/PLA and Poly-ε-caprolactone/PEC) at different mass ratios (Pure PLA, 3-to-1, 1-to-1, 1-to-3 and Pure PEC), for controlled release of a chosen bioactive substance (tolfenamic acid). For this purpose, the prepared porous films were charged under corona discharge in a standard triode system (consisting of a charging electrode/needle supplied with 5 kV of a chosen polarity, a grid supplied with 1 kV with the same polarity as the charging electrode/needle and a grounded electrode) with either positive or negative charges. A set number of chitosan and casein multilayers were deposited on the surface of the charged porous films using a standard layer-by-layer (LbL) deposition technique, with the bioactive material being loaded in the casein layers. The drug release kinetics and the total amount of released drug in a standard dissolution medium were determined with the use of a spectrometer.

Acknowledgements:
The authors gratefully acknowledge the support of the project MUPD23-FTF-014/25.04.2023, Department of Scientific Research at the Plovdiv University.

1.13. Poly(Lactic Acid)-based active packages loaded with polyphenolic compounds

Sofia Milenkova*, Maria Marudova, Asya Viraneva
Faculty of Physics and Technology, University of Plovdiv "Paisii Hilendarski",
24 Tsar Asen Str.,4000 Plovdiv, Bulgaria
* – sophiamilenkowa@gmail.com

Extension of shelf life of food products is a long time desired and tested outcome of different innovative packaging techniques and materials. When it comes to novel materials, biopolymer-based ones stand out. Most of them possess proper mechanical and permeability properties, however not all of them are able to inhibit microorganism development and food spoilage. But when a biopolymer-based film is combined with active compounds, such as polyphenolic ones, an antioxidant effect along with antimicrobial one are observed. The aim of the present study is to evaluate the potential of poly(lactic acid) film incorporated with different polyphenols. The obtained polymer-polyphenol structures are characterized mechanically regarding their Young modulus, strain of break, stress at break and relaxation times. Their wettability and water vapor transmission rates are also examined. As they are intended to be applied as packaging materials, their water uptake is evaluated. Since the structures will be embedded with polyphenolic compounds, their morphology and antioxidant activity are obtained.

Acknowledgements:
This study is financed by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project DUECOS BG-RRP-2.004-0001-C01.

1.14. Photoswitchable molecular systems based on spironaphthoxazines for detection of metal ions

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, 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, Bucharest 060021, Romania
[4]A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, 119991, Russia
* stelamin@ic.bas.bg

The development of photoactive molecular systems and the further improvement of their functional activities is currently of great research interest closely related to environmental and human health protection, as well as industrial and biomedical technologies. This advanced and prospective scientific direction involves the molecular design and synthesis of novel photochromic systems, aiming to resolve a number of practical issues. In particular, the recognition of metal-ion moieties with photochromic molecules is one of the important research activities. Here we report novel molecular systems based on spiroindolinonaphthoxazines (SO) bearing various substituents in their naphthoxazine and indoline ring molecular moiety [1]. The molecular design of such systems aims their application for detection and quantification of heavy metal ions at a concentration less than 10^{-5} M in aqueous solutions. We studied the effects of both the molecular structure of the synthesized SO-based systems and their solvation in various solvents (organic and inorganic) on the optical absorption properties and the complexation of the SO molecules with some metal ions, including harmful heavy metal ions [1,2]. The optical probe of the generation of the open form of SO molecular systems having an absorption band in the visible region of the spectrum, around 630 nm, and the obtained photo-physical characteristics of SOs, highlight the photo-chemical mechanism of the photo-transformations of the involved molecular moieties in the synthesized SO compounds, which might enable new channels of their photo-excitation and novel photo-controllable applications.

References:

1. S. Minkovska, G. B Hadjichristov, A. Neacsu, V. Chihaia, Y. V. Fedorov, Photoswitchable Photochromic Chelating Spironaphthoxazines: Synthesis, Photophysical Properties, Quantum-Chemical Calculations, and Complexation Ability, ACS Omega 9(4), 2024, 4144−4161.
2. G. B. Hadjichristov, S. Minkovska, Spirooxazine-based optical sensing of metal ions using laser beam, Optik 299, 2024, 171546.

Acknowledgements:

The authors gratefully acknowledge the financial support of the project H2020-MSCA-RISE-2020 101007669: Chemistry of Platinum Group Metals CHemPGM.

1.15. Combining gravimetric with electrical transduction methods for the detection of volatile organic compounds (VOCs) by Langmuir-Blodgett films from metal-organic framework (MOF) MIL-101(Cr)

G.R. Ivanov[1], Y.G. Marinov[2], T.E. Vlakhov[2], A. Amova[1], G.B. Hadjichristov[2]
[1] University Laboratory "Nanoscience and Nanotechnology",
University of Architecture, Civil Engineering and Geodesy, blvd. H. 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) are organic chemical compounds found in various products that easily vaporize and reach in the environment under normal conditions. They adversely affect the environment and human health. Hence, portable in-field chemical sensors with the possibility for continuous monitoring of VOCs are in great demand. Such sensors should have a smooth thin sensing layer for fast detection. After this layer captures the studied VOC, the signal has to be transduced into a proper electrical signal for further manipulation and display. The best method for producing the sensing layer is the Langmuir and Blodgett (LB) method for layer-after-layer deposition. Previously, we measured VOCs with LB films from lipids and gravimetric detection using a 434 MHz two-port Surface Acoustic Wave (SAW) resonator with gold electrodes [1]. We used the interdigitated electrodes of the SAW resonators to add the Electrical Impedance Spectroscopy (EIS) detection method to the gravimetric detection, thus increasing the method's selectivity [2]. We extend these to using an LB monolayer from a highly porous and stable Metal Organic Framework (MOF) MIL-101(Cr) to detect VOCs. An LB monolayer from this MOF is approximately 4 times lighter than a lipid monolayer, which yields a high resonator Q-factor, a prerequisite for a sensor with an excellent Limit of Detection (LOD). Simultaneously this MOF layer absorbs significantly more mass from the tested VOCs – chloroform and acetone. Thus, a highly sensitive gravimetric sensor is available. This is complemented by a simple concentration dependence of the EIS measurements on the same device. So a highly sensitive chemical sensor for VOCs can be prepared with the suggested approach.

References:

3. Avramov, I.D.; Ivanov, G.R. Layer by Layer Optimization of Langmuir–Blodgett Films for Surface Acoustic Wave (SAW) Based Sensors for Volatile Organic Compounds (VOC) Detection. Coatings 2022, 12, 669.
4. Ivanov, G.R.; Venelinov, T.; Marinov, Y.G.; Hadjichristov, G.B.; Terfort, A.; David, M.; Florescu, M.; Karakuş, S. First Direct Gravimetric Detection of Perfluorooctane Sulfonic Acid (PFOS) Water Contaminants, Combination with Electrical Measurements on the Same Device - Proof of Concepts. Chemosensors, 2024, 12, 116.

Acknowledgements:

This work is supported by the Bulgarian National Science Foundation contract No. KP-06-N68/3/2023. T. Vlakhov gratefully acknowledges the programme "Young Scientists and Postdoctoral Researchers–2 "approved by DCM 206/07.04.2022 for the year 2024.

1.16. Ion-conducting nematic nanocomposites from nematic liquid crystals and single-walled carbon nanotubes: enhancement by nanodoping

Todor E. Vlakhov*, Yordan G. Marinov, Georgi B. Hadjichristov
Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee Blvd., BG-1784 Sofia, Bulgaria
* todor_vlakhov@issp.bas.bg

We have investigated flexible films (thickness about 50 μm) of room-temperature nematic nanocomposites produced from nematic liquid crystals pentylcyanobiphenyl (5CB), polymer polyethylene oxide (PEO) complexed with the salt sodium metaperiodate ($NaIO_4$) as an ion donor, and by inclusion of finely dispersed single-walled cabon nanotubes (SWCNTs). The composition of the films was: 5CB:PEO weight ratio 70:30 wt.%, $NaIO_4$ 5 wt.%, and the concentration of SWCNTs was varied from 0 to 0.25 wt.%. The diameter and the average length of SWCNTs were 1.5 nm and 7 μm, respectively. The modifications of the properties of PEO-5CB-$NaIO_4$-SWCNTs films due to inclusion of SWCNTs at various concentrations were inspected. The microstructure of the films was characterized by polarizing optical microscopy, XRD and SEM. The nanocomposites were studied by DSC, flexo-dielectro-optical spectroscopy and complex electrical impedance spectroscopy in the frequency range from 0.1 Hz to 1 MHz of the applied electric field, and in the tempearture range 20 – 40 °C. It was found an improvement in the morphology, as well as enhanced ion conductivity and dielectric permittivity of PEO-5CB-$NaIO_4$-SWCNTs sodium-ion-conductive films due to the doping with SWCNTs. Thus, such nematic nanocomposites have a potential for dielectric, ionic, soft-electronic and sensor applications.

Acknowledgements:
Work supported by the Ministry of Education and Science of Bulgaria (MESB), through the National Research Fund of Bulgaria (research project „Liquid crystal nanocomposites for applications in photonics, sensors and biomedicine", No. KP-06-N58/6/2021). T. Vlakhov gratefully acknowledges the financial support by the MESB under the National Research Programme „Young scientists and postdoctoral researchers–2" approved by DCM 206/07.04.2022, for the year 2024.

1.17. Studying the impact of physicochemical profile of metal-phenolic films on the sensitivity and selectivity of QCM-based alcohol sensors

Karekin D. Esmeryan*, Yuliyan Lazarov, Yulian Fedchenko, Ekaterina I. Radeva
Acoustoelectronics Laboratory, Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72, Tzarigradsko Chaussee Blvd., 1784 Sofia, Bulgaria
* – karekin_esmerian@abv.bg

A major challenge in the production of alcohol (for recreational or industrial applications) is the accurate monitoring of the methyl fraction, since any unintentional inhalation or ingestion of methanol, may inflict tissue damage, blindness, and even death.
Despite the widespread use of alcohol, some existing technological constraints contribute to the occurrence of incidents, mostly in the alcohol industry. So far, the authentication of spirits is mainly performed by gas or liquid chromatography, nuclear magnetic resonance or ionization spectrometry that require transportation of the samples to laboratory facilities. In this way, receiving timely information (point-of-use) about the quality of the alcohol is impeded, purely due to logistical reasons. Since the initial manifestations of alcohol intoxication are nonspecific, the lack of accurate data on the content of the drink can delay the diagnosis and the provision of specialized medical assistance, and in countries where the alcohol consumption is forbidden, the fear of punishment leads to the flourishing of "black market' and increase the risk of intoxication due to the lack of effective control measures.
One of the potential solutions to the aforementioned problems is called "quartz crystal microbalance" (QCM) - a miniature (size up to 25.4 mm) piezoelectric disk-shaped quartz resonator with two metal electrodes (usually made of gold) mounted on the lower and upper surfaces of the crystal. When the sensing electrode is coated with a metal-phenolic film, the QCM is capable of detecting methanol content up to seven times below the tolerable level in alcoholic beverages, while operating in conditions of equilibrium vapor pressure, ensuring a constant gas concentration and eliminating the use of flow meters, valves and connecting pipes, which is a prerequisite for implementing the measuring equipment in a stand-alone instrument for point-of-use analysis in night clubs and/or drinking establishments. To accomplish such an ambitious task, the effect of physicochemical profile of the metal-phenolic coating must be elucidated in order to design a sensor with optimal sensitivity and selectivity, even in the presence of interfering compounds.
In this proceeding, we reveal novel results concerning the alterations in gas sorption characteristics of our sensor device as a function of the morphology and chemistry of the metal-phenolic film. It is demonstrated that the latter is strongly dependent on the initial stoichiometry of composite $FeCl_3$-phenol solutions, resulting in predictably tunable sensor response towards methanol, ethanol, isopropanol and water vapor. These findings are the first step of designing a powerful and portable point-of-use alcohol sensor, appropriate both for industrial and private use (e.g., during home alcohol distillation).

Acknowledgements:
This research was performed thanks to the financial support of Bulgarian National Science Fund under grant No. KP-06-H77/3/28.11.2023.

1.18. Petroleum vapors sensor with polyvinyl trimethylsilane sensitive coating

Borislava Georgieva[1,2*], Alexander A. Grechnikov[3], Yuliyan Lazarov[1], Velichka Georgieva[1]

[1] Georgi Nadjakov Institute of Solid State Physics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria
[2] Institute of Electronics, Bulgarian Academy of Sciences, 72 Tsarigradsko Chaussee, 1784 Sofia, Bulgaria
[3] Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, 19 Kosygina Str., Moscow, 119991, Russia
* b.georgiewa@abv.bg

Petroleum hydrocarbon vapors are among the most ubiquitous atmospheric pollutants. Long-term exposure of animals and humans to hydrocarbon vapors can cause various diseases and disruption of vital organs. On-line monitoring of petroleum pollutions using portable gas sensors is an urgent task. Among various types of gas sensors, a particular place is occupied by mass-sensitive sensors based on quartz crystal microbalance (QCM), which exhibit such advantages as high mass-sensitivity, digital conversion of the measured mass value to the output signal, and a high conversion linearity. The analytical performance of such sensors strongly depends on the properties of a sensing coating deposited on the QCM electrodes.

In this work, we report on a QCM sensor coated with a polyvinyl trimethylsilane (PVTMS) film for the detection of petroleum vapors in air. The sensor's operation is based on the change in the QCM resonance frequency, which occurs upon the sorption of hydrocarbon molecules by the PVTMS coating. PVTMS with a molecular mass of 8.5×10^5 Da was dissolved in toluene, the solution was applied on both sides of the QCM by droplet deposition and dried at 100°C. We used 16-MHz QCMs fabricated on AT-cut quartz plates. The sensitivity to petroleum vapors of the PVTMS films was measured on a laboratory setup. Nitrogen or air were used as carrier gases. The petroleum hydrocarbon vapors concentrations in the test chamber were created by diluting saturated vapors with a carrier gas. The sensing properties of the PVTMS films were estimated by measuring the frequency-time characteristics of the QCM at different petroleum vapors concentration.

The influence of the polymer coating mass on the sensor's performance characteristics was studied. The optimal mass of PVTMS film was found, at which the signal-to-noise ratio was maximum. Based on the frequency-time characteristics measured, the adsorption and desorption processes kinetics were studied and the sensor's response and recovery times were estimated. It was demonstrated that the sorption of petroleum hydrocarbons on PVTMS is fully reversible. The dependences of the sensor's response on the concentration showed a good linearity in the petroleum vapors pressure range 10^{-3}-10^{-1} of the saturated vapor pressure. It was found that the sensor exhibits a relatively high selectivity in the presence of water vapor in the relative humidity range of 0-50%.

The results obtained demonstrate that the developed QCM-sensor with polyvinyl trimethylsilane sensitive coating could be successfully used to detect petroleum vapors in air.

1.19. Investigation of partial Al^{3+} substitution on the properties of Y-type $Ba_{0.5}Sr_{1.5}MgNiFe_{12-x}Al_xO_{22}$ hexaferrites

B. Georgieva[1*], S. Kolev[1,2], K. Krezhov[1], Ch. Ghelev[1], D. Kovacheva[3], P. Tzvetkov[3], L.-M. Tran[4], M. Babij[4], 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] – Institute of Low Temperature and Structure Research, Polish Academy of Sciences,
ul. Okólna 2, 50-422 Wroclaw, Poland

* – b.georgiewa@abv.bg

We report the effect of partial Al^{3+} substitution of the magnetic (Fe^{3+}) cation on the magnetic properties in $Ba_{0.5}Sr_{1.5}Me_2Fe_{12}O_{22}$. The Me^{2+} position in the Y-type hexaferrite crystal structure is occupied by non-magnetic (Mg^{2+}) and magnetic (Ni^{2+}) cations. The Y-type hexaferrite powders were synthesized by citric acid sol-gel auto-combustion followed by thermal annealing at 1180 °C in air to obtain $Ba_{0.5}Sr_{1.5}MgNiFe_{12-x}Al_xO_{22}$ (x = 0.08, 1) materials. The X-ray diffraction (XRD) patterns confirmed the phase formation of the Y-type hexaferrite structure. To determine the magnetic phase transitions, the ZFC/FC magnetizations were measured in a magnetic field of 50 Oe, 100 Oe and 500 Oe between 4.2 K and 300 K and complemented with hysteresis loops recorded at the end temperatures. To specify the detected magnetic phase transitions, the *ac*-magnetization was measured in an alternating magnetic field with an amplitude of 10 Oe and a frequency of 1000 Hz. A magnetic phase transition from a spiral magnetic order to a conical spin order was observed at lower temperatures. In addition, a few metamagnetic transitions in the 4.2 – 300 K temperature range were detected for x = 0.08.

Acknowledgements:
Borislava Georgieva was supported by the Bulgarian Ministry of Education and Science under the National Research Programme "Young scientists and postdoctoral students-2" approved by DCM 206/07.04.2022. This work was supported by the Bulgarian National Science Fund under contract KP-06-N48/5, 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.

1.20. Inertial sensor to determine the ballistic resistance state and traumatic effect of multilayer lightweight armor made of (UHMWPE), polyvinyl botyral and nanoparticles SiC

Pavlina Nikolova*, Petya Nedylkova, Alexander Kolev
[1] – Defense Institute, Sofia, Bulgaria
* – p.nikolova@di.mod.bg, p.gencheva@di.mod.bg, a.kolev@di.mod.bg

The concept of network-centric warfare arose in response to the latest technological advances in the information age [1]. In the present material, the authors propose a connection with the addition of an additional information channel for reporting the individual condition of the soldiers on the battlefield covered by the system. After extensive research and analysis, as well as the scientific-applied interest of the project, the research team focused on the methods of obtaining information about the state of the individual means of ballistic protection (the ballistic armor of the combat suit of the soldier and the guard).
High strength polymer fabrics and materials are widely used for lightweight protective systems due to their mechanical properties and impact resistance [2,3]. High-quality polymer fibers such as aramid (aromatic polyamide), ultra-high molecular weight polyethylene (UHMWPE) and Zylon poly (p-phenylene - 2, 6 - benzobisoxazole), etc. have remarkable properties such as lightness, flexibility, high Young's modulus and good impact resistance, which makes them attractive for the production of advanced protective means [4-6].
This work presents the ballistic performance and trauma effects of multilayer Dyneema® UHMWPE impregnated with polyvinyl butyral and a mixture of micro- and nanoparticle SiC [6, 7, 8].

References:

1. Cebrowski A., *Military Technology*, iss. 5 2003, pp. 16-22
2. Deju Z., Aditya V., Barzin M., Subramaniam, *Compos. B Eng* 2014; 56: 254-262.
3. Yang CC, Ngo T., Tran P. *Mater. Des.* 2015; 85: 282-295. doi: 10.1016/j.matdes.2015.07.014. [
4. Liu J., Long Y., Ji C., Liu Q., Zhong M., Zhou Y. *Internal J. Impact Eng.* 2018; 112: 52-65. doi: 10.1016/j.ijimpeng.2017.10.001.
5. Chang CP, Shih CH, You JL, Youh MJ, Liu YM, Ger MD. *Polymers (Basel)*. 2021 Sep 13;13(18):3080. doi: 10.3390/polym13183080. PMID: 34577980; PMCID: PMC8467087.
6. P. Gencheva, K. Kostova, D. Kirkov, S. Aleksandrov, *XX National Textile Conference 2018 "Traditions and Innovations in Textiles and Clothing"*, October 2-4, Sofia, Bulgaria, Textile & Garment Journal, ISSN 1310-912X, (2018), p. 268-272.
7. H. Iv. Hristov, H. P. Hristov, K. Kostova, P. Gencheva, Nanopowder in aramid fabrics for improved ballistic protection, nato unclassified+aus+swe+fin, sto-rws-avt-267, paper nbr 13 – 5, 2018 Mr.
8. H. Iv. Hristov, H. P. Hristov, A. Kolev, P. Gencheva, K. Kostova, Y. Karakaneva, I. Gabrovski, S. Alexandrov, Research on application of light materials for ballistic protection, sto – tr-bgr-gbr-avt-15-p1, isbn 978 -92-837-2288-5, 2020

Acknowledgements:

The National Scientific Program - Security and Defense is financed by the Ministry of Education and Science of the Republic of Bulgaria in implementation of the National Strategy for the Development of Scientific Research 2017-2030 and was adopted by Decision of the Council of Ministers No. 731 of October 21, 2021.

ABSTRACTS OF SECOND POSTER SESSION

2.1. Titanium Dioxide Thin Films Prepared on Different Substrates by Sol–Gel Process: Optical and Morphological Properties

T. Ivanova[1], A. Harizanova[1], N. Petkov[2], V. Dulev[1], A. Benkovski[1*], M. Ganchev[1]

[1] – Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences, Tzarigradsko chaussee 72, 1784 Sofia, Bulgaria

[2] – Physical Sciences, Munster Technological University, Rosa Avenue, Bishopstown, Cork, Ireland and Tyndall National Institute, Lee Maltings, T12 R5CP Cork, Ireland

* – kappu96000@gmail.com

TiO_2 is wideband semiconductor with optical band gap of 3.0–3.2 eV, absorbs UV light, with high refractive index (> 2), high transparency almost 90% in the visible spectral range. This metal oxide is of current research as functional material, due to the interesting properties, stability and low cost. TiO_2 is the n-type semiconductor and serves as the UV light absorber [1]. One interesting application is transparent solar cells. Developing heterostructure with TiO_2 for photovoltaic cell has gained huge research interest. Due to the stable formation of electric field at the interface, photo-generated carriers can be collected more efficiently, resulting in device performance improvement [1].

In this study, sol-gel TiO_2 thin films formed by spin coating on Si, glass and ITO substrates were obtained and characterized using Field emission scanning electron microscopy (FESEM), FTIR spectroscopy and UV-VIS spectroscopy. The impact of the film thickness (different number of layers), annealing temperatures (300, 400 and 500°C) and the type of substrates on the morphology, optical transmittance and vibrational properties were investigated. The work function (WF) of the samples was also determined with a Scanning Kelvin Probe (SKP5050). TiO_2 films on glass substrates revealed a decrease of the film transparency with increasing the film thickness and after annealing at 400 and 500°C. FESEM images manifested that the films began to crack at these technological conditions. Meanwhile, TiO_2 films obtained on ITO substrates exhibited very high transmittance in the visible spectral range up to 85%, despite the number of layers and the thermal treatmeants. FESEM study showed very uniform, smooth surface with small grained structure.

References:

1. T. T. Nguyen, M. Patel, S. Kim, R. A. Mir, J. Yi, V. Dao, J. Kim, Transparent photovoltaic cells and self-powered photodetectors by TiO_2/NiO heterojunction, Journal of Power Sources, 481, 2021, 228865. https://doi.org/10.1016/j.jpowsour.2020.228865.

2. M. Patel, S. Ghosh, J. Park, J. Song, D.-W. Kim, J. Kim, A study of the optical properties of wide bandgap oxides for a transparent photovoltaics platform, Journal of Materials Chemistry C, 11, 2023, 14559-14570. https://doi.org/10.1039/D3TC03122E

Acknowledgements:

The authors kindly acknowledge financial support from the Bulgarian National Science Fund (BNSF) under the project Development and Investigation of metal oxide heterostructures for transparent solar cells, KP-06-N78/7, (5 December 2023).

2.2. Development and Research of a Graded AlTiN Hard Coating

Ekaterina Zlatareva[1*], Vasiliy Chitanov[1], Lilyana Kolaklieva[1], Stefan Kolchev[1], Tetyana Cholakova[1], Roumen Kakanakov[1], Chavdar Pashinski[1,2]

[1] – Central Laboratory of Applied Physics, Bulgarian Academy of Sciences,
61 Sankt Peterburg Blvd., 61, 4000 Plovdiv, Bulgaria
[2] – Department of Mechanics, Technical University-Sofia, Bt. Plovdiv,
25 Tsanko Dyustabanov St., 4000 Plovdiv, Bulgaria
* – ekpepe31@gmail.com

The present study is a part of a larger project of developing multicomponent hard, wear-resistant coatings for industrial applications. A graded AlTiN hard coating with very good mechanical properties, adhesion and wear resistance was obtained as a result of the selected technological regime.

The coating was deposited via Unbalanced Magnetron Sputtering in Closed Magnetic Field (UDP850/4, Teer Coatings) on a HSS substrate. Its thickness was determined by ball-cratering method (Calotet CAT2, Anton Paar). Mechanical properties and adhesion were investigated by nanoindentation and scratch testing (Compact Platform, Anton Paar). The resistance to dry wear was examined by ball-on-disk test using a tribometer (UMT Tribolab, Bruker). Morphology and elemental composition were investigated using a SEM (SU5000, Hitachi) equipped with EDS (Thermo Scientific, USA).

Ti, TiN, and AlTiN layers were carefully designed to obtain a graded coating with balanced characteristics. The TiN layer was separately deposited for comparative testing. Nanohardness of 25.6 GPa and modulus of elasticity of 322 GPa were determined. Any cracks and critical loads were not detected during the scratch test up to 30 N. Coefficient of friction of 0.12 was measured against the diamond indenter. After adding of Al, the nanohardness increased to 28.1 GPa while maintaining the value of the coefficient of friction and the adhesion. The coefficient of friction against corundum counter body was 0.64. The morphological examination showed dense structure without significant defects. The elemental composition of the main layer was: Al – 26.0 at. %, Ti – 32.1 at. %, and N – 42.4 at. %.

The coating considered could be used as a basis for the development of multicomponent coatings, including application as a component of multilayer coatings.

Acknowledgements:
Research equipment of Distributed Research Infrastructure INFRAMAT, part of the Bulgarian National Roadmap for Research Infrastructures, supported by the Bulgarian Ministry of Education and Science was used in this investigation.

2.3. Chemical Bath Deposition of Tin Sulphide Thin Films

Vladimir Dulev[1*], Alexander Benkovsky[1], Daniela Lilova[2], Ekaterina Radeva[1], Stanka Spasova[1], Rumen Stoikov[1], Vassil Palankovski[1], Maxim Ganchev[1]
[1] Central Laboratory of Solar Energy and New Energy Sources – Bulgarian Academy of Sciences
[2] University of Chemical Technology and Metallurgy
* vladogotin64@gmail.com

Tin monosulphide (SnS) layers are successfully deposited on glass substrates covered by TiO_2 or ITO using a simple and economic chemical bath deposition method. The effect of annealing on the structure, surface morphology and optical properties are studied to understand the possible ways for achieving an appropriate material for photovoltaic application. Differential scanning calorimetry measurements of residual powder material reveals a region of well-defined heat absorption (endothermic process) near 160 °C and a weak exothermal reaction at 340 °C upon annealing up to 450 °C. X-ray diffractometry shows the presence of monophase material of orthorhombic SnS. Optical investigations of the deposited thin films show a band gap near 1.9 eV for allowed direct transitions for samples annealed at 100 °C, which varies slightly as the temperature of annealing increases up to 260 °C. This result is attributed to quantum confinement in the nanocrystalline grains comprising the film. Raman spectra for the annealed thin films indicates presence of SnS_2 for the samples annealed at temperatures above 200 °C while only tin monosulphide could be identified for lower temperatures.
The Work Function measurements present levels near 4,83 eV and deviations for 1 mm^2 surface scans are less than 1%.

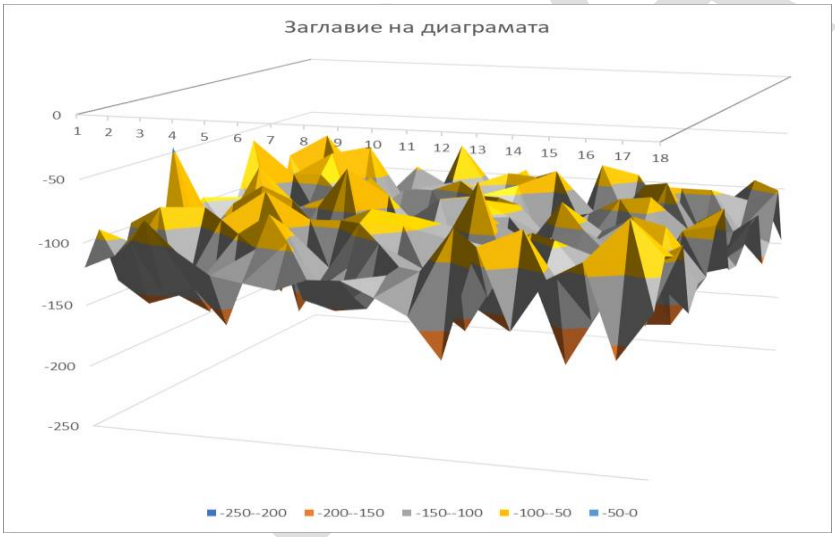

Figure 1: Work Function scan measurement of SnS thin films deposited by chemical solution.

Acknowledgements:
This work is supported by COST Action 21148 ReNewPV by EC funding, Bulgarian National Science Fund under contracts KP06 COST/16/14.12.2023 and KP06-H77/12.14.2023 and bilateral collaboration contracts between the Bulgarian Academy of Sciences the Estonian Academy of Sciences, and the Romanian National Academy. The investigations were performed on the Research infrastructure of Energy Storage and Hydrogen Energetics, funded by the Bulgarian Ministry of Science and Education.

2.4. Study of the nonlinear optical properties of glasses doped with gold nanoparticles using the z-scan method

Krum Shumanov[1], Georgi Yankov[1*], Stefan Karatodorov[1], Ekaterina Iordanova[1], Victoria Atanassova[1], Nikolay Nedyalkov[2], Lubomir Aleksandrov[3]
[1] – Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee, Blvd., 1784 Sofia, Bulgaria
[2] – Institute of Electronics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee, Blvd., 1784 Sofia, Bulgaria
[3] – Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences,
Akad. G. Bonchev Str, bl. 11, 1113 Sofia, Bulgaria
* – gjankov@issp.bas.bg

The study uses the Z-scan method to analyze the nonlinear optical properties of glasses doped with gold nanoparticles. Fused quartz and standard glass are used to calibrate the method, ensuring reliable measurements of glasses with and without nanoparticles. The study aims to determine the impact of gold nanoparticles on the nonlinear refractive index and the multiphoton absorption coefficient. Results show a significant increase in nonlinearity in glasses doped with nanoparticles compared to undoped glasses and fused quartz. Polycrystalline structures have been observed and confirmed through second harmonic generation, highlighting the nonlinear properties of the materials. Thermal treatment of the samples leads to significant differences in multiphoton absorption between annealed and unannealed glasses. Additionally, glasses doped with gold nanoparticles regain their original color when irradiated with wavelengths close to the resonance frequencies of the nanoparticles, making them promising for applications in optical memory. These findings emphasize the importance of the materials used to develop new photonic and optoelectronic technologies, showcasing their potential for innovation in optics and nanotechnology.

Acknowledgements:
The present work is funded by the Bulgarian National Science Fund by Grant No. КП-06-Н58/7 "Plasma dynamics and formation induced by femtosecond infrared laser pulses in transparent media".

2.5. Low temperature investigation of nanosized $BaFe_{12}O_{19}$ powders

Ch. Ghelev[1*], P. Peneva[1], K. Krezhov[1], S. Kolev[1,2], B. Vertruyen[4], F. Boschini[4], R. Closset[4], A. Mahmoud[4], L.-M. Tran[3], M. Babij[3], A. Zaleski[3], M. Ptak[3], 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 Low Temperature and Structure Research,
Polish Academy of Sciences, ul. Okólna 2, 50-422 Wroclaw, Poland
[4] –Greenmat, Chemistry Department, University of Liege, 11 Allée du 6 Août, 4000 Liège, Belgium
* – chavdarghelev@yahoo.com

Modern technologies require miniaturization and transfer to nanoscale technologies. In general, the nanoscale effect on the crystalline and magnetic structure in polycrystalline transition metal oxide compounds is of great importance. M-type hexaferrites have attracted strong attention for many years due to their exceptional magnetic properties favorable for various specific applications, including permanent magnets, high-density recording media, spintronics, multiferroicity and microwave absorption devices, among many other uses. We present our studies on structural and low-temperature properties of nanosized barium hexaferrite powders, namely, nanosized $BaFe_{12}O_{19}$ powder synthesized by an ultrasonic-assisted co-precipitation. The average particle size of the $BaFe_{12}O_{19}$ powder was in the range from 25 nm to 90 nm depending on the synthesis conditions.The particles had irregular shapes ranging from spherical to plate-hexagonal grains. The *ac*-magnetization was measured in an *ac*-magnetic field with an amplitude of 10 Oe and a frequency of 1 kHz to detect magnetic phase transitions in the temperature range 4.2 – 300 K. An anomaly of the magnetic behavior at the low temperature around 150 K was observed for the $BaFe_{12}O_{19}$ powder consisting of particles with a sizes of about 25 nm. To understand better this phenomenon, we measured the temperature-dependent (80 – 300 K) evolution of Raman scattering for the sample with the smallest particles using excitation at 830 nm. The Raman spectroscopy confirmed this anomaly, which can be most likely attributed to spin-phonon coupling. These spin-phonon interactions at the low temperature of 150 K for the nanocrystalline $BaFe_{12}O_{19}$ powder is reported for the first time as far as we know.

Acknowledgements:
The work was supported by the Bulgarian National Science Fund under contract KP-06-N48/5, by a joint research project between the Bulgarian Academy of Sciences and the Institute of Low Temperature and Structure Research, Polish Academy of Sciences and by a joint research project between the Bulgarian Academy of Sciences and WBI, Belgium.

2.6. Optical materials for the electronic industry from fluorite

Margarita Metodieva Goranova[1], Katerina Lazarova[2]
[1] – Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko chaussee, Sofia 1784, Bulgaria
[2] – Institute of Optical Materials and Technologies "Acad. Yordan Malinovski",
109 Akad.G.Bonchev, Sofia,1113 , Bulgaria
* – lozanova_1970@abv.bg

For the production of optical elements for the electronic industry, raw materials from minerals with certain constants in an appropriate percentage ratio are also used. Natural fluorite is used in optics - for the production of lenses for telescope and microscope objectives due to its low dispersion.
Laboratory measurements were carried out on 25 mm diameter and 2.5 mm thick plates of fluorite polished on both parallel sides. UV-VIS-NIR spectrophotometer Perkin Elmer Lambda 1050 with integrating sphere - spectral range: 175 nm – 3300 nm and FT-IR spectrophotometer Vertex 70 (Bruker) - spectral range: 10000 cm^{-1} - 30 cm^{-1} (1-300 μm) were used. The data obtained from the measurements are presented in the form of reflection and transmission spectra.
In this study, diffuse reflectance of fluorite was measured with the integrating sphere of a Lambda 1050 spectrophotometer, which collected the reflected energy from the sample surface.
The spectral transmittance of the fluorite sample in the optical range of the spectrum was also measured. The examined sample was also measured on a Fourier-transform infrared FT-IR spectrophotometer Vertex 70 (Bruker).
Interpretation of the obtained spectra was performed. Optical constants of the samples were determined. The surface roughness of the samples was investigated with a Zeta-20 3D optical profilometer. The contact angle with a drop of water was measured with a tensiometer.
When examining fluorite from the "Mihalkovo", "Slavyanka" and "Chiprovtsi" deposits, a similar mineral composition was found, with fluorite ranging from 40% to 70% with the participation of calcium carbonate, silicon dioxide and others. That is why the spectra obtained from the data from the measurements in ISSP "Acad. Georgi Nadjakov", when compared with a reference spectrum from a reference database, inclusions of these main rock-forming minerals are observed.

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

2.7. Optical spectra in SWIR based on data from Icelandic spar measurements in Bulgaria

Margarita Metodieva Goranova
Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko chaussee, Sofia 1784, Bulgaria
* – lozanova_1970@abv.bg

Iceland spar optical material are selected according to their optical properties, which are required for optoelectronic applications.
Special methods are required for the processing of the mineral, due to the complex internal structure of the crystal and the fact that crystals of perfect and large sizes are rarely found in nature.
For the study of optical spectra of Icelandic spar was used short-wave infrared radiation because it passes through material at great depth and has been found to give optimal results when analyzing carbonate minerals. This gives a basis in this range to expect more accurate results from the interpretation of the spectra.
A sample of Icelandic spar was measured at the Institute of Solid State Physics "Acad. Georgi Nadjakov", Laboratory "Optics and Spectroscopy" with FT-IR spectrometer Vertex 70 (Bruker) in the SWIR (Short Wave InfraRed) range of spectral transmission and reflectance with a Perkin Elmer Lambda 1050 UV-VIS-NIR spectrophotometer.
The results are presented in graphic form in the limits of the spectral transmittance of Icelandic spar from 1 μm to 6 μm. They are compared to a reference spectrum with a spectral transmittance that has been determined for the 2.4 mm thick Icelandic spar optical material in infrared technology.
The obtained form of the spectrum from the data of these measurements in ISPP "Acad. Georgi Nadjakov" with an FT-IR spectrometer Vertex 70 (Bruker) in the SWIR (Short Wave InfraRed) range of spectral transmission, is identical to that of Icelandic spar in the spectral transmittance range from 1 μm to 3 μm, where transmittance matching is also observed.
The purpose of this study is to interpret SWIR (Short Wave Infrared) spectra of Icelandic spar, which are complementary to those available up to this point and are useful for rapid comparative interpretation with analogous spectra.

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

2.8. Spin-induced strongly correlated magnetodielectricity, magnetostriction effect and spin-phonon coupling in helical magnet $Fe_3(PO_4)O_3$

Arkadeb Pal[1,2]*, T. W. Yen[1], V. G. Sathe[3], Y. C. Chuang[4], and H. D. Yang[1]
[1] – Department of Physics, National Sun Yat-sen University, Kaohsiung 804, Taiwan, R. O. C.
[2] – Zernike Institute for Advanced Materials, University of Groningen,9700 AB, Netherlands
[3] – UGC-DAE Consortium for Scientific Research, Khandwa Road, Indore-452001, India
[4] – National Synchrotron Radiation Research Center, Hsinchu, 30076, Taiwan, R. O. C.
* – arkadeb.pal@rug.nl

The demand for advanced spintronics devices has spurred research into multifunctional materials responsive to various external stimuli. These materials exhibit a range of properties resulting from the coupling of microscopic order parameters like spin, orbital, lattice, dipole, and phonon. Focus has been on discovering new multiferroic and magnetodielectric materials for various real-world applications. However, such materials are scarce due to the antagonistic origins of their magnetic and electric properties, often limited by low critical temperatures (<40 K). Tailoring materials with higher critical temperatures remains a challenge, with only a few compounds like CuO (T_c ~ 230 K) and certain hexaferrites displaying coupled properties at considerably high temperatures. On the other hand, Spin-phonon coupling (SPC) is a captivating phenomenon in strongly correlated systems, where magnetic and structural phase transformations are reflected in phonon spectra. SPC serves as a gauge for monitoring various exotic properties such as magnetoelectric coupling, spin Seebeck effect, magnetostriction effect, phonon Hall effect, spin-Peierls transition, and thermal Hall effect in multiferroics. In this report, we demonstrate a spectrum of simultaneously occurring and highly-entangled intriguing phenomena induced by helical spin ordering in a polar and spin-frustrated magnetic system $Fe_3(PO_4)O_3$. Such phenomena include magnetodielectric coupling with a weak ferroelectric ordering, clear magnetostriction effect manifested as a dramatic down-turn in the thermal variation of lattice parameters, and strong spin-phonon coupling (which displays a unique anomalous hardening and softening of various phonon modes) at temperatures as high as T_N = 163 K. The observed dielectric peak is seemingly associated to a structural distortion via the strong magnetostriction effect.

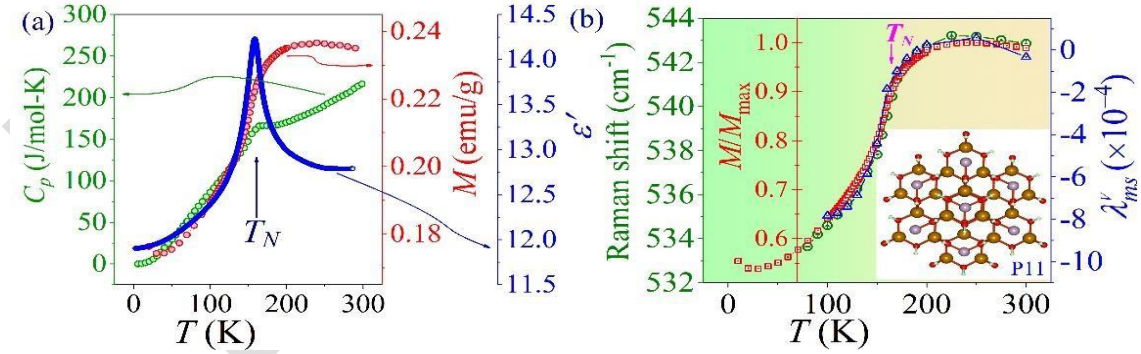

Figure 1: (a): Specific heat (C_p), Magnetization (M), and dielectric constant (Ɛ′), variations as a function of temperature. (b): Raman shift, magnetization, and volume magnetostriction coefficient variations as a function of temperature. All these curves unambiguously suggest the highly entangled behavior of spin, lattice, phonon, and dipolar degrees of freedom in this system.

References:

1. Pal et. al., Phys. Rev. B **106**, 094404 (2022)

Acknowledgements:

A.P thank the European Commission MSCA Postdoctoral Fellowship (101110742).

2.9. Metallic Glass from the Point of View of the Molecular Entropy Theory

Hristo Solunov *
Plovdiv University "Paisii Hilendarski", 24 Tsar Asen St., Plovdiv, Bulgaria
* – solunov@uni-plovdiv.bg

The molecular entropy theory describes the glass transition as a cooperative molecular process. Two main parameters in the theory are the size of the cooperative cluster and the average potential barriers for the rearrangement of the cluster. The equation for measuring the temperature dependence of both these parameters has been found. The product of these two parameters forms the temperature dependence of the activation energy governing relaxation times, viscosity, and diffusion in glass formation. We found that for all glass-forming substances, including metallic glass, the glass-transition temperature is strictly proportional to the activation energy of the cooperative cluster at this temperature. Furthermore, we found that the size of the cooperative cluster at the glass-transition temperature is the molecular basis of the dynamic fragility (steepness) index. The dynamic fragility index reflects only cooperativity, not the second important quantity for glass formation, namely the height of the potential barriers for cooperative rearrangement. The potential barriers of metallic glasses are measured and compared with the same quantity in low-molecular-weight glasses.

2.10. Preparation and spectroscopic characterization of nano-sized glass-ceramics obtained from a sodium silicate glass with high Fe and Mn concentrations

Ivalina Avramova[1*], Ruzha Harizanova[2], Irena Mihailova[2], Zara Cherkezova-Zheleva[3], Daniela Paneva[3], Georgi Avdeev[4], Christian Rüssel[5]

[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 Catalysis, Bulgarian Academy of Sciences, Akad. G. Bonchev Str., bl. 11, Sofia 1113, Bulgaria

[4] – Institute of Physical Chemistry, Bulgarian Academy of Sciences, Akad. G. Bonchev Str., bl. 11, Sofia 1113, Bulgaria

[5] – Otto Schott Institute of Materials Research, University of Jena, Fraunhoferstr. 6, 07743 Jena, Germany

* – iva@svr.igic.bas.bg

The possibility of applying glass-ceramics with ferrite nano-crystals to electronics and medicine determinedthe interest in the synthesis of glasses and nano glass-ceramics in the system $Na_2O/MnO/SiO_2/Fe_2O_3/FeO$. Glasses with different MnO and Fe_2O_3-concentrations in the range from 5 to 15 mol% were prepared. For a composition with an MnO to Fe_2O_3ratio close to 0.5, the glassy samples were heat treated at temperatures from 510 to 700°C for times from 10 min to 100 h. The resulting phases and microstructures were characterized by X-ray diffraction with $Cu_{K\alpha}$-radiation as well as by electron microscopy. A solid solution with spinel structure and a chemical compositionbetween $MnFe_2O_4$ (jacobsite) and Fe_3O_4 (magnetite) crystallized at comparatively lower temperatures and shorter crystallization times, while aegirine, $NaFe(SiO_3)_2$, was additionally formed at higher temperatures and applying longer crystallization times. Here, the average crystallitesize of the jacobsite-based phase varied between 4 to 10 nm as determined by X-ray diffraction. The average particle sizes determined from the electron microscopy micro-graphs revealed that for crystallization times longer than 2h, the size of the formed nano-crystals slightly changed and they had sizes from 10 to 40 nm. The obtained glass and glass-ceramics were further characterized by X-ray photoelectron spectroscopy. It is suggested that Mn was mainly present as Mn^{2+}, while Fe occured as both Fe^{2+} and Fe^{3+}.Mössbauer spectroscopy per-formed on the initial glass and the glass-ceramics at room and liquid nitrogen temperatures also confirmed the occurrence of Fe^{2+}(in octahedral coordination) and Fe^{3+}(both in octahedral and tetrahedral coordination).

Acknowledgements:
The authors are grateful to the Bulgarian National Science Fund, project KP-06-N48/4 for the financial support.

2.11. XPS study of ALD HfO_2/Al_2O_3 stacks on Si

A. Paskaleva[1*], D Spassov[1], I. Avramova[2]
[1] – Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko chausee, Sofia 1784, Bulgaria
[2] – Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences,
Acad. Georgi Bonchev Str., Bl. 11, Sofia 1113, Bulgaria
* – paskaleva@issp.bas.bg

The HfO_2/Al_2O_3 nanolaminates as well as Al doped HfO_2 layers have recently focused the attention of the microelectronics community as promising materials for application in a number of emerging memories. Previously, we have demonstrated feasibility of creating a flash memory device based on atomic layer deposited HfO_2/Al_2O_3 nanolaminates and Al-doped HfO_2 layers [1]. In this work we report results of X-ray photoelectron spectroscopy (XPS) study of two types of HfO_2 based stacks – nanolaminated HfO_2/Al_2O_3 and Al- doped HfO_2. The stacks are obtained in a frame of single low temperature ALD process. The XPS lines of Hf 4f, O 1s, Al 2p, C 1s, Si 2p in case of as-deposited stacks and oxygen annealed ones (800 °C for 1 min) were traced. The results are compared with data obtained from thick (20nm) HfO_2 and Al_2O_3 layers deposited at the same conditions as the HfO_2/Al_2O_3 stacks. The Hf 4f lines from all samples are deconvoluted into two doublet lines: high binding energy one ($4f_{7/2}$ ~ 17.5 eV; $4f_{5/2}$ ~ 19.2 eV) and low binding energy (BE) one ($4f_{7/2}$ ~ 16.9 eV; $4f_{5/2}$ ~ 18.6 eV). The low BE component dominates Hf 4f spectra of the as-grown nanolaminated and doped samples, whereas its presence in single HfO_2 layer is minimal. The annealing increases the intensity of the high BE part and slightly decreases the intensity of low BE one. The O1s spectra is also composed by 2 peaks: main at 530. 2 ± 0.2 eV attributed to O-metal bonds and 532.0± 0.3 eV line attributed to O-O bonds of interstitial O atoms and is representative of oxygen vacancies. The Al 2p peak of the HfO_2/Al_2O_3 layers is at ~ 74.2 eV, which is lower than expected for Al-O bonds in Al_2O_3. Therefore, it is interpreted as an indication of presence of Hf-Al-O bonds.

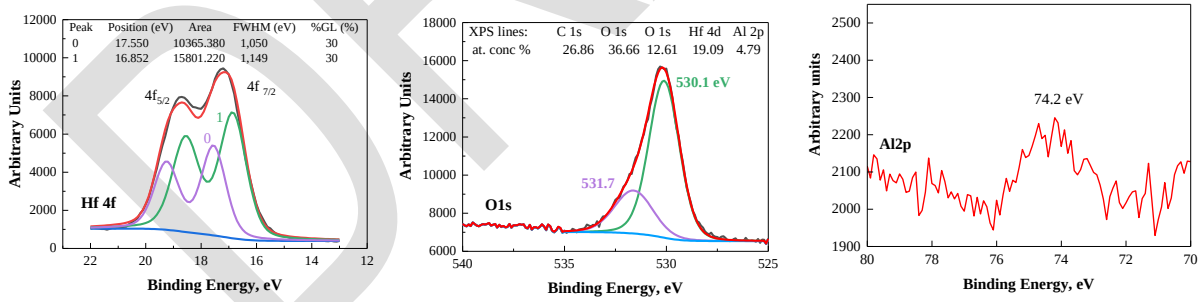

Figure 1: Hf 4f, O 1s and Al 2p XPS lines of as-grown HfO_2/Al_2O_3 nanolaminate.

References:

1. D. Spassov, A. Paskaleva, Challenges to Optimize Charge Trapping Non-Volatile Flash Memory Cells: A Case Study of HfO_2/Al_2O_3 Nanolaminated Stacks. Nanomaterials, 13, 2023, 2456.

Acknowledgements:

The work is supported by Bulgarian National Science Fund under project KP-06-N37/32

2.12. Evaluation of write/erase operations performance in HfO_2/Al_2O_3 based flash memory stacks

D. Spassov, A. Paskaleva, T. Stanchev*, Tz. Ivanov
Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko chausee, Sofia 1784, Bulgaria
* – stanchev@issp.bas.bg

The evolution of non-volatile flash memories working on charge trapping effect demands gradual shift towards replacement of Si_3N_4 with high-*k* trapping dielectrics. Atomic Layer Deposition (ALD) fabricated HfO_2-Al_2O_3 dielectric system seems to be quite suitable as a possible substitute since both HfO_2 and Al_2O_3 are well established in the advanced microelectronics. Apart from the memory windows, another important characteristic from application point of view is the speed with which write and erase operations proceed. Here we report the obtained results from the assessment of the write/erase performance of two types of HfO_2-Al_2O_3 charge trapping stacks (nanolaminated and doped) in dependence on memory capacitor configuration, post-deposition annealing in O_2 and applied write/erase voltage pulse amplitude. It is demonstrated that write operation in capacitive memory cell critically depends on the density of inversion charge carriers. Therefore, write operation was carried out under illumination. The annealing in O_2 at 800°C is found to deteriorate the write process, increasing the pulse duration for beginning of efficient electron trapping, especially at low write voltages.

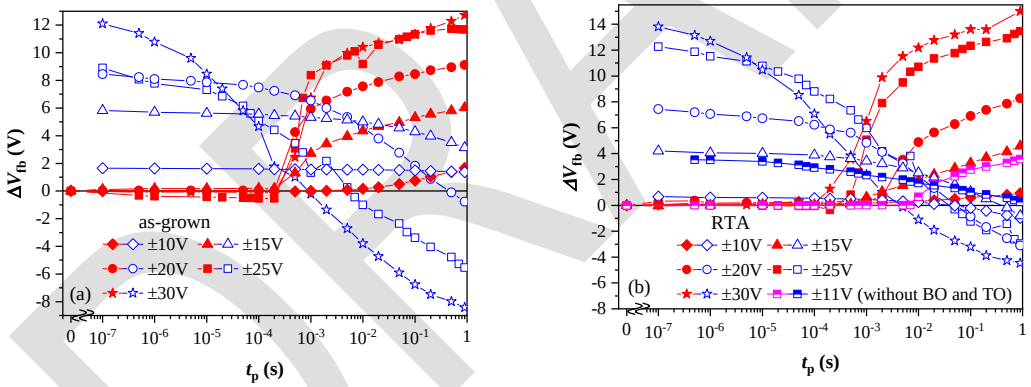

Figure 1: Dependence of the flat-band voltage shifts on the applied write/erase voltage and the pulse durations for memory capacitors with 5×(20cyHfO_2:5cyAl_2O_3), 20 nm Al_2O_3 blocking layer (BO) and 2.4 nm SiO_2 tunnel oxide (TO).

Acknowledgments:
The work is supported by Bulgarian National Science Fund under project KP-06-N37/32

2.13. A study to determine the optical constants of PVD ZrO_2 layers

A. Tenev*, E. Stoyanova, I. Miloushev, T. Tenev, K. Antonova
Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko chaussee, Sofia 1784, Bulgaria
* – a.tenev@issp.bas.bg

Modern optical systems consist of many elements with different functional purposes and almost all of them use multilayer interference coatings. Coating structures can contain from 1-2 to over 50-100 layers of different materials. Most often in practice, structures are made of 2 or 3 materials with a low, high and sometimes medium refractive index. In addition to the value of the refractive index, many other requirements are placed on the qualities (properties) of the layer, such as adhesion, strength, compatibility, hardness, etc.
Although thin film devices differ in the details of their construction, all except for the single layer metal mirrors, are based on the principle of interference. This principal determines the material parameters of prime interest to the thin film designer. In the ideal case the properties of a thin film are completely determined by just two parameters: thickness and refractive index.
Thickness variation due to the deposition process is well understood and correctable. Variation in the refractive index due to the deposition process is a considerably more complex problem. The real challenge of thin films is that they do not behave as simple thin slabs of the bulk material from which they are made. The optical properties of thin films depend on many variables that pertain to the method used for their fabrication. In order to design and produce an optical coating with required properties and parameters, it is necessary to determine in advance the optical constants of the layers to be produced.
There is a great demand of the production of hard amorphous coatings, and the reduction of stress. There are difficulties in maintaining a constant stoichiometry and reproducibility of index. A further aspect of growing interest is their stability under the influence of large fields. One of the materials that receives enough attention is zirconium dioxide (ZrO_2).
In this study, on the example of the deposition of ZrO_2 layers in a high-vacuum technological system Syphony 9 (Tecport Optics), by means of spectrophotometric and ellipsometric measurements, the optical constants of this material were determined according to deposition conditions and thickness of the layer. The reliability of the data for the optical constants determined according to this scheme has been proven by the production of several AR coating.

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

2.14. Ion irradiation assistance alters the microstructure and optical constants of vacuum deposited ZrO_2 thin layers

E. Stoyanova*, A. Tenev, I. Miloushev, T. Tenev, K. Antonova
Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko chaussee, Sofia 1784, Bulgaria
* – e.stoyanova@issp.bas.bg

ZrO_2 often is used as the dielectric material to replace SiO_2 in the nano-technological applications due to its electrical insulating and thermodynamic stability. Moreover, the ZrO_2 thin layers are preferable for their optical characteristics such as high transparency (if properly prepared), high refractive index, high laser induced damage threshold. These desirable properties are strongly dependent on the technological conditions. This is the reason for many publications describing different ways of ZrO_2 layers deposition to be issued during the last few decades. The big number of the parameters to be optimized cannot give unique recipe for a certain device development due to the individual equipment's characteristics. In the present work thin layers of ZrO_2 are deposited by e-beam evaporation in two different techniques in order the optical characteristics of both the series to be compared. One set of samples are fabricated by ion-assisted deposition (IAD) using equal quantities of argon and oxygen ions. The second set of samples are prepared without IAD but the substrates are heated up to 250°C during evaporation. The films' thicknesses in the two series are chosen so to obtain enough spectral extremums for correct determination of the optical constants: 50, 200 and 400 nm. To avoid a possible lack of oxygen in the layer formation which leads to a high optical absorption, oxygen gas maintaining a constant pressure in the chamber is added.

The optical properties of the produced ZrO_2 layers are studied using UV-Vis-NIR, Lambda 1050, Perkin Elmer and FTIR Vertex 70, Bruker spectrophotometers. The former is used for layer's thickness and optical constants determination by the reflection and transmission spectra while the second permits the investigation of the microstructure and the way of the film formation. The obtained refractive indices for the two series of preparation vary between a few tenths and are higher for the layers with IAD.

The layers' composition and microstructure with the thickness growing are discussed on the base of the FTIR spectra and are measured in the ATR geometry. The results reveal some contents of water in both kind of the samples but with different bonding nature of the H_2O molecules. Besides, the IAD technology exhibits the formation of micro-crystallites of ZrO_2 (far IR bands of Zr-O vibrations are registered). Thus, a certain packing in the layer happens and it is confirmed by the refractive index values.

At the end on the base of the described above technology an AR mirror for a special application is elaborated and its spectrum is presented.

Acknowledgements:
This work was supported from the Bulgarian Ministry of Education and Science, National Science Fund, grant No КП-06-Н57/5 (2021).
Special thanks to Dr. Daniela Kovacheva from the Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, for the carrying out the XRD spectra.

2.15. Physical properties of fermions obeying exclusion and superexclusion principles

Piotr Kuterba*, Maciej Fidrysiak, Danuta Goc-Jagło and Józef Spałek
Institute of Theoretical Physics, Jagiellonian University
* – piotr.kuterba@uj.edu.pl

In this work we investigate influence of the exclusion and superexclusion principles (the latter postulated by strongly correlated fermions) on the basic statistical properties of the corresponding fermions. In particular, by incorporating the Zeeman field into the model we examine the changes in spin-dependent energy levels as a function of both temperature and lattice occupation number.

References:

1. Spałek J., Kokowski M., Honig J.M., Low-temperature properties of an almost-localized Fermi liquid Phys. Rev. B., 39, 7, 4175-4185 (1989).
2. Spałek J., Wójcik W., Statistical thermodynamics of strongly correlated electrons in a narrow band: Fermi liquid versus spin liquid Phys. Rev. B., 37, 4, 1532-1538 (1988).
3. Hatsugai Y., Kohmoto M., Exactly Solvable Model of Correlated Lattice Electrons in Any Dimensions J. Phys. Soc. Jpn., 61, 6, 2056-2069 (1992).

2.16. Functionalization of metallic polycrystalline thin films with tryptophan for surface enhanced Raman spectroscopy (SERS) applications

Temenuga Hristova-Vasileva[1,2*], Rosen Todorov[2]
[1] – Institute of Solid State Physics, 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
* – teddie@issp.bas.bg

The formation of composite materials in the SERS technology, where metallic nanoparticles (mostly silver and gold) are mixed with organic molecules in order to achieve an enhanced Raman scattering is a subject of common interest. Two ways for surface enhancement of a Raman signal exist – an enhancement caused solely by presence of surface plasmon resonance in a basic metallic template and by using a functionalized composite material, obtained by chemical reaction between the enhancing metal and an organic molecule. Such functionalized materials provide more stable and repeatable Raman signal and favorable conditions for determination and characterization of biomaterials.

The functionalized composites are mainly prepared by addition of metallic nanoparticles to colloid and sol solutions of organic compounds, which leads to chemical reaction between them and further reduction of the metals toxicity level. However, the main disadvantage of this approach is the inhomogeneity of the mixtures due to the unavoidable precipitation of the nanoparticles. On the other hand, if such chemical reaction occurs on the surface of a stable polycrystalline thin film, deposited on an inert substrate, the problem will be easily solved.

The L-tryptophan, as many other amino acids, is zwitterionic by nature and the presence of separately active positive (NH^{3+}) and negatively (COO^{-}) charged groups in it is a favorable condition for functionalization due to the possibility for selective chemical reaction with only one functional group and thus polarization of the functionalized molecule. A precondition for protonization of the L-tryptophan molecule in water solutions is the acidity of the solvent.

In this sense, we are presenting here a SERS investigation of the changes in the L-tryptophan structure in aqueous solutions at variation of the pH from neutral to acidic and in situ functionalization of Ag, In and $AgIn_2$ metallic thin films with optimal L-tryptophan concentrations.

Despite that indium and its compound $AgIn_2$ enhance lower Raman signal compared to silver, they react better with the L-tryptophan by preferably bonding with the positively charged amino group and by this way forming a uniform row of polarized L-tryptophan molecules on the surface, while in the Ag samples both carboxylate and amino groups react throughout the whole investigated range of concentrations.

The enhancement of the Raman signal of the as-prepared Me/L-tryptophan composite structures was evaluated by measurement of the Raman spectra of Gentazon eye drops solution, containing 0.1 mg/ml betamethasone and 0.3 mg/ml gentamicin.

2.17. On-ground observations of solar over-irradiance effects and their influence on low-voltage electric power grid

Nikolay Tyutyundzhiev[1], Lyubomir Angelov[1], Christo Angelov[2], Todor Arsov[2], Nikola Serafimov[2]

[1] – Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences
[2] – Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences

The variability of solar activity during 25-th Sunspot cycle demonstrates the vulnerability of energy fluxes on Earth and the fragility of biological life conditions. The negative impact on Earth atmosphere and human society includes solar visible, UV-A, UV-B over-irradiance, IR extra-heating, magnetic storms, power grid failures etc. In the recent years accurate measurements of the solar irradiance at short intervals are needed to truly understand the variability of energetic input to Photovoltaic (PV) grid-connected generators. In this work selective wavelength measurements are performed in order to distinguish, predict power disturbances. Correlations between solar events and LV power grid fluctuations are investigated. New hybrid balancing strategies for remote SCADA control are proposed and tested.

Acknowledgements:
This work was supported by a grant of the National Science Fund of the Republic of Bulgaria under project №: КП-06-Н64/3, 15.12.2022 and by means of an infrastructure, financed by "National Road Map for Scientific Infrastructure, financially supported by the Ministry of Education and Science of Bulgaria", ACTRIS BG (Contract №: D01 – 365 / 04.12.2023).

2.18. Comparative gamma background measurements, spectrum horizontal mapping and vertical profile in Sofia, Beli Iskar and at high mountain station BEO Moussala

Todor Arsov[1], Christo Angelov[1], Nikola Serafimov[1], Nikolay Tyutyundzhiev[2]
[1] – Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences
[2] – Central Laboratory of Solar Energy and New Energy Sources, Bulgarian Academy of Sciences

Gamma background spectrum, horizontal mapping and its vertical profile is a challenge in the contemporary understanding of radiation monitoring. This concerns especially areas with complex terrain and restricted access, very often difficult for investigation. By means of a state of the art Unmanned Aerial Vehicle (UAV) and suitable detectors, gamma background mapping, as well as its vertical profile and cosmic ray influence could fulfill its purpose of a powerful scientific tool.
Preliminary measurement results from Sofia area (550 m a.s.l.), Beli Iskar region (1500 m a.s.l.) and Musala peak (2925 m a.s.l.) vicinity are presented and discussed correspondingly.

Acknowledgements:
This work was supported by a grant of the National Science Fund of the Republic of Bulgaria under project №: КП-06-Н64/3, 15.12.2022 and by means of an infrastructure, financed by "National Road Map for Scientific Infrastructure, financially supported by the Ministry of Education and Science of Bulgaria", ACTRIS BG (Contract №: D01 – 365 / 04.12.2023).

2.19. Femtosecond laser modification of optical thin films

Victoria Atanassova[1*], Georgi Yankov[1], Ekaterina Iordanova[1], Tihomir Tenev[1], Ilko Miloushev[1]
[1] Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Tzarigradsko Chaussee, Blvd., 1784 Sofia, Bulgaria
* vatanassova@issp.bas.bg

Ultra-short laser pulses, particularly femtosecond lasers, play a crucial role in photonics applications due to their high precision and minimal heat conduction during material processing. The combination of ultra-short pulse duration and high radiation intensity enables various mechanisms of laser-matter interactions, allowing for precise and selective modification of material surfaces. Femtosecond laser treatment permanently alters surface characteristics at micro- and nano-scales, impacting surface topography, crystalline structure, and chemical composition, thereby enhancing material functionality [1, 2]. This study investigates the mechanisms and effects of femtosecond laser-induced surface modifications on optical thin films, specifically Al_2O_3 and SiO_2 coatings on borosilicate substrates. We conducted the research using a femtosecond laser system, including the 'Mai Tai® SP' oscillator, the 'Empower® 45' pumping laser, and the Ti: Sapphire regenerative amplifier model 'Spitfire Ace' with a pulse duration of approximately 35 fs and a maximum pulse energy of around 6 mJ, generating a central wavelength of 800 nm. We assessed the physicochemical properties of the samples before and after treatment using SEM for surface morphology, spectrophotometry for optical reflectance, and the Z-scan method for nonlinear refraction index and nonlinear absorption coefficient.

References:

1. Xintao Zhi, Xiaopeng Li, Songmei Yuan, Dasen Wang, Kehong Wang. Mechanic properties modification of SiO_2 thin films by femtosecond laser. Optik, Vol. 251, 2022, 168404, https://doi.org/10.1016/j.ijleo.2021.168404.
2. Kaixin Yuan, Feng Geng, Qinghua Zhang, Yaguo Li. Femtosecond laser strengthening of electron-beam deposited SiO_2 thin film on fused silica substrates. Thin Solid Films, Vol. 780, 2023, 139959, https://doi.org/10.1016/j.tsf.2023.139959.

Acknowledgements:

This research was funded by the Bulgarian National Science Fund under the National Scientific Program "Petar Beron i NIE", contract No. KP-06-DB/9.

LIST OF PARTICIPANTS

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
Arsov Todor	Institute for Nuclear Research and Nuclear Energy - BAS	Sofia, Bulgaria	arsoff@inrne.bas.bg
Atanassova Victoria	Institute of Solid State Physics - BAS	Sofia, Bulgaria	viki.atanassova@gmail.com
Avramova Ivalina	Institute of General and Inorganic Chemistry - BAS	Sofia, Bulgaria	iva@svr.igic.bas.bg
Babeva Tsvetanka	Institute of Optical Materials and Technologies	Sofia, Bulgaria	babeva@iomt.bas.bg
Banerjee Sarbajit	Department of Chemistry; Department of Materials Science & Engineering, Texas A&M University	Texas, USA	banerjee@chem.tamu.edu
Baranovski Svetlana	Faculty of Physics, Philipps University Marburg	Marburg, Germany	svetlana.baranovski@physik.uni-marburg.de
Baranovskii Sergei	Faculty of Physics, Philipps University Marburg	Marburg, Germany	baranovs@staff.uni-marburg.de
Benkovski Alexandar	Central Laboratory of Solar Energy and New Energy Sources - BAS	Sofia, Bulgaria	kappu96000@gmail.com
Boyadjiev Stefan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	boiajiev@gmail.com
Chamati Hassan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	chamati@issp.bas.bg
Chitanov Vasiliy	Central Laboratory of Applied Physics - BAS	Plovdiv, Bulgaria	vchitanov@gmail.com
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
Dinescu Adrian	IMT Bucharest	Voluntari Romania	adrian.dinescu@imt.ro
Donchev Vesselin	Faculty of Physics, Sofia University	Sofia, Bulgaria	vtd@phys.uni-sofia.bg
Dudek Maciej	Academy WSB	Cracow, Poland	macmatematyka@gmail.com
Dulev Vladimir	Central Laboratory of Solar Energy and New Energy Sources - BAS	Sofia, Bulgaria	vladogotin64@gmail.com
Esmeryan Karekin	Institute of Solid State Physics - BAS	Sofia, Bulgaria	karekin_esmerian@abv.bg
Fabian Margit	HUN-REN Centre for Energy Research	Budapest, Hunagry	fabian.margit@ek.hun-ren.hu
Fedchenko Yulian	Institute of Solid State Physics - BAS	Sofia, Bulgaria	yulian@dir.bg
Georgiev Velizar	Institute of Solid State Physics - BAS	Sofia, Bulgaria	velizar@issp.bas.bg
Georgieva Borislava	Institute of Electronics - BAS	Sofia, Bulgaria	b.georgiewa@abv.bg
Georgieva Nikoleta	University of Chemical Technology and Metallurgy	Sofia, Bulgaria	n.ivanova@uctm.edu
Georgieva Veselina	Faculty of Physics and Technology, Plovdiv University "Paisii Hilendarski"	Plovdiv, Bulgaria	vesngeorgieva@gmail.com
Ghelev Chavdar	Institute of Electronics - BAS	Sofia, Bulgaria	chavdarghelev@yahoo.com
Goranova Margarita	Institute of Solid State Physics - BAS	Sofia, Bulgaria	lozanova_1970@abv.bg
Grigorov Aleksandar	Plovdiv University "Paisii Hilendarski"	Plovdiv, Bulgaria	aleksandar.grigorov@uni-plovdiv.bg
Guerra Vasco	IPFN, IST, Universidade de Lisboa	Lisboa, Portugal	vguerra@tecnico.ulisboa.pt

Hristova-Vasileva Temenuga	Institute of Solid State Physics - BAS	Sofia, Bulgaria	teddie@issp.bas.bg
Iglič Aleš	University of Ljubljana, Faculty of Electrical Engineering, Laboratory of Physics	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.	Nanotechnology Laboratory, University of Architecture, Civil Engineering and Geodesy	Sofia, Bulgaria	george@at-equipment.com
Korutcheva Elka	Universidad Nacional de Educación a Distancia Institute of Solid State Physics - BAS	Madrid, Spain Sofia, Bulgaria	ekorutch@gmail.com
Koutzarova Tatyana	Institute of Electronics - BAS	Sofia, Bulgaria	tanya@ie.bas.bg
Kralj Samo	Solid State Department, Jožef Stefan Institute	Ljubljana, Slovenia	samo.kralj@um.si
Krezhov Kiril	Institute of Electronics - BAS	Sofia, Bulgaria	kiril.krezhov@gmail.com
Kuterba Piotr	Institute of Theoretical Physics, Jagiellonian University	Kraków, Poland	piotr.kuterba@uj.edu.pl
Lazarova Madlena	Institute of Chemical Engineering - BAS	Sofia, Bulgaria	mplazar@abv.bg
Makedonski Lyubomir	Medical University of Varna, Department of Physic and Biophysic	Varna, Bulgaria	makedonski@mu-varna.bg
Marinov Yordan	Institute of Solid State Physics - BAS	Sofia, Bulgaria	ymarinov@issp.bas.bg
Mihaylova Lydia	Aquachim EAD	Sofia, Bulgaria	Lydia.Mihaylova@aquachim.bg
Milenkova Sofia	Faculty of Physics and Technology, Plovdiv University "Paisii Hilendarski"	Plovdiv, Bulgaria	sophiamilenkowa@gmail.com
Milushev 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	ICube/University of Strasbourg-CNRS	Strasbourg, France	paul.montgomery@unistra.fr
Mukherjee Deshabrato	Hungarian Research Network, Centre for Energy Research, Institute of Technical Physics & Materials	Budapest, Hunagry	mukherjee.deshabrato@ek.hun-ren.hu
Nedyalkova Petya	Defence Institute "Prof. Tsvetan Lazarov"	Sofia, Bulgaria	p.gencheva@di.mod.bg
Nikolova Krastena	Medical University of Varna, Department of Physic and Biophysic	Varna, Bulgaria	kr.nikolova@abv.bg
Pal Arkadeb	University of Groningen, Zernike Institute for Advanced Materials	Groningen, Netherlands	arkadeb.pal@rug.nl
Paskaleva Albena	Institute of Solid State Physics - BAS	Sofia, Bulgaria	paskaleva@issp.bas.bg
Petrik Peter	HUN-REN Centre for Energy Research, Institute of Technical Physics and Materials Science	Budapest, Hungary	petrik.peter@ek.hun-ren.hu
Reynolds Steve	University of Dundee	Dundee, UK	s.z.reynolds@dundee.ac.uk
Reznik Alla	Physics Department, Lakehead University	Thunder Bay, Canada	areznik@lakeheadu.ca
Solunov Hristo	Plovdiv University "Paisii Hilendarski"	Plovdiv, Bulgaria	solunov@uni-plovdiv.bg
Stanchev Todor	Institute of Solid State Physics - BAS	Sofia, Bulgaria	stanchev@issp.bas.bg
Stefanov Georgi	Aquachim EAD	Sofia, Bulgaria	Georgi.Stefanov@aquachim.bg
Stoyanova Elena	Institute of Solid State Physics - BAS	Sofia, Bulgaria	e.stoyanova@issp.bas.bg
Stoyanova Milena	Sofia University "St. Kliment Ohridsky"	Sofia, Bulgaria	milenas@phys.uni-sofia.bg

Strijkova Velichka	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	vily@iomt.bas.bg
Tabakova Ivanka	Institute of Solid State Physics - BAS	Sofia, Bulgaria	media@issp.bas.bg
Tenev Alexander	Institute of Solid State Physics - BAS	Sofia, Bulgaria	alexander.tenev@gmail.com
Tenev Tihomir	Institute of Solid State Physics - BAS	Sofia, Bulgaria	tenev@issp.bas.bg
Todorov Rosen	Institute of Optical Materials and Technologies - BAS	Sofia, Bulgaria	rossen@iomt.bas.bg
Vanderbemden Philippe	University of Liege, Institut Montefiore	Liege, Belgium	Philippe.Vanderbemden@uliege.be
Velkova Irina	Institute of Solid State Physics - BAS	Sofia, Bulgaria	velkova@issp.bas.bg
Viraneva Asya	Plovdiv University "Paisii Hilendarski"	Plovdiv, Bulgaria	asia83@abv.bg
Yankov Georgi	Institute of Solid State Physics - BAS	Sofia, Bulgaria	gjankov@issp.bas.bg
Zahariev Nedelcho	Institute of Solid State Physics - BAS	Sofia, Bulgaria	zahariev@issp.bag.bg
Zamfirescu Marian	National Institute for Laser, Plasma and Radiation Physics - INFLPR	Magurele, Romania	marian.zamfirescu@inflpr.ro
Zid Maha	Jožef Stefan Institute	Ljubljana, Slovenia	Maha.Zid@ijs.si
Zlatareva Ekaterina	Central Laboratory of Applied Physics - BAS	Plovdiv, Bulgaria	ekpepe31@gmail.com