BOOK OF ABSTRACTS

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BOOK OF ABSTRACTS

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ABSTRACTS

S0 – PLENARY SESSION
Nowadays, the use of renewable gases as fuels and the circular economy of carbon dioxide constitute ones of the major world challenges. The production of renewable hydrogen and the conversion of CO\textsubscript{2} into value-added chemicals and/or fuels, using renewable energy and earth-abundant elements as well as environmental friendly materials are key priorities. In this talk, we report on flow-cell type device for bias-free conversion of water and CO\textsubscript{2}, which by design is integrated, scalable to large areas, and compatible with earth-abundant and cheap photovoltaics and appropriate electrocatalysts. The presented device/cell is composed of a photocathode performing the reduction of molecules (H\textsubscript{2}O or CO\textsubscript{2}) and a dark anode for the oxygen evolution reaction (OER). Consequently, catalyst materials are essentials for increasing selectivity and productivity towards determined reactions. So, aside of the system design constraints, parameters as over-potential values or charge transfer resistances are determining the final energy balance as well as the overall efficiency and productivity.

In this contribution the mechanisms and criteria for selecting feasible catalyst for cathode and anode will be presented and discussed.

The proposed photocathode consists of a triple junction silicon solar cell, which has been chemically protected and electrically connected to three-dimensional (3D) appropriate metallic foam or carbon paper coated with selected bimetallic catalyst nanostructures (<50 nm) or, alternatively, catalysts supported on MOF.

For the OER part, we employed also bimetallic nanoparticles loaded on Ni foam. Three-dimensional (3D) nickel foam (NF) was used as scaffold material and the coating process was adapted for large area electrodes regarding scalability, particle size and distribution. This 3D electrode configuration resulted in impressively low overpotentials for the electro-oxidation at high current densities.

Special attention will also be paid on the conditions for diminishing as much as possible the overall cell voltage. For it, aside the development of highly efficient cathode catalysts, the development of high-performance catalysts for the oxygen-evolution reaction (OER) is also of paramount importance for achieving a cost-effective conversion of renewable electricity to fuels and chemicals.

Both optimized electrodes are integrated in a complete flow-cell for solar-driven water splitting or CO\textsubscript{2} conversion that applied a bipolar membrane to separate catholyte and anolyte compartments. According to these achieved performances using earth-abundant catalysts and silicon based photovoltaics, we demonstrate industrial feasibility and competitiveness of the electrochemical production of hydrogen and the electrochemical conversion of CO\textsubscript{2} as alternative for the future energy models considering solar and dark refineries as energy paradigms delivering high current densities at low voltage cells improving energy balance with high stability.
SO 02

MULTIDISCIPLINARY RESEARCH AT THE IBR-2 REACTOR

Valery Nickolaevich Shvetsov, Egor LYCHAGIN

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Frank Laboratory of Neutron Physics is one of the laboratories of the Joint Institute for Nuclear Research (Dubna, Russia), that investigates the neutron as an elementary particle, and employs the neutron as an instrument to investigate the structure and dynamics of condensed matter, including crystals and nanosystems, functional materials, complex liquids and polymers, rocks, etc.

The IBR-2 reactor operating at FLNP since early 80-th of the last century with its unique technical approach produces one of the most intense neutron fluxes at the moderator surface among the world's reactors: \( \sim 10^{16} \text{n/cm}^2/\text{s} \), with a peak power of about 1850 MW in pulse.

In 2007, the reactor reached the service life limit on fuel burn up and fluence on the reactor vessel and was shut down for modernization and replacement of the primary reactor equipment. The main objectives of the modernization were to increase safety, reliability and experimental possibilities of the reactor for the next 25 years of operation. During the modernization period 2007 – 2010 the first of three cryogenic moderators was put into operation. The next one is planned to be commissioned by September 2019 and the last one by the end of 2021.

At the 14 beam ports of the IBR-2 we have 16 instruments for neutron scattering, radioanalytical laboratory for neutron activation analysis and irradiation facility. Among neutron scattering instruments FLNP has seven diffractometers, one SANS instrument, three reflectometers, two inelastic scattering spectrometers and one facility for neutron radiography and tomography. Two beamlines are used for the research in nuclear physics.

Status of the IBR-2 experimental facilities and cryogenic moderators will be presented as well as the plans for instrumentation development.

**Keywords**: pulsed fast reactor; neutron scattering; condensed matter physics; neutron nuclear physics; neutron activation analysis; instrumentation for neutron experiments.

SO 03

NEWS FROM ELI-NP

Calin Alexandru UR

1Extreme Light Infrastructure - Nuclear Physics, IFIN-HH, Bucharest-Magurele, Romania

Extreme Light Infrastructure - Nuclear Physics is implementing two unique systems to deliver extreme light with unprecedented features for experiments. A high power laser system will provide two laser beams with 10 PW power each. By focusing these extreme laser beams on targets will allow ELI-NP to achieve levels of laser intensities of about \( 10^{23} \text{W/cm}^2 \), levels that were never attained before. A second system will deliver gamma beams with variable energy over a broad range of up to 20 MeV, quasi-monochromatic, linearly polarized and with high spectral density.

The availability in premiere of such extreme beams of electromagnetic radiation opens new opportunities for studying advanced research topics on both fundamental physics and applied physics.

The ELI-NP team has defined the first day experiments and is currently implementing the experimental setups, designed in collaboration with a broad worldwide scientific community, to perform them.

High power lasers are opening the pathway towards new schemes of producing high-intensity short-duration secondary radiation pulses and thus providing new perspectives for applied physics research. A special emphasis is given to research topics related to the improvement of life quality such as medical imaging, tumour irradiation, radioisotopes production but other topics related to particle acceleration, space technology, industrial imaging, nuclear safety are pursued as well.

**Keywords**: high power lasers, gamma beam, medical applications, industrial applications.
ABSTRACTS

S1 – Materials Physics

- Semiconductors, Dielectrics and Organic Materials
- Spintronics, Magnetism and Superconductivity
- Crystal growth, Surfaces, Interfaces and Thin Films
- Polymers and Amorphous Materials
ON THE EXCHANGE INTERACTIONS IN R-Co COMPOUNDS WHERE R IS A RARE-EARTH OR YTTRIUM

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The exchange interactions in RCo\(_n\) compounds, where R is rare-earth or yttrium and 2 ≤ n ≤ 8.5 are analysed starting from 4f-5d-3d model. The R5d (Y4d) band polarization M\(_{5d}\) is the key point is stabilizing the magnetic order. In a first approximation, this is determined by the additive contributions of M\(_{5d}(f)\) term, due to 4f-5d exchange and M\(_{5d}(d)\) one resulting from short range 5d-3d interactions, hybridization effects, respectively.

For a given series, the M\(_{5d}(f)\) follows a linear trend, as function of De Gennes factor, with different rates for light and heavy rare earth compounds. The M\(_{5d}(d)\) contribution is dependent on the local environment of a given R atom. The Curie temperatures, for a given series with both light and heavy rare earths, follow the same linear dependence when plotting as function of M\(_{5d}\). In pseudoternary compounds, the R5d band polarizations mirror all the changes in magnetic properties, being the key point in stabilizing the magnetic order. Finally the complex and interdependent exchange interactions, within the spatial extension of the unit cell, are analysed.

Keywords: cobalt-rare-earth compounds, exchange interactions, R5d band polarization.

COLORING AND DIELECTRIC PROPERTIES OF PHOSPHOTELLURITE GLASSES

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Phosphotellurite glasses are now widely used due to the phosphate glass former ability, mainly by melt quenching technique [1]. Compositional, these glasses include other oxides besides tellurite one with higher melting point compared with the phosphate component. Depending on the method of preparation and melt quenching parameters, the phosphotellurite glasses are more or less red colored [2]. The origin of this color is connected with the presence of tellurium element which influences the mechanical properties from brittle to a rigid structure of phosphotellurite glasses.

Figure 1. Absorption and color of the phosphotellurite glasses
The 40%ZnO+40%P2O5+20%TeO2 glasses, obtained by melt quenching method, are analyzed both from the experimental and theoretical point of view to explain the red color of these phosphotellurites. The parameters of these glasses, like the dimension of tellurium clustering and dielectric constant of glasses, are discussed to identify the origin of the physical properties of phosphotellurites.

**Keywords**: phosphotellurite glasses; optical spectroscopy; theoretical model; melt quenching.

**References**:

**S1 L3**

**A2-B6 THIN FILMS USED IN SOLAR CELLS FOR TERRESTRIAL AND SPACE APPLICATIONS**

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Due to their physical and chemical properties (such as suitable band gaps, large absorption coefficients and good chemical stability) CdS, ZnS, ZnSe, ZnTe and CdTe thin films are interesting materials for electronic and optoelectronic devices, including particularly, the photovoltaic cells for both terrestrial and space applications. For this specific application, it is of prime importance to study the influence of ionizing radiations on the structural, electrical and optical properties of the component materials on a hand and on the photovoltaic structures based on them, on the other hand.

In this paper, thin films of CdS, ZnSe, ZnS and CdTe, prepared on thermal vacuum evaporation and rf-magnetron sputtering were characterized from structural, morphological, optical and electrical point of view before and after irradiation with protons and alpha particles of 3 MeV and the fluencies of $10^{14}$ protons/cm$^2$ and $10^{13}$ alpha particles/cm$^2$, respectively.

Using these thin films the conventional photovoltaic cells based on ITO/CdS/CdTe/Cu:Au heterojunction, and new Glass/ITO/ZnS/ZnSe/CdTe/Cu:Au structures based on ZnS and ZnSe as window layers, were produced and characterized before and after irradiation with protons and alpha particles, in the above conditions. The effects of irradiation were studied by investigating the changes in the structural, morphological, electrical and optical properties of the component thin films and prepared cells. Action spectra of the external quantum energy (EQE) and the current-voltage (I-V) characteristics in AM 1.5 conditions (the density power of the incident light is equal with 100 mW/cm$^2$) corresponding for conventional CdS/CdTe heterojunctions and double-heterojunction ZnS/ZnSe/CdTe photovoltaic structures were investigated before and after irradiations. The parameters characterizing a photovoltaic cell, short-circuit current, open circuit photo-voltage, fill factor were calculated before and after protons or alpha particles irradiation and the obtained values are compared. A discussion about the possible origin of those defects is given. In the case of component thin films the defects induced by irradiation with protons and alpha particles are point like defects like vacancies of Cd, or Zn or S. In the case of photovoltaic structures, it was found that proton and alpha particles irradiation in the above mentioned conditions results mainly in the introduction of defects at the CdS/CdTe interface and at ZnS/ZnSe/CdTe interface in the case of Glass/ITO/ZnS/ZnSe/CdTe/Cu:Au structures in superstrate configuration, respectively.

**Keywords**: CdS, ZnS, ZnSe, CdTe
CARBON-TITANIUM NANOSTRUCTURES: SYNTHESIS AND CHARACTERIZATION

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Carbon-Titanium (C-Ti) multilayer nanostructures were deposed by Thermionic Vacuum Arc (TVA) technology. The layers consisting of about 100 nm Carbon base layer and seven 40 nm alternatively Ti and C layers were deposed on Silicon substrates. The thickness of such a multilayer structure was up to 500 nm. On the other hand, in order to obtain Ti doped Carbon multilayer structures with various Ti content, a 20 nm thick Ti interlayer was first deposed on Si substrate and then seven successively Ti doped Carbon layers, each of these having a thickness of up to 40 nm were deposed. To perform the successively Ti doped layers with various Ti content were changed the discharge parameters for C and Ti plasma sources to obtain the desirable Ti atomic concentration. By changing of substrate temperature between room temperature and 300°C and on the other hand the bias voltage up to -700V, different batches of samples were obtained for this study.

To characterize microstructure properties of as prepared C-Ti multilayer structures were used Electron Microscopy techniques (TEM, SEM, STEM), X-Ray Photoelectron Spectroscopy and Raman Spectroscopy. The measurements reveal the content of diamond-like sp³ and graphite-like sp²; the ratio sp³/sp² increases when the bias voltage increases. Also, in the case of Ti doped multilayer structures, HRTEM and SAED patterns reveal an increase of amount and size of TiC nanocrystals with the increase of energy of Ti ions determined by increase of Ti anode potential. For tribological characteristics determination, systematic measurements were performed using a ball-on-disk system with normal force of 0.5, 1, 2, 3N respectively. The coefficient of friction depends on the substrate temperature and on the bias voltage. In the case of Ti doped multilayer structures the friction coefficient depends by the Ti content, pure C and amount of TiC nanocrystallites. The microhardness of the coatings was measured by dynamical microindentation method with Nanotest 550 instrument. The results are associated with the occurrence of atomic diffusion processes at Ti/C interface and with the amount of TiC nanocrystallites. To characterize the electrical conductive properties, the electrical surface resistance versus temperature have been measured, and then the electrical conductivity. Using the Wiedeman-Frantz law was calculated the thermal conductivity, which increase with increase of the temperature, according to the decrease in the proportion of TiC phase.

Keywords: TVA, C-Ti multilayer, TEM, SEM, STEM, EDX, XPS, Raman spectroscopy, tribological properties, electrical properties.

BASIC NEW DATA IN FERROELECTRIC TRANSITION OF TGS CRYSTAL

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Triglycine sulphate crystal (TGS for short) has a second order phase transition around 49°C. Pure (and doped) single crystals were grown from solution, in paraelectric phase at 52°C by slow solvent evaporation. Samples were cleaved perpendicular on the “b” crystallographic axis (1 mm / 0.8 cm²), polished and silver electrodes were painted.

Dielectric dispersion of pure TGS samples was studied by dielectric spectroscopy on a large frequency (1 x 10⁷ Hz) and temperature (-120 to +65°C) ranges, crossing up and down the Curie point (CP ≈ 49°C) several times. Both components of permitativity increases more than one order of magnitude in ferroelectric phase, crossing down the CP in the first run. Surprisingly, a metastable zone down the CP, not mentioned in the literature, on the first temperature stage 49-45°C was found, where “strange” crystal properties arrows. Other
temperature stages 45-40°C, 40-35°C, 35-30°C was clearly discerned (Ferroelectrics 506 493 (2016) 165-171) and (2016) 216-228. On the bases of other experiments, we have found that crossing down the CP the system become metastable due to the relaxation process of ferroelectric domains (JOAM 20 (2018) 676-681).

Some other new data shall be presented. In the Cole-Cole representation, mainly two relaxation types were found. The higher frequency one, with a relaxation time of $\tau_{H} \sim 5 \cdot 10^{-7}$ sec, has a non-Arrhenius temperature dependence and is due to the Glycine I (GI) group from the structure. This can be associated the "critical slowing down" mechanism related with the long distance order in the lattice and the second order transition in TGS. The lower frequency relaxation ($\tau_{L} \sim 10^{-3}-10^{-4}$ sec), related with the ferroelectric domain evolution has an Arrhenius temperature dependence with the activation energy of $0.65-0.70$ eV. An unusual, "middle" frequency relaxation ($\tau_{M} \sim 10^{-4}$ sec), not mentioned in the literature so far, was found on the temperature range Tc-35°C. We found that this relaxation is correlated with the dynamic of other glycine group GII-GIII from the TGS structure, joined by a Hydrogen bridge.

It was established that the ferroelectric transition of TGS was really closed down 30°C.

**S1 L6**

**TUNING OPTICAL AND MORPHOLOGICAL PROPERTIES OF POLYMER NANOFIBERS OBTAINED BY ELECTROSPINNING TECHNIQUE**

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The electrospinning technique is a very facile method for producing polymer fibers with nano and micrometric diameters. The process is scalable, flexible and low-cost because does not require complicated devices or high temperatures. The advantages offered by the electrospinning technique when producing polymeric fibers are given by the simplicity of the method. Thus, one can use an electric field to draw fine nanofibers from solutions. The polymer fibers can be further functionalized using nanoparticle addition or further chemical or electrochemical deposition of various compounds on the surface of the electrospun nanofiber [1-3]. Functionalized meshes of nanofibers obtained by the electrospinning technique have been successfully used as thermochromic, magnetochromic, and electroluminescent devices. Bundles of such nanofibers were prove to be able to mimic the human muscles’ movements [4, 5].

Morphology control is allowed by the possibility of controlling all the process parameters (temperature, viscosity of polymeric solution, applied voltage, distance between electrodes, etc.). Electrospun polymeric nanofibers have multiple applications in medicine but they also permit manipulation of light at nanometric dimensions when doped with organic dyes or different nanoparticles. Dye doped polymers were studied in details, from the point of view of the emission tuning with morphology and with composition [6-9].

We present our studies regarding the tuning of the properties of polymer nanofibers produced by electrospinning. Our main objective was to produce polymer nanofibers doped with different dyes and tailor their optical and morphological properties.

**Keywords:** electrospinning, polymer nanofibers, functionalized nanofibers, optical properties.

**Acknowledgments:** The authors acknowledge the financial support received through IFA CEA Project No. C5-08/2016.

**References**

ADVANCES IN Ge NANOCRYSTALS-BASED STRUCTURES FOR SWIR SENSORS AND NON-VOLATILE MEMORIES

Catalin PALADE, Adrian SLAV, Ana-Maria LEPADATU, Ionel STAVARACHE, Ioana DASCALESCU, Ovidiu COJOCARU, Ioana LALAU, Sorina LAZANU, Constantin LOGOFATU, Toma STOICA, Valentin Serban TEODORESCU, Magdalena Lidia CIUREA

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The use of oxide films with embedded Ge nanocrystals (NCs) is beneficial for photosensing in short wave infrared (SWIR) range as they ensure the increase of transition probability and tuning of energy band gap by means of quantum confinement [1]. Regarding the non-volatile memories, the floating gate of Ge NCs in oxide is a better solution than that with Si NCs as the quantum confinement is stronger in Ge.

In this work we present photosensitive Ge NCs-oxide films in SWIR and trilayer structures with floating gate of Ge QDs -oxide layer having memory properties. Both films and structures were obtained by magnetron sputtering deposition followed by rapid thermal annealing (RTA) for Ge NCs formation. The technological processes were conducted under optimal conditions for targeted properties.

Ge NCs-TiO$_2$ films with 5 nm Ge NCs size (HRTEM) show a optical band gap of 1.14 eV [2]. The optical spectral constants (n and k) in VIS-NIR were determined (experiment and simulation) for the first time, and their behaviour was correlated with technological parameters for Ge NCs formation. The photosensitivity in SWIR was evidenced by measuring the spectral photocurrent on coplanar structures of Ge NCs-TiO$_2$ layer/SiO$_2$/c-Si substrate under monocromatic modulated light. The spectral photocurrent is enhanced by the presence of Ge NCs with 5 nm size in TiO$_2$ matrix and exponentially increased by the gating effect and surface photovoltage.

Ge NCs-SiO$_2$ films are deposited by magnetron sputtering on heated Si substrate at 400 °C. The ITO/5 nm Ge NCs in SiO$_2$/n-Si/Al structures have high photosresponse in a broad band of 450–1300 nm. So, the high responsivity of 5AW$^{-1}$ and photo-detectivity higher than 10$^{14}$ Jones were obtained.

HfO$_2$/Ge QDs-HfO$_2$/HfO$_2$/p-Si trilayers were also obtained by magnetron sputtering deposition in a single run followed by RTA under suitable conditions (e.g. 600 °C) [3,4]. The intermediate layer with role of floating gate is formed of Ge QDs (2–3 nm, hexagonal phase) arranged in a single layer, that are separated by HfO$_2$ NCs (8 nm size, tetragonal/orthorhombic structure). These Ge QDs are positioned at the boundaries crossing of HfO$_2$ NCs. Also, Ge (other than Ge QDs) is found at HfO$_2$ NCs boundaries in the floating gate and inside the lattice of gate HfO$_2$ probably forming GeHfO$_4$. These memory structures have high performance, so the memory window is 3.8–4 V and the retention time is given by 14% capacitance decrease only, in the first 3000–4000 s and a 50% capacitance reached after 10 years.

Keywords: Ge nanocrystals, SWIR photosensing, non-volatile memory structures

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References
The great properties of zinc oxide (ZnO) triggered lately an extensive interest among scientific community due to the distinctive advantages of this material, such as a wide band gap (3.37 eV), a large exciton binding energy (60 meV), as well as good piezoelectric characteristics. In addition, it is a non-toxic and transparent oxide with biocompatibility properties and good chemical, mechanical and thermal stability. All these features make ZnO suitable for a wide range of applications in electronics and optoelectronics. Interestingly, ZnO can be also easily nanostructured in many ways, allowing for a huge variety in its structural morphology. In particular, the ZnO quasi–one-dimensional (1D) nanostructures have been widely explored lately, as these unique elongated architectures could provide extremely large surface-to-volume ratios, bringing thus valuable benefits for device applications.

In this context, this lecture will present several simple and cost-effective strategies to prepare dense arrays of ZnO quasi-1D nanostructures (i.e. nanorods or high aspect-ratio nanocolumns with hexagonal symmetry) perpendicularly-aligned on top of various substrates. Both, template-assisted and template-free ZnO electrochemical synthesis routes will be reviewed, focusing on the complex interplay between processing parameters and substrate properties, which could yield large high-quality arrays of such vertical ZnO nanostructures. It has been found that under specific preparation conditions, highly-oriented ZnO 1D nanostructures can be obtained, featuring reasonable aspect-ratios, an excellent crystallinity, as well as a very good piezoelectric response. The described approaches are promising, as they open the pathway towards fabrication of chipper and more performant ZnO-based electronic and optoelectronic nanostructured devices.

Keywords: ZnO quasi-1D nanostructures; nanoporous anodic aluminum oxide templates; polycarbonate track-etched membranes; electrochemical synthesis.

References:
The use of high pressure allows a fundamental way to change the physical properties of various compounds, since the pressure directly affects interatomic distances and affects the angles of interatomic bonds, thereby changing the structure of the compound. Such changes are well identified using neutron diffraction methods, which make it possible to simultaneously observe changes in both the crystalline and magnetic structures of the compounds and to find the positions of light elements in their crystal lattice. However, the use of the high-pressure method in neutron scattering experiments is made difficult by the relatively low intensities of neutron sources in the modern world.

One of the most powerful sources of neutrons is the IBR-2 pulsed reactor, which has one of the highest neutron fluxes in the world. Thanks to unique technical solutions, it was possible to maintain a high neutron flux density at the end of the 30 meter base of the 6th rector beamline and create a unique station for the study of microsamples under high pressure - the DN-6 diffractometer. The use of a parabolic neutron beam focusing system in combination with a wide solid angle of the detector system, as well as a serious suppression of the radiation background at the station hub at the moment, allows to obtain high-quality neutron diffraction patterns from samples of less than 0.01 mm3. This fact made it possible to use not only high-pressure cells with sapphire anvils, but also diamond cells, which allow to obtain pressures of up to 1/2 megabar. Some examples of recent studies at pressures up to 40 GPa are presented.

Keywords: co-doped zinc oxide, RF magnetron sputtering, XRD, AFM, Raman

References:
EFFECT OF ANNEALING ON STRUCTURAL PROPERTIES OF ELECTRODEPOSITED CZTS THIN FILMS

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The production of renewable energy is based on three conditions: a clean and non-limited energy source, high conversion efficiency and a conversion device made of widely abundant components and produced by low energy consumption processes. In this respect, photovoltaic uses the most suitable energy source which is solar light. Copper, zinc, tin and sulfur (CZTS), is a semiconductor with a band gap of about 1.5 eV, which makes it suitable for incorporation in photovoltaic devices, as an absorber in thin films solar cells. Moreover, the abundance of its elements and its non-toxicity makes CZTS an excellent candidate for large scale utilization. Many physical and chemical techniques have been employed for preparing CZTS thin films as a light absorber such as atom beam sputtering, RF magnetron sputtering, hybrid sputtering, thermal evaporation, sulphurisation of electron beam evaporated precursors, pulsed laser deposition and spray pyrolysis technique, ultrasonic spray pyrolysis, sol–gel spin coating technique. In this field the electrochemical route appears of great interest because easy to conduct, it is a non-vacuum and low-cost technology, working at room temperature and using non-toxic solvents and reagents, with high throughput and high materials utilization. Moreover, the electrodeposition has the advantage of being an industrially established process of a large area semiconductor deposition with superior uniformity in composition.

In this work, we report an electrodeposition process based on citrate buffer electrolyte to fabricate Cu2ZnSnS4 (CZTS) absorber film. The effluence of the annealling effect was studied. The electrochemical studies were performed using the cyclic voltametry analysis and the electrodeposition was held using the chronoamperometry method. The films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and (ICP) analysis.

Keywords: CZTS Thin Film, Electrodeposition, Annealing, Photovoltaics

LASER SYNTHESIS OF HYBRID MATERIALS FOR REMOVAL OF PHARMACEUTICAL PRODUCTS FROM AQUEOUS SOLUTION

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The problem of pharmaceutical product residues in wastewater is of great importance, especially for human health. One of the frequently used antibiotics against gram-positive and gram-negative bacteria is chloramphenicol. The presence of chloramphenicol residues in the environment represents a serious problem, specially owing to the formation of antibiotic – resistant bacteria. Moreover, chloramphenicol is known as a carcinogenic substance, generating also blood disorders and anemia.
The aim of this work is to develop new photocatalytic hybrid organic-inorganic materials based on transition metal oxide, carbon nanomaterials, and organic molecules with high photodegradation efficiencies. To this purpose we used a laser-based technique, called matrix assisted pulsed laser deposition. The catalytic properties of the synthesized nanocomposite layers were assessed through the UV light assisted degradation of chloramphenicol molecules. It has been proven that the hybrid organic-inorganic materials are suitable for the light induced degradation of chloramphenicol, allowing also to the elimination of the by-products formed under UV light irradiation. The reusability of the hybrid layers was also tested through repetitive degradation cycles of methyl orange probe molecules.

**Keywords:** noble metal free photocatalysts; transition metal oxides; organic molecules; organic-inorganic nanomaterial hybrids

**Acknowledgements**
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**S1 O5**

**STRUCTURAL AND MAGNETIC PROPERTIES OF YCo₄B AND YCo₄Si COMPOUNDS UNDER HIGH PRESSURES**

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The study of YCo₅₋ₓMₓ (M = Fe, Co, Ni) intermetallics is one of the actual task of condensed matter physics, due to the large variety of physical phenomena found in materials based on them. Such phenomena as the magnetism of collectivized electrons, giant magnetoresistance, magnetocaloric effects (FEM), and the volume collapse of the crystal lattice were found in these compounds, which makes them promising materials for magnetic refrigerators, permanent magnets, etc.

The RCo₅ and YCo₅₋ₓMₓ compounds crystallize in CaCu₅-type structure with space group P6/mmm. In this lattice, the cobalt atoms occupy 2c and 3g sites and form ferromagnetic ordering. These compounds are sensitive to changes in interatomic distances that can lead to significant changes in their magnetic properties and the simultaneous using of high-pressure cells give opportunity to control the changes of the interatomic distances.

In our work the results of the investigation of of YCo₄B and YCo₄Si by the method of neutron diffraction at high pressures are presented. The crystal structure and magnetic properties of YCo₄B intermetallic compound were studied by means of neutron diffraction at pressures up to p = 6.5 GPa. No structural transitions are evidenced. The cobalt moments at 2c and 6i sites decrease, upon lattice compression, with a rate dlnM_{Co}/dp = 0.11 GPa⁻¹. The evolutions with pressure of band structures have been also analysed and the computed cobalt moments, which have been compared with those experimentally determined. The YCo₄Si have been studied in a wide range of pressures and temperatures 0 ≤ p ≤ 5.3 GPa and 10 ≤ T ≤ 300 K, respectively. The Curie temperature reducing with same baric coefficients -10 K/GPa for cobalt atoms in both 2c and 3g positions is observed under pressure. The suppression of cobalt magnetic moments in these positions has been found as well. This phenomena is associated with change of cobalt ions spin states from the high spin to the low spin in YCo₄Si.

This work was supported by the Russian Foundation for Basic Research grant 17-02-00112-a.

**Keywords:** intermetallics, neutron diffraction, high pressures, band structures
MAGNETIC AND FERROELECTRIC PROPERTIES, CRYSTAL AND MAGNETIC STRUCTURES OF SRFE\(_{11.9}\)IN\(_{0.1}\)O\(_{19}\)

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The investigation of strontium ferrites partially substituted with diamagnetic ions (Al, Nb, Zn etc.) \(^1,2\) has attract an attention due to their high functional properties. The high coercive force (\(H_c \sim 160 \times 10^3\) A/m) with a sufficiently high residual induction allows to receive permanent magnets with a satisfactory specific magnetic energy. Their high electrical resistivity (\(\rho \sim 10^8\) Ohm\(\cdot\) cm) allows to use hexaferrite magnets in the presence of high-frequency magnetic fields. Currently, these materials have received practical application in magnetic recording devices of information \(^3\), as permanent magnets \(^4\) and absorption area of decimeter and centimeter electromagnetic radiation.

Recently, a large ferroelectric polarization was found in strontium \(^5\) and barium \(^6,7\) hexaferrites that opened a new direction for potential multiferroic candidate to the conventional ferrimagnetic oxides, such as SrFe\(_{12}\)O\(_{19}\), which holds similar perovskite-like lattice units in its hexagonal structure. The perovskite BiFeO\(_3\) shows weak magnetism, which somehow limits its practical application. Therefore, preparation materials where a large ferroelectricity and strong ferromagnetism coexist would be a milestone for modern electrics and functionalized materials. However, the reasons of appearance of ferroelectric polarization in barium ferrites are still not clear.

The sample SrFe\(_{11.9}\)In\(_{0.1}\)O\(_{19}\) has been obtained by conventional solid reaction method. Its crystal and magnetic structure has been investigated by neutron diffraction method in a wide temperature range. The presence of spontaneous polarization has been discovered at room temperature. The refinement their crystal structure have been carried out in frameworks of centrosymmetric P6\(_3\)/mmc (\(\#\) 194) and non-centrosymntric P6\(_3\)/mc (\(\#\) 186) space groups. Analysis of refinement results allows explaining reasons of appearance electric polarization in strontium hexaferites as result of unequal distortions of neighbouring octahedrons (tetraedrons and trigonal-bipyramids).

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References:
EVALUATION OF CHITOSAN/PVP HYDROGELS CONTAINING IBUPROFEN AND NANO SILVER PREPARED BY E-BEAM CROSS-LINKING

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Chitosan/Poly(N-Vinyl-2-Pyrrolidone)(PVP) hydrogels were prepared by e-beam radiation cross-linking as wet dressings for rapid healing and pain release of infected skin wounds. PVP, a synthetic polymer and chitosan, a natural polymer are biocompatible and have presented a great variety of interesting properties for biomedical, pharmaceutical, cosmetic and biotechnological applications [1]. In this study two different hydrogels compositions based on chitosan solubilization using acrylic acid or lactic acid were prepared and was determined that the best hydrogels properties were found to be for those prepared at 15-20 kGy in acrylic acid (AA) solution. The hydrogels structural and compositional features have been investigated according to: gel fraction, sol-gel analysis, swelling studies, network parameters, FT-IR and XPS analysis. The stability of hydrogels in simulated physiological condition of a infected wound (variation of pH in range 5.2-9.2 and in conditions of different body temperatures within 37-41°C range) was also investigated.

The cross-linked hydrogels showed a gel fraction (over 90%), the swelling capacity reaching the equilibrium state after 8 hours of immersion in different pH buffer solutions and it was observed that the best swelling capacity was obtained at the 15 kGy. The hydrogel shape was maintained more than 48 hours in buffer tampon solutions (pH = 5.2-9.2) and simulated body temperatures. The investigation of hydrogels network parameters indicated the formation of a cross-linked microstructure with a mesh size of 5.8-72.2 nm. The chemical composition of the hydrogels was evaluated by means of X-ray Photoelectron Spectroscopy (XPS) measurements. The hydrogels were tested in order to determine the loading capacity (LC) of ibuprofen (IBU) and Ag nanoparticles and it was determined that ensuring the possibility of incorporating of a therapeutic dose of at least 200 mg of IBU. The IBU was released up to 60% in the first 120 min, having a release maximum after 6h. The hydrogels prepared in AA solutions showed the best efficiency of colloidal Ag absorption ranging from 43 to 86%.

Keywords: hydrogel, e-beam irradiation, ibuprofen, nanosilver.
Acknowledgements: This work was supported by project Nucleu LAPLAS VI 16N/08.02.2019.
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THERMOELECTRIC TRANSPORT THROUGH A QUANTUM DOT CONNECTED TO GRAPHENE LEADS: TRANSITION FROM THE COULOMB BLOCKADE TO THE KONDO REGIME

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We theoretically analyze thermoelectric properties of a quantum dot connected to pure monolayer graphene source and drain electrodes. The system is described by the pseudogap Anderson Hamiltonian [1,2].
The equation of motion technique \[3-5\] within the nonequilibrium Green’s function formalism \[5\] is used to employ the current-voltage characteristic of the system. The retarded Green’s function of the dot is computed within the Lacroix decoupling scheme \[3\] using the Meir approximation \[4\]. The Coulomb interaction between localized electrons in the quantum dot is assumed to be finite. The thermal transport through the dot is analyzed assuming a linear response regime. We find that a transition from the Coulomb blockade to the Kondo regime in thermoelectric transport through the quantum dot takes place when the coupling strength between the dot and graphene electrodes is gradually increased. The current-voltage characteristic of the dot within the Coulomb blockade regime contains two steps. The appearance of these steps is caused by the discreetly changing electron number in the dot. The main dot level is tuned by the gate voltage through a metallic gate electrode. In our system, in contrast with other studies for quantum dots coupled to metallic contacts \[3-6\], the temperature-dependent Kondo resonances show up in the density of states only for nonzero values of the chemical potentials within the Kondo regime. This is due to the linear energy dispersion of the graphene leads.

**Keywords:** quantum dot, graphene, Coulomb blockade, Kondo effect.

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**S1 O9**

**HYSTERESIS IN PEROVSKITE SOLAR CELLS: CHARGE ACCUMULATION VS. CHARGE COLLECTION MODELS**

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Currently there are two main types of models which explain the J-V hysteresis in perovskite solar cells: charge accumulation models and charge collection models. Starting from the basic assumption that ions migrate under the influence of the internal electric field in the PSC under bias, our extended model based the dynamic electrical model (DEM) accounts for capacitive effects related to interfacial charge accumulation and for the modulation of the charge collection efficiency. In this context, as there are currently more and more reports of perovskite solar cells without J-V hysteresis, it is crucial to distinguish between genuine performance improvements and measurement artifacts \[1,2\]. We investigate how far the hysteresis-free behavior of perovskite solar cells can be reproduced using particular pre-conditioning and measurement conditions. We focus on two of the parameters that influence the dynamic J-V scans, namely the bias scan rate.
and the bias poling voltage, and point out the measurement conditions for achieving a hysteresis-free behavior. We also discuss the suitability of defining a hysteresis index (HI) for the characterization of dynamic J–V scans.

![Graph showing hysteresis](image)

Fig 1. The hysteresis magnitude and type for R–F scans depend on the pre-poling conditions and bias scan rate.

**Keywords**: perovskite solar cell, J-V hysteresis


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**S1 O10**

**PHYSICAL PROPERTIES OF NANOSTRUCTURED Nd_{0.6-x}Bi_xSr_{0.4}MnO_3 COMPOUNDS**

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The physical properties of Nd_{0.6-x}Bi_xSr_{0.4}MnO_3 compounds where x = 0, 0.05, 0.1, 0.15 and 0.2 are reported. The compounds were prepared using the sol-gel route. X-ray diffraction studies confirm that all samples crystallize in orthorhombic structure having Pnma space group. The powders consist of spherical particles that tend to agglomerate, with average grain sizes of about 40-50 nm. The transition metal-insulator and Curie temperatures decrease slowly with increasing the Bi content and was explained by the Bi(6s) - O(2p) hybridization. In the spectral region between 2 eV and 5 eV there are several contributions from the Mn 3d, and of extensively hybridized Mn(3d)-O(2p) states. The magnetization does not saturate in magnetic fields up to 12 T. The difficulty of approaching a magnetic saturation state can be due to the absence of true long-range FM coupling due to the small grain size of the samples obtained by sol-gel method. It was shown that smaller sizes grains can create strain at the grain boundaries and give rise to more non-FM or weak antiferromagnetic regions which disturb the long-range FM order [1]. Large magnetoresistance in magnetic field of 10 T and 12 T were measured. The low temperature metallic behavior could be explained by electron-electron and electron–magnon scattering processes. The analysis of the core level XPS spectra proves the existence of both Mn^{3+} and Mn^{4+} ions in all samples, as well as the localization of Bi^{3+} ions in the perovskite lattice. The XPS valence-band are dominated by extensively hybridized Nd 4f–O 2p states, with contributions from Mn 3d-O 2p bonding and Mn 3d states. Finally, the electronic, transport and magnetic properties are analyzed.

**Keywords**: Manganites, Nanoparticles, Magnetic properties, Magnetoresistance.

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**Reference**:

IONIC EXCHANGE MEMBRANES BASED ON QUATERNIZED POLYSULFONES: DIELECTRIC RESPONSE

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Due to the increasing need from the membrane technologies for diverse applications, from biomedicine to electronics, development of new generation of materials with electroactive properties and significant impact on the future technological systems was imposed. In this context, the quaternized polysulfones (PSFQ) integration in blend with a hydrophilic polymer (cellulose acetate phthalate, CAP), represents an innovative way to improve the workability, hydrophilicity, and electrical performances (i.e., dielectric properties and conductivity (see Fig.1)), required by the ionic exchange membranes (IEMs) applications.

Fig. 1. Dielectric response for PSFQ/CAP blend (70/30 wt./wt.): Variation of the dielectric constant (ε’, (a)) and electrical conductivity (σ, (b)) versus frequency at different temperatures

Analyzing the dielectric response for the investigated blends was observed that the dielectric constants increase with temperature, as result of the improved polarization and more intense oscillation of the molecules present in films arising from the dipole orientation and trapped charge carriers. Additionally, the results obtained from conduction studies showed that the electrical conductivity, besides electronic conduction is accompanied by an ionic conduction, due to the quaternary ammonium group from the PSFQ.

In conclusion, the obtained data for the dielectric constant and electrical conductivity were demonstrated that the studied blends possesses enhanced dielectric quality of vital importance in their applications as ion-exchange membranes.

Keywords: dielectric properties, electrical conductivity, ionic exchange membranes.

PHYSICAL PROPERTIES OF RF-SPUTTERED ZNS AND ZNSE THIN FILMS USED FOR DOUBLE-HETEROJUNCTION ZNS/ZNSE/CDTE PHOTOVOLTAIC STRUCTURES

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Due to their excellent optoelectronic properties, AII-BVI binary semiconducting compounds have attracted considerable attention. In this work, polycrystalline ZnX (X= S, Se) and CdTe thin films were prepared by RF-magnetron sputtering and by thermal vacuum evaporation (CdTe films), respectively, in order to fabricate glass/ZnS/ZnSe/CdTe/Cu:Au structures in superstrate configuration. The structural properties of ZnX (X=S, Se) and CdTe thin films were investigated by X-ray diffraction (XRD), which revealed that ZnX and CdTe thin films are polycrystalline with a pronounced (111) texture. It was observed that after irradiation with protons crystallite sizes decreased while mechanical strains increased. X-ray reflectometry (XRR) was used to evaluate the thickness and the roughness of the films. The values obtained for thicknesses were between 58 nm and 163 nm and for surface roughness were between 1.7 and 2.4 nm. Morphological investigations of surfaces of ZnX and CdTe thin films were made by scanning electron microscopy (SEM). Investigated films present relatively smooth surfaces, with compact and uniform aspects and with no drops formed during sputtering processes. Also, absorption and transmission measurements were carried out for all samples deposited onto optical glass. In the case of ZnSe layers, optical bandgap values were between 2.31-2.7 eV and 3.10-3.65 eV for ZnS films. Furthermore, in Vis-NIR region, transparency is larger than 60% for both ZnSe and ZnS films. Afterwards, it was made a study on the ZnS/ZnSe/CdTe double-heterojunction properties and it was shown how these properties are influenced by irradiations with high energy protons (3 MeV, 10^{13} fluency).

Keywords: AII-BVI semiconductors, RF-magnetron sputtering, protons irradiation

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S1 O13

THERMAL AND ELECTROCHEMICAL CHARACTERIZATION OF THE GRAPHENE MODIFIED CATION-EXCHANGE MEMBRANES FOR WATER ELECTROLYSIS

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Proton Exchange Membrane Water Electrolysis (PEMWE) is expected to lead to a major breakthrough among current water electrolysis technologies. One of major current technical challenges in PEMWEs is the limited proton conductivity. Nowadays, graphene is considered one of the most promising candidates for improving the ionic transport properties, isotopic selectivity and conductivity throughout the unique two-dimensional structure. In this paper, we report on the development of graphene composite membranes containing different graphene loadings for PEMWE applications. Commercial graphene was incorporated into the Nafion® solution (5%), and fabricated by doctor-blade method. The nanocomposite membranes were compared with a membrane prepared in the same condition using the ionomer solution, and with a commercial Fumapem® membrane. The effect of graphene filler incorporation was studied by FTIR, TGA, DMA, FE-SEM, water uptake, IEC, and four-points in plane impedance spectroscopy to assess the commercial and graphene-composite PEMs. Thermal characterization of the composite membranes showed by increasing the graphene loading, the \(T_g\) peaks’ intensity decrease and/or is shifted due to the dipolar interaction between the graphene and the membrane matrix, showing the increase of the mechanical stability, IEC, and proton conductivity due to graphene nanoparticles introduction within the Nafion® matrix, that is an improved behaviour when compared to pristine Fumapem® membrane [1]. The membranes behaviour was investigated under ‘real’ electrolyser conditions, by using an in-house 10 cm\(^2\) electrolysis cell.

Keywords: Electrolysis, membrane, proton, graphene.
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References

S1 O14

ROS GENERATION AND PHOTOCATALYTIC ACTIVITIES OF INTERFACE MODIFIED SnO2-TiO2 COMPOSITES

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Generally the nanoporous SnO2 and TiO2 nanoparticles are known by their good photocatalytic properties. Here, the basic mechanism is based on the reactive oxygen species generation (ROS) at the interface between nanoparticles the aqueous solution.

Surface modifications of TiO2 nanoparticles may determine the adjustment of ROS generation efficiency primarily by changing the ionization potential of titania. Also, the presence of various moieties at the solid-liquid interface may adversely affect the photocatalytic efficiency. Instead, the combination in a core-shell structure in which TiO2 forms the outer shell while SnO2 represents the core allows the adjustment of TiO2 ionization potential by its modification at the interface with the SnO2 thus leaving the external surface accessible to the catalytic reactions. Moreover, SnO2 being a conductive material it admits electrons at the top of its conduction band may act as an electron trap which increases the life time of the photoexcited species.

Interface modifications are made in the SnO2 preparation phase by using different quantities of surface-anchoring precursors like polyethylene glycol (PEG) and polyvinylpyrrolidone (PVP). The process was followed by an annealing at elevated temperature. Here the polymers act as stabilizing agents which also significantly affect the size and porosity of nanomaterials. Next the SnO2 nanoparticles were covered with the same quantity of TiO2 and finally annealed to ensure titania crystallization.

The materials were characterized by X-ray diffraction (XRD), photoelectron spectroscopies (XPS and UPS), transmission electron microscopy (TEM) and UV-Vis. EPR coupled with spin-trapping were used to determine the efficiency of ROS generation process. Photodegradation tests were also performed and the results were interpreted in terms of modifications of the energy band alignment at the interface between the two oxides. The modifications of the TiO2 ionization potential induced by the polymer used in preparation controls the ROS generation process and implicitly the efficiency of the photodegradation.

Keywords: composites, SnO2, TiO2, ROS.

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S1 O15

STRUCTURAL AND OPTICAL PROPERTIES OF Ce3+-Mn2+ CO-DOPED LANTHANUM PHOSPHATE FOR CRYSTALLINE SILICON SOLAR CELLS

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Lanthanide ions Ln³⁺ doped rare earth orthophosphate REPO₄ have attracted much attention due to their physic-chemical inericy, photoluminescent properties and various applications such as biomedical labels, plasma display panels, electrical conduction, fluorescent lamps and solar cells [1-2]. Recent years, considerable attention has been paid to the downconversion (DC) process in REPO₄ compounds for improving the efficiency of solar cells, which is important for environmental reasons. The phosphors LaPO₄ (Lanthanum phosphate) doped with Ce(III)/Ce³⁺ and co-doped with Ce³⁺-Mn²⁺ were effectively synthesized by direct precipitation method using nitrates and chlorides as starting materials.

The prepared samples were characterized by powder X-ray diffraction (XRD) to confirm the formation of LaPO₄ nanoparticles with crystal structure monoclinic p21/n and surface morphology was studied by scanning electronic microscope (SEM). Additionally, Fourier transform infrared spectroscopy (FTIR) and thermogravimetric/differential thermal analysis (TG-DTA) were investigated to prove the phosphate vibration bands and the temperature of total dehydration of the rhabdophane phase, respectively.

A strong absorption band between 305 and 315 nm (4f–5d transition of Ce³⁺) and absorption peak at 374 nm (⁶A₁ → ⁴T₂ transition of Mn²⁺) are observed by UV-Vis. On doping Ce³⁺ and Mn²⁺ ions band gap of LaPO₄ decreases from 5.10 eV to 2.73 eV.

The photoluminescence (PL) properties of samples in UV-VIS-NIR region allows to verify the energy transfer (ET) process from Ce³⁺ to Mn²⁺. The down-conversion in Ce³⁺-Mn²⁺ co-doped LaPO₄ phosphors can convert a photon of UV region into photons of visible region of Mn²⁺: ⁴T₁ → ⁶A₁ transition. Indeed, Mn²⁺ is an important luminescence Ln³⁺ ion with typical emission peaks at around 600 nm and Ce³⁺ ion might be an ideal broad band sensitizer for Mn²⁺. This emissions can be candidates for improving spectral response of solar cells [3].

Keywords: Lanthanum phosphate, X-ray diffraction, Luminescence, Solar cell materials.

References:

S1 O16
MAGNETOCALORIC EFFECT IN ALKALI METALS DOPED LANTHANUM MANGANITE PEROVSKITES

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Sodium and Lithium doped lanthanum manganite exhibits an important magnetocaloric effect, which is characterized by a large variation of the magnetic entropy or wide adiabatic temperature change, arising from the application of external magnetic field [1]. This type of perovskite show a paramagnetic and a ferromagnetic phase by changing the doping concentration of the Sodium and Lithium. These materials are promising candidates for magnetic refrigeration at room temperature. The undoped compound LaMnO₃(x=0) is an antiferromagnetic (AFM) which evolves to a ferromagnetic material (FM) when a mixed Mn³⁺/Mn⁴⁺ valency is induced by partial substitution of the monovalent Li⁺ or Na⁺ ions for the trivalent La³⁺ ions. The Mn³⁺/Mn⁴⁺ ratio can play a large role in the various interactions such as double exchange (DE) and superexchange (SE)

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among Mn ions[2]. In this work, La_{1-x}M_{x}Mn_{1-y}Fe_{y}O_{3} (M = Na, Li), (x=0.1,0.2), (y=0,0.1) powders were synthesized by flash combustion method using glycine as fuels and chelating agent. All samples calcined at 1000°C are crystallized in a rhombohedral structure with R3-C space group. The addition of 20 % of Li leads to the formation of LiMn_{2}O_{4} spinel phase as impurity. The structural components in the LaMnO_{3} calcined at various temperatures in the 100–1000°C range are investigated by Fourier transform infrared spectroscopy (FT-IR). The Mossbauer spectrum, recorded at room temperature, represents a paramagnetic character of the manganite. The thermal behavior is examined by thermo gravimetric and differential thermal analysis (TG-DTA). The morphological properties of the nanoparticles are investigated using scanning electron microscopy (SEM) and the magnetic properties are determined by vibrating sample magnetometer (VSM).

Keywords: Perovskite, Flash combustion, Magnetic refrigeration, Magnetocaloric effect.

References

S1 O17
MODELING OF AN ACRT PROCEDURE IN A CZOCHRALSKI CRYSTAL GROWTH PROCESS FOR SOLAR SILICON

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In a Czochralski crystal growth process temperature fluctuations occur near the solid-liquid interface due to the melt convection. These fluctuations of temperature (and impurity concentration) lead to the development of striations in the crystal during the solidification process. In order to minimize the effects of the melt convection, two major approaches are usually taken into consideration: growing a crystal in microgravity-like conditions [1] and the damping of fluid flow by applying external magnetic fields [2]. Another alternative is to use the accelerated crucible rotation technique (ACRT) proposed for the first time by Scheel and Schultz-Dubois [3], [4] in 1971-1972.

In this study, we focused on modeling the temperature and oxygen distribution in a 200-mm Silicon Czochralski process. The temperature boundary conditions are taken from a 2D global numerical modeling. In order to validate the numerical simulations, a reference case with a counter rotation of the crucible and crystal was taken into account. The crystal rotation rate was fixed at 10 rpm and the crucible rotation rate at 6 rpm. The numerical modeling results for the temperature and oxygen concentration fluctuation will be compared to the striations observed by Lateral Photovoltaic Scanning (LPS) along a Silicon crystal. The results indicated a good agreement between frequencies of the crystal striations and the ones of the melt temperature. This is an indication that the crystal striations are generated by the temperature fluctuations.

Two parameters for the ACRT were investigated in order to achieve the best conditions for the Czochralski Silicon growth process: the variation of the crucible rotation rate and the shortening of the period duration. All numerical modeling was performed using the STHAMAS3D software.

Keywords: Czochralski crystal growth, solar Silicon, ACRT, numerical modeling.

Acknowledgements: This work was supported by a grant of Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P1-1.1-TE-2016-0416, within PNCDI III.

References:
Solar energy has great potential to cover society needs in the context of energy crisis the world is facing today. This is however achievable mainly through seeking reliable and cost-effective options to produce more performant photovoltaic devices. In this work, we attempted to construct a more efficient collector electrode/absorber layer interface within a superstrate-type photovoltaic cell.

In particular, back-contacts relying on large and dense arrays of vertically-aligned copper (Cu) nanowires (NWs) have been first fabricated to considerably enlarge the collector surface of the photogenerated carriers, thus to improve the charge collection efficiency in future photovoltaic applications. The Cu vertical NWs have been grown through an electrochemical synthesis within the nanopores of an anodic aluminum oxide (AAO) template. The proposed electrochemical preparation protocol is cost-effective, versatile and allows an easy control of the NWs aspect-ratio and density on the electrode's surface. The superficial morphology and geometrical parameters of the Cu NWs have been subsequently examined by scanning electron microscopy (SEM).

In a second stage, the as-prepared Cu NWs back-electrodes have been covered with a semiconducting cadmium teluride (CdTe) layer, by employing three methods, namely, vacuum thermal evaporation (VTE), magnetron sputtering (MS) and electrochemical deposition (ECD). The aim of this comparative work lies in the investigation of the inorganic CdTe layer's capability to entirely fill-in the gaps between the Cu NWs, securing thus further a high quality holes collector junction of the ensuing photovoltaic element. The obtained results have been discussed taking into account the CdTe synthesis process in relation to the density of the Cu NWs shaping the back-electrode.

Although still in a preliminary phase, this research work deserves further consideration, as the attained results are promising, potentially allowing the production of affordable and more efficient photovoltaic cells.

**Keywords:** Nanostructured back-electrodes; Copper (Cu) nanowires (NWs); Cadmium teluride (CdTe) films; Solar cells

**Acknowledgement:** This work was financially supported by The Romanian National Authority for Scientific Research (UEFISCDI), through the grants 18PCCDI/2018 and PN-III-P4-ID-PCE-2016-0122.
S1 O19

IMPROVED W-MONOBLOCK WITH EMBEDDED FUNCTIONALLY GRADED THERMAL BARRIERS FOR THE DEMO DIVERTOR

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The DEMO divertor should remove in normal operating conditions, a steady heat flux of at least 10 MW/m². The first choice is to use pure Tungsten (W) as armor material and CuCrZr or an ODS CU-alloy as heat sink material, like in ITER. However, taking into account the current design, these materials will not be able to operate in their optimal temperature windows. This window is defined for W by its brittle to ductile transition temperature (BDTT, ~300–400 °C) and its recrystallization temperature (~1200 °C), respectively. If the recovery temperature under neutron irradiation is also considered, the lower limit for W operation might be increased even to about 800 °C. For Cu-based alloys, the optimal operating temperature window is between 180–200 °C and 300–350 °C, with the lower limit derived again from neutron irradiation recovery considerations and the upper limit by the alloy softening temperature. Moreover, W has a low thermal expansion coefficient (CTE), which generates problems related to its joining to the heat sink materials, which have a much higher CTE. The CTE mismatch between those poses a serious concern due to thermal fatigue in the joints. In an improved monoblock, the optimal operating temperature windows should be overlapping while the CTE mismatch should be mitigated to increase the life time of the divertor components. To improve the heat flow through the divertor’ monoblock we have developed thermal barrier materials [1,2] which, by an adequate graded design [3], are able to solve at least partially the operating temperature windows mismatch. Unfortunately, not completely, since even using such interfaces it is possible either to keep all the W monoblock above BDTT and below recrystallization temperature or to have all the W monoblock above the recovery temperature but in the same time the plasma exposed part well above the recrystallization limit. Further we propose to use a W monoblock produced by 2 different W materials, a plasma exposed part created by K-doped W, which has both higher BDTT and recrystallization temperatures, while the main monoblock is a W composite with low concentration dispersed carbides like SiC or ZrC [4], which should have better mechanical properties at low temperature (below BDTT of pure W). The thermophysical properties of the relevant materials are investigated while FEM (finite element method) simulations based on these experimental results are used to show the feasibility of the concept. A field assisted sintering technique (FAST) route [5] can be used to produce the improved monoblocks.

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Keywords: Fusion reactor materials, thermophysical properties, FEM, FAST

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S1 O20

MAGNETIC PROPERTIES OF (Ni;Co)Fe₂O₄/SiO₂ NANOCOMPOSITES

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We present a detailed study of the magnetic properties of the nanocomposites (Ni;Co)Fe₂O₄/SiO₂ and Fe₃O₄/SiO₂ obtained by various preparation routes. Saturation magnetization (Mₛ), remanent magnetization (Mᵣ), squareness (S), coercivity (Hₑ), magnetic moment per formula unit (n₀), and anisotropy constant (K) are very important parameters for a magnetic material to be used in technical applications such as high-density data storage, sensors and microwave devices, and medical applications. The magnetic properties of these nanocomposite systems can be controlled by the chemical composition, the mean size distribution of the nanoparticles and by the nature of the matrix in which they are embedded [1-3]. The shape of the hysteresis loop revealed the dependence of superparamagnetic behavior on the structural properties. The replacement of magnetic Co²⁺ with zero magnetic moment Zn²⁺ in Co-ferrites induces a gradual reduction of magnetocrystalline anisotropy and the decrease of magnetic coercivity [3]. The magnetic properties are strongly affected by the sample composition and cation distribution within the ferrite structure. The Ni-rich nanocomposites presented superparamagnetic behavior, while the Ni-poor nanocomposites ferromagnetic behavior [4]. Both Mₛ and Hₑ increase with the degree of crystallinity, crystallite size and annealing temperature.

Keywords: Nanocomposite; Nickel-cobalt ferrite; Crystallinity degree; Magnetic properties

Acknowledgments
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S1 O21
DEVELOPMENT OF W-W LAMINATES, FIGHTING AGAINST W BRITTLINESS
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W has the highest melting point of all metals, good high temperature strength, high creep resistance and a high thermal conductivity, properties which make W a first choice for fusion reactor materials. Unfortunately, bulk W has low values for tensile ductility, toughness K_c coefficient (crack growth resistance), and thermal expansion coefficient and also a high value of brittle to ductile transition temperature (BDTT). The later can be however decreased by a finer (under micrometer) grain size structure, produced by severe plastic deformation. Recently, it was shown that thin W foils (under 100 microns) are ductile even at room temperature [1] and this particular and paradoxical feature of W can be used to develop possible new Tungsten based structural materials. Attempts to transfer these properties from W foils to W-based bulk materials resulted in the so-called “W-laminates” concept, i.e. multi layered composites from alternate W and other metal foils. Different metals and approaches have been used to create such composites but several shortcomings were observed at high temperature exposure [2] or during neutron irradiation [3]. In this work we show that is
possible to produce by FAST (field assisted sintering technique) W-W laminates, that is without any other interlayer material. Plates and pipes can be obtained using both simple and K-doped W foils. Micro-structural, thermophysical and mechanical properties are investigated. The application potential of such materials in DEMO fusion reactor is evaluated.

**Keywords:** Fusion reactor materials, W-laminates, thermophysical properties, mechanical properties

**Acknowledgement** This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grand agreement No 633053, WP-MAT. The views and opinions expressed herein do not necessarily reflect those of European Commission.

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**S1 O22**

**ELECTRIC FIELD SWITCHING OF MAGNETIZATION IN HM-Co-MgO SYSTEM: EXPERIMENTS, AB-INITIO, MICROMAGNETIC AND ATOMISTIC STUDIES**

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Voltage controlled magnetic anisotropy (VCMA) became in the last ten years a subject of tremendous interest in the field of spintronics [1] due to its promising potential outcome: ultrafast, low power consumption magnetization manipulation in magnetoresistive random access memories with enhanced storage density. This subject led to the investigation of various experimental multilayer architectures and related spintronic devices. They were commonly composed of a heavy metal (HM), a ferromagnet (FM): iron, cobalt or various complex alloys and an insulating (I) dielectric or ferroelectric material, enabling E-field gating of a ferromagnetic material interface in view of anisotropy control [2].

In a first step, our study clearly demonstrates the voltage control of the perpendicular magnetic anisotropy (PMA). The magnetic analysis, based on anomalous Hall effect magnetometry measurements, has been performed on planar Hall-cross geometry micrometric size devices obtained by sputtering deposition of Pt-Co-MgO multilayer stacks grown in UHV on thermally oxidized silicon wafers patterned by UV-lithography and ion beam etching. Their architecture allows the application of a tunable external E-field across the MgO dielectric layer at the top Co/MgO interface. In a next step, the static magnetic experiments have been completed by extended theoretical studies for acquiring a good insight regarding the dynamics of the switching phenomena and also for finding the configuration which exhibits the highest performance in terms of speed and response to the applied voltage. From ab-initio calculations on HM/FM/I stacks we get a deep insight on electronic structure mechanisms involved in PMA and its voltage control. The ab-initio analysis is completed by micromagnetic simulations. Beyond the confirmation of the observed experimental asymmetric variation of PMA with voltage, our micromagnetic simulations provide a clear insight on the toggling reversal magnetization mechanisms within a nanosecond voltage (E-field) pulse range. Moreover the simulations emphasize the dependence of the switching probability to parameters like surface anisotropy, electric and magnetic pulse shape and frequency, etc, allowing predictive sets of parameters for optimum swithing experiments for realistic devices.

**Keywords:** VCMA, electric field switching.

**References**
EFFECT OF ADDITIVES ON THE PROPERTIES OF ELECTRODEPOSITED CZTS THIN FILMS

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This work involves the synthesis and characterization of CuZnSnS4 (CZTS) layers. The films were prepared on Mo/glass substrate by ecofriendly and simple single-step electrodeposition method followed by sulfurization and annealing at 500°C under Argon flow. The effects of acid boric concentrations on the crystallographic structure, composition, morphology and optical properties of CZTS thin films were investigated, with the objectif to understand the growth behavior and to enhance the film properties. The X-ray diffraction (XRD) analysis showed the formation of the specific kesterite structure. The Raman spectra confirmed the existence of the CZTS phases. The scanning electron microscopy (SEM) was employed to inspect the films surface. The results indicated that the concentration of boric acid affects the physico-chemical properties of the films.

Keywords: thin films, CZTS, electrodeposition, structural characterization, optical properties

CARBON NANOMATERIALS OBTAINED BY ELECTRICAL EXPLOSION OF GRAPHITE RODS IN WATER

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A lot of investigations have been carried to obtained spatial forms of carbon by electrical explosion of graphite. The electrical explosion process creates high temperature and high pressure state. The physical basis of electric discharge technology of synthesis of different forms of CNMs consist in the injection into the working medium (a carbon source) of a high energy needed for its heating and subsequent evaporation, resulting in structural and phase transformations of carbon on individual fragments. Using water as reaction media, ultrafast cooling and synthesis of different types of CNM take place. In this work, to obtain CNM by electrical explosion, a high voltage current pulse generators with 1/10 µs, 8/20 µs, 30/60 µs nominal waveforms, accepting a maximum charge voltage of 100 kV and rated energy of 80 kJ was used. A graphite rod with 2 mm in diameter and 30 mm in lengths was electrically exploded in deionized water at high voltage. The current/voltage wave shapes and total energy absorbed into the samples were presented in the
oscillograms. The resulted powders were structural investigated by scanning electron microscopy, X-ray diffraction, and Raman spectroscopy.

Characteristic oscillogram for electrical explosion of graphite at high voltage and 24 kA

SEM image of CNMs resulted from electrical explosion of graphite rod at 24 kA in deionized water

Keywords: graphite, carbon nanomaterials, electrical explosion.

Acknowledgement: This work was performed by the financial support of the Romanian Ministry of Research and Innovation through the Project Nucleu PN18240102.

S1 O25
SINGLE MATERIAL ORGANIC SOLAR CELLS EXHIBITING FULLERENE AS ACCEPTOR AND TRI-OR DIARYL AMINES AS DONORS

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The synthesis, structural investigation and optoelectronic characterization of original Single Material Organic Solar Cells (SMOSCs) obtained using naphthyl-diphenylamine and methyl-diphenylamine motifs for the building of donors and fullerene C60 as acceptor are reported (Scheme 1). The target solar cells proved to have moderate efficiency.

The linkage of the donors and acceptors was carried out by esterification reactions and the spacers contain several methylene units. The structural investigations of compounds AC-29 and AC-30 were based on multinuclear NMR experiments, (HR)MS spectra, while the photovoltaic properties were determined using absorption and emission spectra, cyclic voltammetry and the classic measurements used for solar cells characterization.

Scheme 1. Access to different pyrene and bipyrene derivatives
EXTENSION OF SHORT-WAVE INFRARED DETECTION BY Sn ALLOYING OF Ge NANOCRYSTALS

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New applications in light sensing for process-monitoring, vision systems, diagnose in medicine, pollution monitoring, etc. have increased the scientific interest in obtaining new materials for light emitters and detectors in short-wave infrared (SWIR) wavelength region of 1.5 µm - 3 µm. Materials based on group four elements Ge-Sn are currently intensively studied as non-toxic and Si technology compatible solution, to replace the present III-V alloys dominating the IR detectors market. The major limitation of the Si photonics is the indirect bandgap character of the commonly used IV-group (Si,Ge,C) alloys. The quantum confinement in quantum dots or nanocrystals (NCs) results in local increase of the optical transition probability, but also in lower absorption in the assemble of NCs, as well as blue-shift of the optical bandgap.

For the optoelectronic applications of nanocrystals, the decrease of recombination centers induced by the grain boundaries requires optimized surface passivation of NCs surface. This can be obtained by embedding the NCs in an oxide matrix, a technique well developed for Ge and Si NCs for photonic applications. This is the pathway adopted in this paper for GeSn NCs. The Sn alloying of Ge results in both decreasing the optical bandgap to compensate the quantum confinement blue shift, and in inducing the transition from indirect to direct character of the bandgap. To obtain this transition in GeSn alloys, the Sn concentration must be increased above 8% as theoretically and experimentally demonstrated. In this paper we present the formation and SWIR optoelectric properties of GeSn NCs embedded in SiO2 matrix, obtained by nano-crystallization thermal treatment of GeSnSiO2 layers deposited by magneton co-sputtering of Ge, Sn and SiO2. The Sn and SiO2 concentrations are varied in the ranges 12 to 22 at.% and 11 to 15 at.% respectively. 5% hydrogen added to Ar enhances the nanocrystallization and increases the photosensitivity. The morphology, composition and structure of layers are investigated by HR-TEM, XRD and XPS. Spectral photovoltaic current measured on heterojunctions of GeSn-NCs with p-Si substrate shows extended SWIR sensitivity up to 2.4 µm in samples containing NCs of 15 at.% Sn.

Keywords: GeSn nanocrystals; nanocomposite, magnetron sputtering; spectral photocurrent

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We acknowledge the support of UEFISCDI-contract no. 58/2016, project M-ERA.NET GESNAPHOTO, and of the Romanian Ministry of Research and Innovation: 2019 Core Programs of NIMP and INOE.
COMPARISON OF NEUTRON POLE FIGURES EXTRACTION METHODS ON THE EXAMPLE OF MYTILUS SHELLS

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Crystallographic texture is a set of preferred grains orientation in polycrystal. It is common in the quantitative texture analysis to draw conclusions based on pole figures (PFs) and orientation distribution function (ODF). Pole figures can be extracted from diffraction patterns measured by X-rays or thermal neutrons. There are two local methods of PFs extraction from neutron patterns [1]. The first one is connected with summation of total neutron intensity recorded by detector for specific diffraction reflex. In this case the part of diffraction pattern is divided into three regions. Two parts are used for background estimation and the central part is for intensity estimation. The second method is local approximation of peak intensity with the bell-shaped function. In this case background is approximated with linear function.

The objective of the present work is to compare these two methods by calculating of differences between measured pole figures and ones recalculated from an ODF and by comparing of RP factors. The comparison is demonstrated on the example of the pole figures extracted for Mytilus Edulis shells. The neutron diffraction time-of-flight patterns for these pole figures were measured with SKAT diffractometer situated at the channel 7A-2 of pulsed nuclear reactor IBR-2 (JINR, Dubna) [2].

The extracting of pole figures were carried out by the computer program „Pole Figure Extractor” [1, 3]. The ODFs computation, pole figure reconstruction, calculation of RP factors and differences between measured and reconstructed PFs were made by using MTEX program [4].

It was revealed that the efficiency of extraction methods depends on peak/noise ratio. The local peak fit gives better result (that is the smaller difference between measured and recalculated pole figures) in case of large peak/noise ratio. The summation of the intensities gives the better result for the peaks with a low peak/noise ratio.

Keywords: neutron diffraction patterns, pole figures, crystallographic texture, Mytilus shells.

The JINR – Romania scientific cooperation program 2018-2019 is acknowledged.

References

PRESSURE INDUCED MODIFICATIONS OF THE MAGNETIC ORDER IN THE SPIN CHAIN COMPOUND Ca3Co2O6

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The low dimensional spin chain magnetic systems exhibit a rich variety of challenging physical phenomena like quantum critical point, Bose-Einstein condensation, Haldane gap excitations, exotic magnetic ground states, formation of magnetization plateaus in external magnetic fields, multiferroicity, which are at the current focus of the extensive research.

Among the spin chain systems an interesting model compound, demonstrating a number of the above mentioned phenomena, is Ca₃Co₂O₆. In the rhombohedral crystal structure of Ca₃Co₂O₆ (Fig. 1), the quasi-1D Ising chains are formed due to alternating arrangement of face-sharing Co(II)O₆ octahedra and Co(II)O₆ trigonal prisms along the c axis, which are arranged in a triangular lattice in the ab plane (Fig. 1a). Due to the different crystalline electric field splittings, the Co³⁺(I) and Co³⁺(II) ions with the octahedral the triangular base prism oxygen coordination have the low spin state LS (S = 0) and the high spin state HS (S = 2), respectively.

The structural and magnetic properties of Ca₃Co₂O₆ spin chain compound have been studied by means of neutron and X-ray powder diffraction at pressures up to 6.8 and 30 GPa, respectively. A suppression of the initial spin density wave phase (Tₐ = 25 K) and stabilization of the collinear commensurate antiferromagnetic (AFM) phase at high pressures (Tₐ = 26 K at P = 2.1 GPa) was observed. The pressure behaviour of the competing intra- and interchain magnetic interactions was analysed on the basis of obtained structural data and their role in the formation of the magnetic phase diagram is discussed. The pressure behaviour of the Néel temperature of the pressure-induced AFM phase was evaluated within the mean field theory approach and the good agreement with the experimental value dTₐ/dP = 0.65 K/GPa was obtained.

Keywords: spin chain, neutron diffraction, high pressures

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S1 P3

CRYSTAL AND MAGNETIC STRUCTURE OF THE DISORDERED IRON OXIDES PbFe₀.₅Nb₀.₅O₃: NEUTRON DIFFRACTION DATA

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Among the objects of the study of modern condensed matter physics, a special place is occupied by compounds and materials based on iron oxides with a structural type of perovskite. These materials have a wide range of crystal and magnetic properties depending on the degree of doping, temperature or high pressures. One of the interesting properties of the oxides PbFe₀.₅Nb₀.₅O₃ are the order and disorder of the magnetic and paramagnetic ions in the crystal lattice. This fact strongly affects the magnetic properties that determine the unique magnetic structures: from ferromagnetic to disporportionate.

My talk presents the results of the studies of crystal and magnetic structures of iron oxides with a structural type of perovskite PbFe₀.₅Nb₀.₅O₃ over a wide temperature range using a neutron diffraction at the DN-6 diffractometer of the IBR-2 high-flux reactor in JINR at the Frank Laboratory of Neutron Physics.

Crystal structure of ordered perovskite PbFe₀.₅Nb₀.₅O₃ describes by the trigonal symmetry R₃m.

In disordered perovskite PbFe₀.₅Nb₀.₅O₃, there is the appearance of antiferromagnetic ordering of G-type at low temperatures. I present the crystal lattice parameters, bond lengths, the magnetic moments of iron for this compound and discuss the models of crystal and magnetic structures forming in PbFe₀.₅Nb₀.₅O₃ based on experimental data.
BALLISTIC 3-PORT INTERFEROMETRIC LOGIC GATES IN THE QUANTUM HALL REGIME

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In this study we report that a 3-port interferometer, defined by quantum point contacts (QPCs) in a two-dimensional electron gas (2DEG), and working in the quantum Hall regime, can implement different logic gates at each port depending on the energy of charge carriers and the operating conditions. The input logic states are encoded in the potentials applied on the QPCs that define the interferometer, while the output logic states are determined by the overall wavefunction transmission coefficient at each port. Thus each output is a linear combination of the 3 possible inputs/edge state sources and determines the operating condition of the gate. One may be aware that in this study we have considered the case of spin-independent scattering at potential barriers, which implies from a practical point of view either small-enough magnetic fields or that the spin-orbit coupling can be neglected, or that spin-polarized charge carriers are injected.

The obtained results indicate that 3-port interferometers can offer a novel manner of implementing logic gates in parallel, without increasing significantly the technological challenges to fabricate them.

Keywords: 3-port interferometer, logic gates, 2DEG, quantum computing

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SPECTROSCOPIC PROPERTIES OF ErF$_3$-DOPED BaF$_2$ CRYSTALS

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In the last decade, the trivalent erbium doped MeF$_2$ (Me=Ca, Ba, Sr) crystals has proven to be one of the most attractive rare-earth media for laser applications or optical communications. The BaF$_2$ crystals are transparent in a large spectral region. The aim of this paper is to investigate the spectroscopic properties of the Er$^{3+}$ ions doped BaF$_2$ crystals using Judd–Ofelt analysis.

The 0.2 mol% ErF$_3$-doped BaF$_2$ crystal was grown in our crystal research laboratory using the vertical Bridgman method. Transparent crystal of about 10 mm in diameter and 6 cm long was obtained in spectral pure graphite crucible, in vacuum ($\approx 10^{-1}$ Pa), using a shaped graphite furnace [1]. The pulling rate was 4 mm/h.

Room-temperature, UV-VIS-IR absorption spectra were recorded by Shimadzu 1650 PC and FTIR Nexus 470 spectrophotometers. The emission spectra were recorded at room temperature, using a Perkin-Elmer spectrofluorimeter. The standard Judd–Ofelt model [2,3] was applied to investigate the emission properties of the crystal. The J-O intensity parameters, $\Omega_2$, $\Omega_4$, and $\Omega_6$, were calculated using a set of six absorption bands obtained from the best fit between the measured and calculated line strengths [4]. These intensity parameters were used to determine the radiative transition probability, oscillator strength, branching ratio, and radiative lifetime of the Er$^{3+}$ transitions from the excited-state $J$ manifolds to the lower-lying $J'$ manifolds. The radiative transition probability and radiative lifetimes are compared to those of Er$^{3+}$ transitions in other hosts [5]. Beside the green emission, recently reported by Bitam at.all. [4], a new emission bands were observed after excitation at 290 nm (transition $^4$I$_{15/2} \rightarrow ^4$G$_{7/2}$) in UV spectral region, not reported previously. The emission intensity of UV band is two times higher then the green emission. There is a good match between the predicted results of the J-O model and the experimental ones.

**Keywords**: barium fluoride, erbium fluoride, J-O analysis, spectroscopic properties.

**References**

MODEL FOR THE THERMAL BEHAVIOR OF MAGNETIC NANOWIRES ARRAYS

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The most remarkable advance in recent decades in magnetism is the trend from bulk macroscopic structures towards systems of microscopic magnetic particles. Moreover, the tendency now is to produce and study organized structures of almost identical magnetic entities. These virtually identical entities organized in geometrically perfect structures have many technological advantages in tailoring the magnetic properties and are consequently intensely studied, with the main aim to understand the complex effect of the inter-particle interactions. When not only the applied field is the input parameter but also the temperature of the sample and
the time dependence of these two factors, the complexity of the models becomes many times too high to be easily tackled with the actual computers.

Many times we are coerced to study simpler structures in which we already understand the static behavior and then to try to discuss the effect of temperature and field dependence of time during a measuring process. In recent years we were able to satisfactorily understand the magnetic behavior of 2D arrays of identical magnetic wires with their axes parallel and all perpendicular to a plane [1-3]. In order to improve the model describing so well the static case of the interacting arrays of nanowires we have added the complete calculus of the energy barriers between the two stable states of the wires (up/down) using in this case the well-known Pfeiffer approximation of the energy barrier in the Stoner-Wohlfarth model [4]. With a Metropolis-Monte-Carlo algorithm one can calculate the probabilities for the switching of the wires which is dependent on the applied field, temperature of the sample and the duration of the experiment. As a test for the algorithm implemented by us we have made first a study of the dependence of the blocking temperature for the array as a function of the geometrical parameters of the system (for two materials – Co and Ni wires). In the presentation we shall describe the effect of the interactions between the wires on the Zero-Field-Cooled (ZFC) curves for the mentioned samples and discuss the results.

**Keywords**: magnetic nanowire arrays, Metropolis-Monte-Carlo algorithm, ZFC.

**References:**

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**S1 P7**

**ON THE CHARACTERIZATION OF OPTICAL SLOT WAVEGUIDES FABRICATED BY AFM NANO-INDENTATION LITHOGRAPHY**

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The slot waveguides are lately studied intensively by researchers, as designing such photonic devices with high geometric accuracy may open new pathways towards construction of modern integrated all-optical devices, such as logic gates, optical diodes and switches, only to mention a few. Among existing architectures, the planar topologies involving bidimensional (2D) building blocks are the most promising, mainly due to the simplicity and cost effectiveness of the fabrication methods involved.

In this work, we report preliminary results on the preparation and characterization of such 2D-engineered slot waveguides. The fabrication method involves multi-step nano-indentation lithography with the help of an atomic force microscope (AFM), on either bare silicon (Si) substrates, or optical glass coated by DC magnetron sputtering with thin silver (Ag) films. The superficial morphology of the prepared slot waveguide configurations is analyzed by AFM and scanning electron microscopy (SEM). Further, subsequent optical properties are evaluated by optical microscopy. Ultimately, the transmission coefficient is extracted and analyzed as a function of the waveguide excitation conditions.
The proposed fabrication protocol based on AFM nanolithography is particularly promising, as it may allow the facile implementation of various slot waveguides with easily tunable configuration, such as plasmonic logic gates, where the gate dimension requires precise control of the slots geometrical parameters.

**Keywords:** slot waveguides; 2D materials; AFM nanolithography; plasmonic logic gates.

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**S1 P8**

**PREDICTION OF ELECTRONIC PROPERTIES BY MACHINE LEARNING TECHNIQUES**

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We explore the possibility of predicting the electronic properties by machine learning techniques. As test systems, graphene nanoflakes (GNFs) with embedded hexagonal boron nitride (h-BN) domains are investigated by combined ab initio density functional theory calculations (DFT) and machine learning techniques. The h-BN domains can be of regular shape, i.e. rectangular, or random. We develop two artificial neural network (ANN) models able to reproduce the gap energies with high accuracies and investigate the tunability of the energy gap, by considering a set of GNFs with embedded rectangular hBN domains. In one ANN model, the input is in one-to-one correspondence with the atoms in the GNF, while in the second model the inputs account for basic structures in the GNF, allowing potential use in up-scaled structures. The approach based on ANNs is therefore a feasible route, providing a reduction of the computational effort, while retaining a high accuracy and therefore may be employed for optimizing the design and selecting candidates of nanostructured graphene based materials for specific electronic properties. The methods presented here can be applied to other systems, such as high entropy alloys.

Fig1. Graphene nanoflake passivated with hydrogen and hexagonal boron nitride domains.

**Keywords:** graphene - h-BN nanoflakes, DFT, artificial neural networks


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**S1 P9**

**TERAHERTZ CHARACTERIZATION OF (Ba,Sr)TiO₃ FERROELECTRIC FILMS GROWN BY PLD AND RF MAGNETRON SPUTTERING**


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(Ba,Sr)TiO$_3$ (BST) ferroelectric solid solutions, in both bulk and thin/thick film form, have been intensively studied during the last 30 years for their integration in electrically-controlled devices. Here we report on the synthesis and characterization of BST thick films grown by pulsed laser deposition (PLD) and radio frequency magnetron sputtering methods. Samples with various strontium content were deposited on single-crystal substrates (Si, MgO, Al$_2$O$_3$) with low absorption in terahertz domain. Morphological, structural and optical investigations of the samples were performed by Atomic Force Microscopy, X-ray Diffraction and Spectroscopic Ellipsometry. As a result of a parametric study, single-phase BST films with thicknesses higher than 1 micrometer where selected for terahertz characterization. The measurements were carried out by using the Aispec IRS 2000 PRO terahertz time-domain spectrometer on transmission set-up in the 0.5 - 3 THz range. The time-domain data have been transformed to frequency-domain in an approximate manner with a commercial software (TeraLyzer). Experimental data will be discussed and compared with respect to substrate type and thickness of the films.

**Keywords**: Barium strontium titanate, ferroelectric thick films, terahertz spectroscopy.

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**S1 P10**

**CARBON-PLATINIUM NANOSTRUCTURES USED IN CATALYTIC PROCESSES**

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The latest generation catalysts for ORR (Oxygen Reduction Reaction) require the use of Pt-based materials as they have demonstrated the highest efficiency in terms of both activity and durability. However, the high cost and deficiency of Pt, added to long term thermal stability and limited tolerance to impurities of Pt-based catalysts, remain important bottlenecks for combustion cells.

Carbon nanoparticles are often used as catalyst support due to their stability in both acidic and basic media, good electrical conductivity and high specific surface area.

The carbon support can influence the performance of the catalyst in the fuel cells, such as mass transport and electrical conductivity, the electrochemical active surface, and the stability of the nanoparticles during operation. At the moment, there are a number of Pt-based catalysts on the market that use carbon nanoparticles as a support.

In this paper there are presented some C/Pt-based nanostructurated catalysts obtained by laser pyrolyses technique; theses nanostructures are characterized by TEM, SEM, STEM, XPS and Raman techniques..

**Keywords**: ORR, Pt-based catalyst, carbon nanoparticles.

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**S1 P11**

**RHEOLOGICAL RESPONSE IN CELLULOSE ACETATE/ TETRAETHYL ORTOSILICATE BINARY SYSTEMS**

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In the present work we report the rheological response through dynamic viscosity of cellulose acetate (CA) solutions in tetrahydrofuran (THF), in absence and presence of tetraethyl ortosilicate (TEOS) in different amounts (1.0-2.0 wt./wt.), over a range of shear rates between 0.1-100 1/s, at temperature of 25°C.
The dynamic viscosity dependence on shear rate was plotted and compared with the results obtained by other researchers for similar systems [1].

From Fig. 1 were observed a Newtonian behavior for CA, as well as a thinning behavior for CA/TEOS binary systems. Decreasing of the dynamic viscosity with increasing of the shear rate may be a consequence of the polymer backbone disentanglement, and orientation of the polymer chain in the flow direction during the rheological measurements. Also, for CA/TEOS solutions an increase in viscosity with TEOS content was found. This behavior is justified by the fact that -OH groups of cellulose acetate and Si-OH belonging to TEOS, are able to form new hydrogen bonds gradually leading to gelling process [2].

Fig. 1. Dynamic viscosity, \( \eta \), dependence on shear rate, \( \dot{\gamma} \), for cellulose acetate and cellulose acetate/tetraethyl orthosilicate binary system

The results obtained in present study has aimed the highlighting the solutions rheological response, being the basis for future preparation of neat cellulose and cellulose/tetraethyl orthosilicate (TEOS) composite membranes applied in a wide variety of fields from industrial to medical i.e., as membrane for adsorption, separation, catalysis, sensors, drug delivery or tissue regeneration [3,4].

**Keywords:** dynamic viscosity, thinning behavior, gelling process.

**References.**


S1 P12

**STRUCTURAL CHARACTERIZATION OF ZNO NANORODS/GRAFHE COMPOSITES SYNTHESIZED BY HYDROTHERMAL METHOD**

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Zinc Oxide (ZnO) is a multifunctional semiconductor material and its used in applications involving sensors, light-emitting diodes (LEDs), piezoelectric devices, solar cells. Graphene, exhibits properties such as ultrahigh electron mobility, large surface area, high chemical and thermal stability, excellent electrical and optical properties.

The goal of this study is to obtain the porous 3D graphene network on nickel foam template by chemical vapor deposition (CVD) at high temperatures using methane as carbon source. ZnO-graphene (ZG) composite was developed using hydrothermal method to deposit zinc oxide directly on the 3D graphene network.
The prepared ZG were structurally characterized by X-ray diffraction, Raman technique and Scanning Electron Microscopy. The analysis of X-ray diffraction showed that the samples had hexagonal wurtzite structure. From SEM imagine we obtain hexagonal ZnO nanorods structures.

ZnO-graphene were synthesized in order to develop a good material for energy applications.

**XRD patterns of ZnO nanorods/graphene composites synthesized by hydrothermal method**

**SEM images of ZnO nanorods/graphene composites**

**Keywords**: ZnO, nanorods, graphene, semiconductor.

**Acknowledgement**: This work was performed by the financial support of the Bilateral Collaboration Romania-Russia, project position 32 from the JINR Order no. 397/27.05.2019, and the contract no. 30PFE/2018 between National R&D Institute for Electrical Engineering ICPE-CA and Romanian Ministry of Research and Innovation.

**S1 P13**

**INVESTIGATION OF ZNO/GRAFHENE NETWORKS NANOSTRUCTURES OBTAINED BY MAGNETRON SPUTTERING TECHNIQUE**

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Over the last decades, the semiconductor materials were considered as very attractive materials for application in sensing devices, solar cells, as well as in energy storage and conversion.

Combining ZnO with conductive materials such as carbon nanostructures (e.g., carbon nanotubes, graphene, graphene oxide) has shown an improved electrical conductivity of the final composite. Because these ZnO/carbon composites already offer significant technological impact in a wide field of applications, the development of new synthesis methods for conductive ZnO/graphene networks nanostructures with a large surface area has become one of the main research focus in the field of materials for energy applications.

**SEM images of graphene and ZnO thin film deposited on graphene by magnetron sputtering technique**
The graphene networks were obtained by chemical vapor deposition on nickel foam catalyst using a gas mixture of methane as carbon source, argon, and hydrogen at atmospheric pressure for 60 minutes. In this work, ZnO/graphene networks nanostructures were developed using magnetron sputtering technique to deposit zinc oxide directly on the graphene networks.

The graphene networks and the ZnO/graphene networks nanostructures were investigated by scanning electron microscopy, X-ray diffraction, and Raman spectroscopy.

**Keywords**: graphene networks, zinc oxide, nanostructures, magnetron sputtering.

**Acknowledgement**: This work was performed by the financial support of the Bilateral Collaboration Romania-Russia, project position 32 from the JINR Order no. 397/27.05.2019, and the contract no. 30PFE/2018 between National R&D Institute for Electrical Engineering ICPE-CA and Romanian Ministry of Research and Innovation.

**Keywords**: Calcium phosphate glasses, Magnetic properties, Magnetic susceptibility.

**References**:  

**S1 P15**  
**OPTICAL AND CONDUCTIVE PROPERTIES OF THE COMPOSITES BASED ON IRON OXIDE AND CARBON NANOTUBES**  

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Composites based on Fe$_2$O$_3$ and double-walled carbon nanotubes (DWNTs) were prepared by hydrothermal (H) method and the mechanico-chemical (MC) interaction of the two constituents. Using the two methods, the DWNTs/Fe$_2$O$_3$ composites with a DWNTs concentration equal to 8 and 27 wt.%, were prepared. Studies of scanning electron microscopy (SEM) demonstrate that the two synthesis methods, i.e. H and MC, lead to the spherical particles with size ~2.21 - 6.2 μm and ~ 48.52 nm, respectively. A core-shell structure of the DWNTs/Fe$_2$O$_3$ composites is invoked by SEM. The presence DWNT is proved by X-ray diffraction (XRD),
Raman scattering and dielectric spectroscopy. XRD studies performed on the DWNTs/Fe₂O₃ composites, synthesized by H and MC ways, highlight two broad lines at 25° and 44° belonging to DWNTs over which is overlapped a series of sharp lines in the 30° ≤ 2Θ ≤ 70° range coming from the Fe₂O₃ particles. Raman spectra of these composites are characterized in: i) the low frequencies range, by four lines peaked at 224, 288-396, 496 and 604 cm⁻¹ assigned to the A₁g, E₂g, A₁g, E₈ vibrational modes of Fe₂O₃ [1] and ii) the high frequencies range, by two bands having maxima at 1348 and 1585 cm⁻¹ assigned to the disorder state or defects (D) induced to the graphitic lattice and tangential mode (TM) of DWNTs, respectively [2]. The Fe₂O₃ particles assembling onto the DWNTs surface induce a progressively changing of the ratio between the intensities of the two bands, D and TM, from 0.18 to 0.87 and 0.96, as increasing the DWNTs concentration from 0 wt.% to 8 and 27 wt.% in the DWNTs/Fe₂O₃ composite weight. This fact confirm a DWNTs functionalization with Fe₂O₃ particles. Dielectric spectroscopy studies carried out on the Fe₂O₃ particles highlight several dielectric relaxation processes and an intrinsic electric conductivity. The relaxation processes can be assigned to intra-granular or inter-granular mechanisms. Mössbauer and SQUID magnetometry measurements performed on DWNTs/Fe₂O₃ composites infer the formation of maghemite like Fe oxide particles in case of the MC method and of mainly hematite like particles in case of the H method of synthesis, with the hematite like particles much better formed and of larger size as in case of the maghemite ones. Regardless of the synthesis methods, the DWNTs/Fe₂O₃ composites show a single dominant conduction mechanism in the low relative frequencies range (1Hz-10kHz). These results indicate that DWNTs generate bridges between Fe₂O₃ particles, allowing movind of electrical charge over longer distances.

Keywords: iron oxide, double-walled carbon nanotubes, optical properties, dielectric spectroscopy.

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References

S1 P16

INTERFACES IN CoFe₂O₄@TiO₂:Tb MAGNETIC RECOVERABLE NANOCOMPOSITES WITH ENHANCED PHOTOCATALYTIC ACTIVITY

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Photocatalytic technology represents the most important routes for removing organic pollutants from wastewater. One major challenge in photocatalysis applications is the separation and recovery of nanosized photocatalyst particles from the treated water. In this regard, the use of magnetically separable composite photocatalysts represents a convenient approach for wastewaters treatment.

The purpose of the present work is to study the influence of synthesis conditions on morpho-structural, optical, magnetic and photocatalytic properties of CoFe₂O₄@TiO₂:Tb composite nanoparticles. The CoFe₂O₄@TiO₂:Tb core-shell nanoparticles were prepared by a two-stage process: first CoFe₂O₄@TiO₂:Tb nanoparticles were obtained by chemical coprecipitation method and then they were coated with terbium doped TiO₂ nanocrystallites by a sol-gel process. Finally, the samples were calcined at 550°C in order to get the anatase phase of titanium dioxide.

The composites were characterized by using X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM and high resolution-TEM), Photoelectron Spectroscopies (XPS, UPS), FT-IR and Raman Spectroscopy. Also, magnetization behaviour and photocatalytic properties were investigated. Electron Spin Resonance (ESR) experiments coupled with spin-trapping technique were carried out in order to evidence the production of reactive radical groups at the solid–liquid interface of TiO₂.
The photocatalytic tests demonstrated that the composite nanoparticles exhibit good photocatalytic activity toward the degradation of RhB solution. The high photocatalytic activity of CoFe$_2$O$_4$@TiO$_2$:Tb composites can be attributed to the synergetic effects of different components from the composite nanostructures.

**Keywords:** nanocomposites, titania, magnetic photocatalyst.

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S1 P17

AB INITIO INVESTIGATION OF ENERGY LEVELS STRUCTURE AND SPIN-HAMILTONIAN PARAMETERS OF Cr$^{3+}$: Al$_2$O$_3$ LASER CRYSTALS

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Corundum ($\alpha$-Al$_2$O$_3$) crystals doped with transition metal (TM) ions have wide applications in solid state laser devices [1]. The crystal $\alpha$-Al$_2$O$_3$ crystallizes in the $R3c$ space group (No. 167) with six chemical formula units in one unit cell [2]. Al$^{3+}$ ions are coordinated by six O$^{2-}$ ions in Al$_2$O$_3$ crystals, and the local structure of [AlO$_6$]$^9-$ clusters have octahedral symmetry with slight distortion along a threefold axis coinciding with the c crystaline axis of crystal. When TM ions are doped into Al$_2$O$_3$ crystals, they will substitute Al$^{3+}$ ions without charge compensation and the space group will decrease to No. 146 (trigonal symmetry).

In this paper we present, in the unified frame, the results of the ab initio investigation of energy levels structure, ligand field and spin-Hamiltonian parameters for trivalent chromium doped $\alpha$-Al$_2$O$_3$ crystal. Our calculations are based on a new methodology [3] applied to cluster [CrO$_6$]$^3-$ embedded in an extended point charge field of host matrix ligands. After DFT optimization of the doped crystal, the ab initio energy calculation of the electronic states and corresponding wave functions of Cr$^{3+}$ is documented from the complete active space self-consistent field (CASSCF). The improved energy states from N-electron valence second order perturbation theory (NEVPT2), second order dynamic correlation dressed complete active space (DCD-CAS2), difference dedicate configuration interaction with three degrees of freedom (MRDDCI3) and spectroscopy-oriented configuration interactions (SORCI), has been analyzed. The ab initio ligand field theory (AILFT) [4] procedure allows extracting all LF parameters and spin-orbit coupling constant for studied case. In addition, spin-Hamiltonian parameters ( zero-field splitting (ZFS) parameter $D$ and $g$-factors $g_\parallel$ and $g_\perp$ for the ground state $^4A_2$ of Cr$^{3+}$ ion in corundum are presented in detail, taken into account the full configuration interaction.

The obtained results are discussed and the comparisons with measured values from literature [5] show a reasonably agreement, which justifies this new route of investigation.

**Keywords:** Cr$^{3+}$:Al$_2$O$_3$, ab initio, energy levels, spin-Hamiltonian parameters.

**References**


S1 P18

PVDF MEMBRANE MODIFIED WITH Cu DOPED ZnO NANOPARTICLES FOR WATER TREATMENT BY ULTRAFILTRATION AND PHOTOCATALYSIS

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Photocatalysis technology is an effective and green method for the removal of organic pollutants from water. The catalyst loss in separation process from suspension system represents an important drawback of photocatalytic technology. This issue could be solved by immobilization of catalyst on porous materials like activated carbon and membranes. Membrane filtration technology can efficiently separate suspended solids, bacteria and macromolecule solutes. By combining photocatalysis and membrane filtration technology the efficiency for treatment of pollutants can be enhance due to a series of synergistic effects which appears. Based on the above mentioned, in this study were synthesized and characterized Cu doped zinc oxide (ZnO) nanoparticles. The obtained nanoparticles were blended in polyvinylidene fluoride (PVDF) membrane casting solution to prepare nanocomposite ultrafiltration membrane with photocatalytic activity under light irradiation. The synthesized nanoparticles were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), UV-Vis, EPR and XPS spectroscopy. The effect of the embedded nanoparticles on morphology, band gap energy and photocatalytic performance of PVDF prepared membranes was studied. SEM images showed significant changes in cross-section morphologies of the composite membranes. Rhodamine B (RhB) dye solution was used to evaluate photocatalytic activity of catalyst and composite membrane. The photocatalytic mechanism was elucidated based on the identification of radical oxygen species involved and in accordance with energy bands alignment, and porosity. The presence of radical species at the solid–liquid interface was evidenced using ESR experiment coupled with spin-trapping technique.

Keywords: PVDF membrane, Cu doped ZnO, photocatalysis.

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S1 P19

SYNTHESIS AND CHARACTERISATION OF MWCNTs DECORATED WITH TiO2:Mn NANOPARTICLES

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Multi Walled Carbon nanotubes (MWCNTs) have attracted a lot of attention in last decades due to their unique molecular geometry, the excellent electronic, thermal, and mechanical properties [1]. Incorporation of metal oxides with CNTs will lead to the formation of nanocomposites having the properties of both components, which would be useful for PEC water splitting and photocatalysis as CNTs are very good electron acceptor [2].

In this paper we report a simple strategy for decoration of MWNTs with TiO2:Mn nanoparticles by a polymer wrapping-technique that is non-invasive, and does not introduce defects to the structure of CNTs. At a constant MWCNTs : TiO2 ratio, the Mn doping concentration influence on the composite properties was
studied. The composites were characterized by using XRD, RES, TEM and HRTEM, XPS and UV-Vis Spectroscopy. The photocatalytic activity of the nanocomposites was evaluated by photodegradation of Rhodamine B (RhB) in a Laboratory-Visible-Reactor system with a 400 W halogen lamp (Osram) which emits in visible range.

The results revealed that by adjusting the composition of components, one can control the decoration efficiency and, by consequence the application areas of these composite nanoparticles.

**Keywords:** composite nanoparticles, TiO$_2$:Mn, decoration, MWCNT.

**Acknowledgments:** Financial support from the Romanian Ministry of Research and Innovation, Core Programme, Project PN19-35 02 03 is gratefully acknowledged.

**References**

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S1 P20

**SOL-GEL SYNTHESIS AND CHARACTERISATION OF Co-BASED SOFT MAGNETIC NANOCOMPOSITES**

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The soft magnetic nanocomposites, based on FeCo/Al$_2$O$_3$ and Co/SiO$_2$ nanoparticles were prepared using chemistry routes. These magnetic nanocomposites consist on magnetic nanocrystallites, arranged in a crystalline matrix and were synthesized using the sol-gel route, starting from salts of Fe, Co, Al and respectively tetraethyl orthosilicate (TEOS) [1]. The presence of the oxide layer, consisting on Al$_2$O$_3$ or SiO$_2$, combined with the magnetic properties of FeCo compound or Co, leads to the development of novel materials with improved magnetic and electric performances: high saturation magnetisation, low coercivity and increased resistivity [2,3]. The main advantages of these nanocomposite magnetic materials are the following: (i) due to the enhanced resistivity, the losses by eddy currents are reduced and (ii) the metallic elements with high saturation magnetization and high Curie temperature, such as Fe and Co, possess performant intrinsic magnetic properties. These benefits recommend the Co-based electrically insulated nanopowders, after consolidation by sintering, as potential candidates for high frequency applications: rotoric cores for high speed motors, inductors, cores for planar transformers etc. The paper presents the experimental results concerning the chemical synthesis of Co-based, electrically insulated nanopowders and their structural and magnetic properties.

**Keywords:** FeCo/Al$_2$O$_3$ and Co/SiO$_2$ nanoparticles, sol-gel technique, soft magnetic, high frequency

**Acknowledgement:** Financial support is gratefully acknowledged from the Romanian Space Agency: the Research, Development and Innovation STAR Programme - Technology Space and Advanced Research (ctr. STAR No. 125/2017 and STAR No. 176/2017).

**References:**
COMPARATIVE ANALYSIS OF ADSORPTION PROCESS OF ISOBUTYL XANTHATE SOLUTIONS ON THE SURFACE OF SPHALERITE USING OPTICAL REFLECTOMETRY

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Continuous reflectance measurement is proposed in this work for the evaluation of the kinetics of adsorption processes at the interface level of K-isobutyl xanthate solution and sphalerite natural mineral, or crystalized ZnS deposited on amorphous substrate. This way important comparative information was obtained regarding time to achieve dynamic equilibrium at the interface level leading to the optimization of froth floatation processes [1].

Reflectance measurements were made at the thin adsorption layer formed between non-activated or activated sphalerite natural minerals, or crystalized ZnS and K-isobutyl xanthate solution. Sphalerite is the most important industrial mineral of zinc and is usually recovered by froth flotation. But its poor response to common xanthate collector is also well known, therefore copper sulphate is used as activator. This shows how important studying activation and collection process is from both theoretical a practical point of view. Because natural minerals also contain trace elements, the obtained results had to be compared with ones from prepared, crystalized, chemically pure samples. Therefore, both nonactivated and activated ZnS was also used in our determinations.

Continuous monitoring of the reflected monochromatic radiation intensity was done at the \( \lambda=0.89\mu m \) wavelength of a GaAs laser. This assured high transmission rates in the xanthate solution, strong reflection on the solid surface, minimal influence of surface defects, easy implementation using a widely available radiation source, and a collimated beam. A single Y-shaped quartz optical fiber was used as common channel distributor.

Reflectance measurements were done at the industrial temperature of 18°C, in the pH range of 7-10, for the xanthate solution concentrations: 10 mg/l, 25 mg/l, 50 mg/l, 100 mg/l and 3000 mg/l [2].

At least a threefold increase of reflectance signal for the activated mineral, with an optimal pH range between 7-8 and a xanthate solution concentration of 50 mg/l was observed. In these conditions, a minimum time to achieve dynamic adsorption-desorption equilibrium of 15-20 minutes was obtained this way. Deviations from the theoretical isotherms were also observed, underlining the need for a more complete theoretical model. Good correlations between determinations for the natural mineral and deposited ZnS crystals were also obtained [3].

**Keywords:** sphalerite natural mineral, isobutyl xanthate, activation, interface layer dynamics.

**Acknowledgements.** The authors acknowledge partial financial support of the TUCN, NUC Baia Mare, Romania – JINR Dubna, Russian Federation joint research projects.

**References.**
The layered perovskites TbBaCo$_2$O$_{5.5}$ have attracted much attention due to the interplay between magnetic and magnetotransport properties. The cobalt oxide materials demonstrate spectacular range of physical phenomena, which are currently extensively explored – giant magneto-resistance, spin state, insulator-metal, orbital and charge ordering transitions.

The physical phenomena observed in the RBaCo$_2$O$_{5.5}$ – based systems are mediated by a complex interplay of spin, charge, orbital and lattice degrees of freedom. A role of particular factors responsible for the formation of magnetic properties can be explored by application of high pressure due to different response of various degrees of freedom on the modification of interatomic distances and angles, driving underlying interactions.

Recently it was found that a gradual insulator-metal transition, accompanied by a structural phase transformation, is induced in TbBaCo$_2$O$_{5.5}$ by application of high pressure at P~5-10 GPa at ambient temperature. In contrast, the pressure effects on the Fe-substituted systems remain poorly explored.

Therefore, the crystal and magnetic structures of the perovskite-like, oxygen deficient layered cobalt oxide TbBaCo$_{1.91}$Fe$_{0.09}$O$_{5.5}$ have been studied by means of neutron and X-ray diffraction at high pressures up to 6.2 and 30 GPa, respectively.

The structural anomalies in lattice compression at P=20-25 GPa were revealed, which could be associated with the insulator-metal transition. At ambient pressure below $T_N=300$K a formation of the complex magnetic structure on the Co/Fe sublattice, comprising the G-type antiferromagnetic (AFM) and ferromagnetic (FM) components, was observed. Below $T=150$K the FM component vanishes. At $T=5$K a presence of the long range AFM order on the Tb sublattice was also revealed. At high pressures, the FM component becomes suppressed and the only G-type AFM order is found for the Co/Fe sublattice.

The Néel temperature decreases noticeably down to 275K at P=6.2GPa with a pressure coefficient $dT_N/dP=-4$K/GPa. The intrinsic mechanisms of the observed pressure-induced magnetic phenomena are discussed.

**S1 P23
RAMAN SPECTROSCOPY STUDIES UNDER HIGH PRESSURE IN WIDE TEMPERATURE RANGE: NEW OPPORTUNITIES**

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The dramatic progress in extreme condition research is caused by a discovery of great number of novel interesting phenomena in condensed matter physics and material science, chemistry, geophysics and planetary research. In a comparison to other experimental methods, the application of high pressure is a direct method of controlled changing of some physical properties by means of variation of interatomic distances and angles.

Raman spectroscopy studies has many advantages for studies of the various materials and involve on both fundamental and applied studies in fields as diverse as chemistry, physics, materials science, surface science, nanoscience, and the life sciences.

Raman spectroscopy is a non-destructive technique providing dynamic and structural information on molecules. It has been applied to analyses of protein dynamics, drug interactions, single cells, bacteria and viruses, and it provides a characteristic signal for certain molecular bonds. The position and intensity of peaks in a Raman spectrum relate to the composition and structure of molecules. The positions of the maxima depend on specific vibrational modes (for example carbon–carbon single-bond or double-bond stretching), and are very sensitive indicators of differences in the molecular structure.

In addition, Raman spectroscopy is an ideal method for identifying polymorphs. It is successfully shows the quantitative polymorphic analysis, because it provides excellent fingerprint spectra specific to each crystal structure.

Present report is focused on resent progress in technics and methods for research under extreme conditions in Frank Laboratory of Neutron Physics: Raman spectrometer with diamond anvils cells. The
prospects for further progress in development of Raman spectroscopy techniques under extreme conditions are discussed.

As an example of high pressure research, the recent results of studies of the spin chain cobaltite Ca$_3$Co$_2$O$_6$ at high pressures are presented.

The Raman-active vibrational modes of Ca$_3$Co$_2$O$_6$ under high pressure were obtained. The pressure-induced variations in atomic dynamics of spin chain cobaltite Ca$_3$Co$_2$O$_6$ are discussed.

S1 P24
FORMATION AND INVESTIGATION OF THE PROPERTIES OF COMPOSITE BASED ON ZIRCONIUM DIOXIDE ZrO$_2$ FOR SENSOR APPLICATION

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At the moment nanotechnology is one of the most promising field of science and technology. Nanomaterials based on zirconium dioxide ZrO$_2$ is of great interest that has been conditioned by its own special characteristics. In particular discreteness of the energy zones, which makes it possible to consider it as a quantum object. Whenever quite high coverage of dielectric permittivity ($\varepsilon = 25$) and high chemical activities allow interaction with the gas atmosphere wide range of heterogeneous processes, including a high-energy (up to $5 \times 10^6$[1]), and containment ions on the surface. That is why nanoparticles ZrO$_2$ of interest to functional application that involves an exchange with an environment.

The reversible absorbing processes on the nanopowders surface can be used in sensor techniques as a humidity sensor. This type of sensors differ advantageously from semiconductor analogues, because it need not burn the adsorbents, has swift action and highly-processible method. The obtaining and investigation of these humidity sensors was a goal for the work.

The planar humidity sensors as films of hydrophilic biopolymer Alginate, which is consist of nanoparticles ZrO$_2$ – 3mol% Y2O3 (YSZ) were made on a dielectric substrate with gold and silver electrodes. The method is a spray-pyrolysis. The production technology have been described in [2].

During the experiment has been proved that humidity sensors received in 4000C are more sensitive in the range of low concentrations of water (humidity less than 30%). While other have a much broader range for 50% humidity. A difference was also established between conductivity various metals on electrodes.

It should be noted that received humidity sensors have biocompatible qualities.

Keywords: perspective building technologies, powder nanotechnologies, zirconium dioxide nanoparticles, biocompatible humidity sensors.

The work was supported through the project H2020/MSCA/RISE/HUNTER/691010 and JINR-Romania Cooperation Programme Project of 2019.

References:
INVESTIGATION OF FERROELECTRIC PROPERTIES OF Al:HfO_2 THIN FILMS OBTAINED BY ATOMIC LAYER DEPOSITIONS ACCORDING TO SLOW THERMAL TREATMENT TEMPERATURE

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The effects of slow heat treatment on crystal structure and ferroelectric properties of Al:HfO_2 films have been investigated. Ferroelectric capacitors based on aluminum (Al) doped hafnium oxide (HfO_2) grown on platinum (Pt)/silicon substrates and Cr/Au top electrodes were fabricated. Formation of orthorhombic phase in thin films Al:HfO_2 was revealed by X-ray diffraction (GIXRD). Recording and investigation of ferroelectric domains in Al:HfO_2 films was performed using the piezoresponse force microscopy (PFM) technique.

Atomic force microscopy (AFM) analyzes indicate a very low average roughness value for all thin films grown less than 0.25 nm. The electrical characterization was evaluated by voltage-to-voltage (C-V) and current-to-voltage (I-V) measurements in the range of 25°C to 350°C. Significant changes in crystal structure were noted with the increase of thermal treatment temperature.

Keywords: Atomic Layer Deposition, hafnium oxide, ferroelectrics.
Acknowledgments: The authors acknowledge the financial support from the Ministry of Research and Innovation, CNCSIS-UEFISCDI for grant number PN-III-P4-ID-PCCF-2016-0033 (GRAPHENEFERRO) and POS CCE, O2.2.1, nr. 254/28.09.2010, Cod SMIS-CSNR: 14040 project.

GENERATOR THERMOELEMENTS OF PARMEABLE MATERIALS

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The use of thermal waste from industry and internal combustion engines is a promising line of solving the tasks of conservation of energy resources. Attractive properties of thermoelectric method of direct thermal into electric energy conversion, namely the absence of movable parts and possibility of functioning under extreme conditions, make thermoelectric generators advantageous over the others. In so doing, it is customary to use thermoelectric modules of homogeneous materials whose maximum value of thermoelectric figure of merit is achieved in a rather narrow temperature range. This is responsible for insufficient efficiency of thermoelectric power converters, hence restricts the possibilities of their practical use.

At the same time, growing interest has been observed recently in the study of permeable thermoelements, where heat input and removal occurs not only on the junctions, but also due to the use of a developed heat exchange surface in the bulk of legs material. Such thermoelements are made permeable for pumping gas or liquid flows, which allows improving the efficiency of thermoelectric energy conversion. The use of permeable structures in thermoelectric modules with Bi-Te made it possible to improve the efficiency of energy conversion by 20%.

Results of investigations of permeable thermoelements based on Bi-Te, Pb-Te, Co-Sb are presented. Optimal parameters and concentrations of doping impurities whereby maximum efficiency of thermal into electric energy conversion is accomplished are determined. Possibility of 1.2-1.4-fold efficiency increase of permeable thermoelements of Bi-Te, Pb-Te, Co-Sb based materials as compared to conventional ones.

Keywords: permeable materials, thermoelectric elements, segmented material.
S1 P27
STRUCTURAL PROPERTIES OF N DOPED SIC NANOSTRUCTURES OBTAINED BY MAGNETRON SPUTTERING METHOD

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Silicon carbide (SiC) is a generic name for a material produced by numerous process routes that result in a host of different external and internal microstructures and, as a consequence, a broad range of properties. The resulting properties of SiC make a substantial variety and number of applications possible, especially for use under challenging conditions.

Si-C nitrogen doped thin films were obtained by Magnetron sputtering method, varying the temperature of the substrate and the quantity of nitrogen. To characterize the structure of as-prepared N-SiC coatings we used Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Raman spectroscopy techniques.

Keywords: SiC nanostructures, Magnetron sputtering method, TEM, RAMAN, N doped, coatings

S1 P28
CuFeCo THIN FILMS: SYNTHESIS AND CHARACTERISATION

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In this study CuFeCo films were deposited by Thermoionic Vacuum Arc (TVA) method was used. Gigant Magnetoresistance (GMR) appears in thin films composed of metallic alternative ferromagnetic and non ferromagnetic layers, when the magnetic grains are isolated in the non magnetic matrix. The electric resistance of the films show a considerable decrease in the presence of the magnetic field. Films with a thickness of 100 nm each were deposited on glass substrate and also on silicon substrate. In order to create the films, two TVA guns have been used, which have evaporated simultaneously, under a pressure of $10^{-6}$ torr, the material from the two melting pots, one of them containing Cu and the other one containing Fe and Co in a proportion of 50% each.

In order to investigate the films, the Scanning Electron Microscopy (SEM) was used, which helped in examining the morphology of the surfaces of the samples. On the surface of the samples crystallities with dimensions of aprox 5-7 nm were identified, disposed in granular formations whose diameters are between 20 and 50 nm. The Energy-Dispersive X-ray (EDX) spectroscopy shows, besides the elements used to obtain the thin film (Cu, Co, Fe), the presence of some foreign elements such as Si, O, Ca, K, part of them due to the glass which has been used as a substrate, but also due to Ni element, which is most probably a processing impurity.

Keywords: TVA, GMR, SEM, EDX.
SPIN-CROSSOVER METAL COMPLEXES OF 2,2’-BIPYRIDINE BASED MACROCYLES

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The spin-crossover (SCO) phenomenon corresponds to the reversible spin-state switching in certain metal complexes, which can be induced by temperature, pressure and light or other external fields. The SCO phenomenon occurs mainly in some first row transition metal complexes of d\textsuperscript{4}-d\textsuperscript{7} electronic configurations. The phenomenon of spin-crossover has an important impact on the properties of a solid material, including colour, magnetic moment, optical density, electrical resistance and thus, materials with SCO are of major interest through their potential applications such as molecular memory, sensors or molecular switches \cite{1}. The associated change in the electronic state between low-spin (LS) and high-spin (HS) states of the metal is related to the population of antibonding orbitals and leads to changes in the bond lengths and volume of the system \cite{2}.

Herein we present the design and synthesis of metal complexes of 2,2’-bipyridine based macrocyles (Figure 1) which might present laser radiation induced spin crossover. Various possible SCO compounds of this class will be considered and the most promising candidate will be synthesized and characterized.

![Figure 1: Schematic representation of SCO 2,2’-bipyridine based macrocyles metal complexes](image)

X: C=O; NHR, NR\textsubscript{2}, CR\textsubscript{2}
M: Ni\textsuperscript{2+}, Fe\textsuperscript{2+}, Cr\textsuperscript{2+}, Pd\textsuperscript{2+}, Pt\textsuperscript{2+}

Keywords: spin crossover, macrocyle, metal complex

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OPTICAL CHARACTERISTICS OF OXIDE THIN FILMS DEPOSITED BY RADIO FREQUENCY MAGNETRON SPUTTERING DEPOSITION

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\textsuperscript{1}married as Garoi
This study reports the influence of the deposition conditions of SiO$_2$ and ZnO oxide thin films on their optical characteristics. These films were deposited by rario frequency magnetron sputtering technique on quartz substrates. The film thickness values of 0.100-0.250 μm were measured using an interferometric method.

The orientation of crystallites, surface morphology, mass density, structure and composition were investigated by X-ray diffraction (XRD), X-ray photon spectroscopy (XPS) and atomic force microscopy (AFM). AFM analyses showed that all the films had a granular-like and pinhole-free microstructure. The surface topography of samples was analyzed using scanning electron microscopy (SEM).

The maxima and minima of transmission and reflection spectra recorded in the range 190 - 2500 nm for the analyzed samples are due to multiple reflections on the surfaces of the film, indicating that the studied oxide films were uniform. Optical constants (refractive index $n$, extinction coefficient $k$, and absorption coefficient $\alpha$) of the ZnO and SiO$_2$ oxide films deposited by radio frequency magnetron sputtering on quartz substrates were determined using Swanepoel’s method. These values vary depending on the the deposition conditions and the thickness of the analyzed sample. The values of the energy band gap were calculated from the absorption spectra, for ZnO and SiO$_2$ samples, deposited onto quartz substrates.

By calculating the average value of the refractive index in the investigated wavelength range it was found that, in general, the refractive index of the layer increased with its thickness. As a result, depending on the deposition conditions, the ZnO and SiO$_2$ oxide films showed a good optical quality and adhesion to the substrate.

**Keywords**: SiO$_2$ and ZnO, thin films, magnetron sputtering, optical quality.

This research was supported by ELI [contract number 17/2017].

S1 P31

**THE THICKNESS EFFECT ON THE GOLD AND SILVER ULTRA THIN FILMS PROPERTIES**

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The radio frequency magnetron sputtering (rfMS) deposition technique had gold and silver ultra thin films, paying particular attention to the technological aspects, and interpreting the results of the analysis respectively amounting to identify them. In the present work, we studied noble metals (i.e. Ag and Au) ultra thin films, with thickness values in the range 2 – 9 nm, prepared by rfMS technique onto glass substrates.

In this study, a stylus profilometer (Ambios, XP–2) was used to measure the thickness of the ultra thin films. A comparative analysis was conducted by measuring the thickness of the corresponding oxide thin films, using SEM, interferential microscopy and stylus profilometry methods. The surface profiles of the investigated samples, indicated that the size of the crystalline grains increased with the thickness.

Films made with smaller thicknesses were less crystalline, with the crystalline grains smaller. AFM images showed that our samples have a grain like surface morphology. The surface roughness played an important role in nucleation and growth processes of thin films. The crystallites orientation, the granulation and columnar growth were more evident in the Au samples.

The thickness effect on the compositional properties of these ultra thin films were discussed based on XPS results. In the case of the sample of ultra thin Au and Ag layers, it had been observed the presence of chemical elements on the surface of the film were analyzed. Above, there were presented the scans showing the presence of Au 4f5 and Au4f7 in the gold nanostructures and of Ag 3d3 and Ag 3d5 silver in the silver nanostructures, which increased with the increase of the predefined thickness of the film using the quartz monitor.

The surface topography of samples was analyzed using scanning electron microscopy (SEM). The XRD patterns indicated the Ag and Au films are crystalline. Also, the Ag and Au ultra thin films have a strong orientation after the main planes perpendicular to the substrate, e.g. (111) for Au and Ag films. The intensities and positions of (111) peaks in the XRD patterns were strongly dependent on the increasing thickness. Thus, increasing the thickness of the thin film greatly improved the crystallinity of the film. These ultra thin layers
present interesting for advanced technologies in terms of basic research and and new potential research for the next-generation of the spatial microsatellites.

**Keywords**: thin films, gold and silver, magnetron sputtering, structural properties

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**S1 P32**

**STUDIES ON THE STRUCTURAL – MORPHOLOGICAL PROPERTIES OF HDPE+\%SiO\textsubscript{2} NANOCOMPOSITES**

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Currently polymer nanocomposites are materials of great commercial and economic importance. The nanocomposite materials exhibit a wide range of properties such as lightweight, chemical resistance, flexibility, toughness, good dielectric properties, thermal stability, electrical insulation, heat shrinkable properties, and relatively low cost compared with other plastics, which make it suitable for many applications. Their large specific surface area (high surface-to-volume ratio) insertion of nanoparticle in the polymer matrix leads to the changes in the intermolecular interaction at the phase interfaces of the resulted materials.

Nanocomposite samples of high-density polyethylene matrix (HDPE+\%SiO\textsubscript{2}) were obtained by thermal pressing (under a pressure of 15 MPa) at a temperature 165°C, followed by rapid cooling in water-ice system. As a filler it has been used an amorphous silica dioxide \(\alpha\)-SiO\textsubscript{2} (Sky Spring Nanomaterials, Inc. Houston, USA) with 20 nm size of spherical particles, specific surface area of \(S=160\text{ m}^2/\text{g}\) and density of \(2.65\text{ g/sm}^3\).

Small-angle neutron scattering (SANS) measurements were performed at the time-of-flight YuMO spectrometer situated at IBR-2 pulsed reactor, JINR, Dubna, Russia. The investigations by small angle X-ray (SAXS) method were performed on a pinhole camera Molecular Metrology SAXS System at the Institute of Macromolecular Chemistry CAS (Prague, Czech Republic) and on a Rigaku X-ray instrument with high-speed Cu rotating anode (SMAXS 3000 Point SAXS system, at MIPT, Dolgoprudniy, Russia) using a standard transmission configuration.

SEM and SANS experiments showed SiO\textsubscript{2} nanoparticles mainly distributed in the polymer matrix as aggregates system. Small angle neutron scattering (SANS) demonstrated in Guinier region that the internal structure of these aggregates could be characterized by the mass fractal dimensions of 2.1-2.5. Analysis of the SAXS data using Guinier's law revealed that the nanocomposites consisted of particles with a broad distribution of sizes from 45 nm to 94.5 nm. Analysis of the experimental data using Porod's law revealed that all the nanocomposite samples formed surface fractal aggregates behaviors.

**Keywords**: high-density polyethylene, silica dioxide, nanocomposite, fractal.

The work was supported by the JINR-Romania Cooperation Programme Project of 21.05.2018 Order No. 323/92.
S1 P33

FACILE PREPARATION IN TWO STEPS OF SOL-GEL COATINGS BASED ON SILICA MATERIALS AND TiO₂ NANO PARTICLES

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TiO₂ nanoparticles has been preferentially applied as photo-catalyst because of its photo-stability, high oxidative power, low cost and non-toxicity [1]. Sol-gel process was found to be a very useful tool to obtain new materials based on TiO₂ for catalysis, chemical sensors, optical gain media, photochromic and non linear applications [2].

In this work, bilayer coatings based on silica materials and TiO₂ nanoparticles deposited on glass surface were prepared by sol–gel process at room temperature. These coatings were realized in a two-step procedure. The sol–gel acidic solutions containing silane precursors with long alkyl chains were deposited by dip-coating onto substrates. Afterwards an alcoholic dispersion of TiO₂ was added onto the silica films surface in order to obtain coatings with photo-catalytic properties.

Physico-chemical properties of sol-gel hybrid films have been investigated using FTIR and UV-Vis spectroscopy techniques, and AFM analysis. The photo-catalytic experiments were developed using methylene blue as a standard contaminant (deposited as alcoholic solution). Absorbance was monitored by Vis spectrometry at various intervals of time during irradiation with visible light. The wettability of coatings was investigated by water contact angle measurements. FTIR spectra confirmed the successful grafting of the silane precursors onto the surface of TiO₂ nanoparticles. AFM analysis indicated that the obtained sol-gel hybrid films present a different microstructure depending on the silica matrix and the existance of nanoparticles. It was observed that the water contact values varies as a function of the hydrophobic functional groups belonging to the silane precursors. The presence of TiO₂ nanoparticles play an important role in the development of the sol-gel hybrid coatings with photo-catalytic properties.

Keywords: sol-gel process, photo-catalytic activity, hydrophobic films

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References:

S1 P34

SPECTROSCOPIC STUDIES OF SAMARIUM IONS IN LEAD BORATE GLASS - CERAMICS

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Trivalent rare earth doped glasses and crystalline matrices have received attention due to their commercial applications in different technologies such as optical fibers, solid state lighting systems or lasers [1-3]. For this study, lead borate glasses with composition \(x\text{Sm}_2\text{O}_3\cdot(100-x)[4\text{PbO}:3\text{B}_2\text{O}_3]\) (where \(x=0, 5, 10, 20, 30, 40\) mol %) were prepared using melt quenching method. Samarium doped lead - borate glass - ceramics were successfully obtained by heat tretment of glasses at different temperature. The samples thus obtained were characterized by X-ray diffraction (XRD), Photoluminescence (PL) and Electron Paramagnetic Resonance (EPR) studies. XRD analysis was used for phase identification and verification of the crystallization progress. In order to possible applications of these materials in the fields of optics, the luminescence properties was investigated. The emission spectra consists of three emission bands in the visible region that corresponds to the \(^4\text{G}_{5/2} \rightarrow ^4\text{H}_1\) (\(J=5/2, 7/2\) and \(9/2\)) transitions of \(\text{Sm}^{3+}\) ions responsible for orange luminescence. CIE chromaticy coordinates was evaluated to understand the utility of these materials in the next generation Solid state lighting technology and laser applications. EPR data show that the samarium ions are incorporated in vitrocermics as \(\text{Sm}^{3+}\) and the gradual increase of the samarium content in matrice determined changes of the EPR spectra.

**Keywords**: glass-ceramics, EPR, luminescence, XRD.

**Acknowledgments.** The financial support of this work was provided by the National Plan for Research-Development, PN-III-P1-1.1-PD-2016, Contract No. 33/2018.

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**S1 P35**

**INFLUENCE OF SAMARIUM IONS CONCENTRATION ON STRUCTURAL AND OPTICAL PROPERTIES OF LEAD BORATE GLASSES AND VITROCERAMICS**

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In this study, the structural and spectroscopic properties of a series samarium doped lead-borate glasses and vitrocermics were reported. The samples in the \(\text{xSm}_2\text{O}_3\cdot(100-x)[4\text{PbO}:3\text{B}_2\text{O}_3]\) composition where \(x=0-40\) mol % \(\text{Sm}_2\text{O}_3\) were prepared by conventional melt-quenching method and characterized by X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and Ultra-Violet Visible (UV-Vis). XRD pattern identified the amorphous nature of glasses. Vitrocementic samples containing crystalline phase were obtained for composition with \(x\geq40\) mol % \(\text{Sm}_2\text{O}_3\). The FTIR data shows that the evolution of the \([\text{BO}_3]\) (the region from 1200 to 1600 cm\(^{-1}\)) and \([\text{BO}_4]\) (the region between 900 and 1150 cm\(^{-1}\)) structural units were modified by increasing of \(\text{Sm}_2\text{O}_3\) content up to 40 mol % in the host matrix. FTIR analysis revealing that samarium oxide induces a rearrangement of the lead-borate network. The intensity of the UV-Vis bands increases and the position of the absorption edge is considerable shifted to larger wavelengths with adding of \(\text{Sm}_2\text{O}_3\) contents in the host matrix. The strong transition present in the UV-Vis spectrum is due to the presence of Pb=O bond in \([\text{PbO}_3]\) structural units which allow \(\pi-\pi^*\) transitions. From the UV-Vis absorption spectra, the optical band gap for the prepared glasses and vitrocermics was estimated. Optical gap energy values are dependent on the concentration of rare earth oxide as dopant.

**Keywords**: glasses, FTIR, optical properties, XRD.
Acknowledgments. The financial support of this work was provided by the National Plan for Research-Development, PN-III-P1-1.1-PD-2016, Contract No. 33/2018.

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S1 P36
PREPARATION, CHARACTERIZATION AND PHOTOCATALYTIC ACTIVITY OF MULTI-WALLED CARBON NANOTUBES DECORATED WITH COBALT OXIDE AND SILVER NANOPARTICLES

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The development of new photocatalysts for environmental pollution remediation has gained increasing interest over the past years. Multi-walled carbon nanotubes (MWCNTs) are presented as suitable candidates for the preparation of photocatalytic composites due to their unique structural, chemical, thermal, and electrical properties [1]. MWCNTs have been shown to synergistically enhance the photocatalytic activity of metal based nanoparticles. Among various other nanomaterials, Co3O4 NPs and Co3O4-Ag nanocomposite demonstrated photocatalytic activities and have been applied to the degradation of dyes [2, 3].

In this work, Co3O4-Ag-MWCNT nanocomposites with different concentrations of the three components were prepared and further characterized using specific techniques, including X-ray diffractometry (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and Brunauer-Emmett-Teller (BET) surface area analysis. The photocatalytic activity of the MWCNT-based nanocomposites was investigated through the Rhodamine B (RhB) dye degradation.

Keywords: MWCNT nanocomposites, cobalt oxide, silver, photocatalysis.

References:

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S1 P37
MAGNETIC NANOCOMPOSITE BASED ON HALF-METALS AND CHALCOGENIDE: STRUCTURAL, MICROSTRUCTURAL AND MAGNETIC PROPERTIES

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Magnetic nanomaterials based on half-metals and chalcogenide not only covers a wide range of application given by the specific properties of its phases, but also represents an interesting theoretical field hold by physical phenomenon which is encountered for this type of materials, at nanometric scale.
The huge potential of these nanoparticles as theranostics materials – one of the most recent medical directions – leads from their magnetic, photoluminescent and drug careers properties. The last property is achieved by attaching different functionalities on the surface of those magnetic nanocomposites. The complexity, diversity and heterogeneity of tumors determine the therapeutic treatment. Regarding the physical phenomena which are encountered, most of them are determinate by the intrinsic physical properties which combine half-metal properties and nanometric scale properties.

Here we successfully obtained FePt@CuS and CoPt@CuS nanocomposites by a simple chemical deposition method. The hard phases were obtained from iron pentacarbonyl-Fe(CO)$_5$ and cobalt (II) acetylacetonate- Co(C$_5$H$_7$O$_2$)$_2$ combined with platinum (II) acetylacetonate - Pt(C$_5$H$_7$O$_2$)$_2$). The reaction was carried out in dioctyl ether and as a dispersing agent oleic acid was used. The reducing agent was 1.2 hexadecandiol. The reaction took place in an inert atmosphere (argon current). The as obtained FePt nanoparticles were annealed at 700 °C in reducing atmosphere (Ar+10%H$_2$). In the second step the CuS shell was added using precursors of copper (copper sulphate) and sulphur (sodium sulphide).

The elemental composition of materials was determined by XPS measurements, the structure and microstructure was checked by XRD and TEM analyses. The magnetic properties were investigated by using VSM magnetometry methods.

**Keywords**: half-metals, copper chalcogenide, theranostics, magnetic nanocomposite.

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**S1 P38**

**INFLUENCE OF Co IONS CONTENT ON THE PROPERTIES OF SnO$_2$ NANOPARTICLES**

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Semiconductor oxide nanoparticles with well-defined size, shape, optical and optoelectronic properties are intensely explored due to their favorable potential in the area of water depollution, more precisely in photocatalysis. Among various metal oxides, SnO$_2$ has become of great interest in the field of photocatalysis due to its different morphologies, high photochemical stability, strong oxidizing power, low-cost, and nontoxic nature [1]. Among all the shapes and morphologies, round shape nanoparticles with excellent crystallinity have a great importance for a photocatalytic reaction because of their higher surface area and colloidal stability in aqueous solution [2]. The drawback of this material is due to the quick recombination of the photogenerated electron and hole. One strategy to prevent the recombination is doping with transition metals [3]. Co doped SnO$_2$ nanoparticles were synthesized by co-precipitation method. The influence of Co ions content on structural, morphological characteristics and optical properties of SnO$_2$ nanoparticles was studied. The photocatalytic activities of the SnO$_2$ nanoparticles were evaluated through a degradation process in the presence of Rhodamine B dye under visible light irradiation as a function of Co concentration. The reactive oxygen species generated in the time of photocatalytic process were evidenced by spin-trapping and by using the electronic paramagnetic resonance.

**Keywords**: SnO$_2$ nanoparticles, Co Ions, photocatalysis.

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**References**

S1 P39

PROCESSING, MICROSTRUCTURE AND MAGNETIC PROPERTIES OF ALNICO RIBBONS

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The experiments consisted in preparation of samples, from Alnico alloy. Melting and alloying was carried out in an induction furnace, Leybold-Heraeus type, starting from pure elements, namely: electrolytic Ni, Co, Cu (99.9% purity), Ti, Al (technical purity) Fe (99.7% purity). The samples were re-melted several times for the homogenization.

From the obtained ingot, there were processed ribbons by melt-spinning technique at different wheel speeds. The obtained ribbons where then heat treated at 850°C for 30 min with and without magnetic field. The samples where cooled very fast till 600°C and another heat treatment was carried out at 600°C for 5 hours.

The crystalline structures of prepared samples have been investigated through X-ray diffraction. Magnetic properties of the samples obtained in the induction furnace was measured with Vibrating Sample Magnetometer (VSM)

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S1 P40

TEMPERATURE EFFECT ON MnO₂ / CARBON NANOTUBES

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Magnetic nanocomposites based on carbon nanotubes (CNT) have a high interest due to their potential applications in various fields such as: water decontamination, sensors for contaminants detection, biomedicine. The CNT can be functionalized with various chemical groups to increase their affinity towards target compounds. Manganese dioxide is one of the most attractive inorganic materials because of its widespread application in catalysts, supercapacitor and lithium batteries and is a promising material for many technology
and it may exist as several crystallographic modifications. The crystal structure determines the functional properties of MnO₂ materials, including their magnetic properties, electrochemical characteristics, molecular absorption and catalytic properties.

In this study, the preparation and characterization (XRD, BET, TEM) of multi-walled carbon nanotubes containing MnO₂ nanoparticles is presented. The effect of thermal annealing on MnO₂ and MnO₂ / CNT was also investigated. Due to their large specific surface area and unsaturated surface atom coordination, CNT provide excellent adsorption properties and chemical reactivity. Therefore, CNT and CNT decorated with MnO₂ annealed at different temperatures were used as adsorbing moities for inorganic and organic pollutants from aqueous solution. The adsorbion of pollutants such as heavy metal ions, antibiotics, dyes or other organic matters have been tested.

Keywords: MnO₂, carbon nanotubes, thermal annealing.

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S1 P41
PREPARATION AND CHARACTERIZATION OF Fe₃O₄/GO - TEMPERATURE EFFECT

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Graphene oxide (GO), one of the most important derivatives of graphene, has a layered structure where oxygen functional groups are presented on its basal planes and edges. Due to large surface area, large amounts of activated functional groups, good dispersion in water and a simple method for preparation, GO can be used in magnetic resonance imaging, magnetic fluid hyperthermia, magnetic separations, biosensors, water decontamination and controlled drug delivery.

The aim of this work consists of preparation and characterization of the Fe₃O₄/GO nanocomposites by co-precipitation of FeSO₄ and FeCl₃ in aqueous solution of GO. Through the attachment of such metal-oxides magnetic nanoparticles at the surface of GO one can prevent the agglomeration of GO nano-sheets and allows that the active nano-blocks to be functionalized adequately. By using magnetite nanoparticles, additionally, the obtained composites possess magnetic properties which are useful, especially, for further magnetic manipulations.

The effect of temperature on the system Fe₃O₄/GO was studied in correlation to their structural properties, morphology and magnetic properties. The characterization of samples was performed by XRD, BET, TEM and magnetization measurements. Due to their high specific surface these materials can be used in applications like adsorption of different pollutants from waters. The process is followed by the magnetic separation of pollutants charged on Fe₃O₄/GO composites.

Keywords: Graphene oxide, Fe₃O₄, nanocomposites.

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S1 P42
ON THE NICKEL MAGNETIC BEHAVIOUR IN RARE-EARTH COMPOUNDS

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The magnetic measurements performed on RNi\textsubscript{n} compounds where R is a rare-earth were generally analysed assuming that nickel is not magnetic when \( n \leq 5 \) or carry a small magnetic moment for \( n = 8.5 \). A small nickel moment has been already evidenced only in GdNi\textsubscript{2} by using magnetic Compton profile [1].

In order to obtain additional data on the nickel magnetic behaviour in the above compounds, XPS measurements and band structure calculations were made. The Ni\textsubscript{2p\textsubscript{3/2}} and Ni\textsubscript{2p\textsubscript{1/2}} core level lines, in the above compounds, essentially reproduce those of pure nickel. The 6 eV satellite lines suggest the presence of unoccupied Ni3d states. Band structure calculations showed also the presence of small nickel moments for RNi\textsubscript{n} compounds with \( n \geq 2 \) or R-Ni-B series. Along a given series, the Ni moments follow linear dependences on DeGennes factor \( G = (g_J - 1)^2J(J+1) \). Their slopes are dependent on site location, decreasing as the number of rare earths situated in their first coordination shell diminishe. The R5d bands are negatively polarized with induced contributions from both 4f-5d and 5d-3d exchange interactions [2].

**Keywords**: rare-earth-nickel compounds, band structures, XPS measurements.

**References.**


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**S1 P43**

**OPTIMIZATION OF THE QUALITY OF ELECTRON DIFFRACTION IMAGE: CHARACTERISATION OF THIN FILMS PRECESSION**

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The advantage of using electron diffraction is the small area taken into study, up to a few square nanometers, but sample can be complex and can affects the results. Nanostructured materials are accurately investigated using TEM (Transmission Electron Microscopy), but compromise must be made when information are acquired using electron diffraction technique. Due to instrument geometries, the errors in electron diffraction data are larger compared to X-Ray diffraction, making the analysis difficult.

For amorphous samples, we cannot separate useful data because of the additional quantity given by scattering on amorphous carbon or formvar film substrate. Crystalline structure analysis can be done in two steps: first, crystallographic information and cell parameters determination and second, refinement of the unit cell, including atom position.

To improve the quality of electron diffraction analysis we use precession technique: First of all, the electron beam is deflected and rotated using the condenser lens. Frequency of rotation is a controllable parameter using electronic equipment. After the beam interaction with the material studied, it is recollimated by means of DeScan lens.

We compared the electron diffraction results in the case of precession method with the conventional electron diffraction method for different thin films, based on software, wich coordinate the precession system with an original hardware system.

**Keywords**: TEM, Electron Diffraction, Precession, Thin Films

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EFFECT OF EUROPIUM SUBSTITUTION ON THE STRUCTURAL AND OPTICAL PROPERTIES OF CH₃NH₃PBI₃ PEROVSKITE FILMS

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In this work, we report the effect of substitution of lead (Pb²⁺) by Europium on the structural, optical and morphological properties of MAPbI₃ was studied aiming for the application in perovskite solar cells as active layer. Surface morphology, crystal phase, transmission spectra and PL proprieties of the active layer were investigated by Atomic force microscopy (AFM), X-ray diffraction (XRD), ellipsometer spectroscopy and photoluminescence spectroscopy respectively. The obtained results indicate that the partial substitution of Pb²⁺ by Europium have an advantage in improving the optical absorption and quality of the perovskite films for 1% and 5% of Europium. These findings presents a great potential of compositional engineering to produce perovskite films with better optical properties and high photovoltaic performance.

Keywords: perovskite films; structural and morphological characterization; optical properties.

TRIANGULAR POLYAROMATIC HYDROCARBONS WITH SPIN

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The spintronics is a desideratum of future technologies which actually is prospected mostly with the tools of modeling, testing in silico various candidates. We present computational predictions and analyses,[1] methodological advances and heuristic conclusions applied on series of polyaromatic systems condensed in the shape of regular triangles, carrying spin, because of topological reasons. A new clue about the classification of title systems in three equivalency classes is presented (see Fig.1). A conjugated hydrocarbon having n-hexagonal rings at one edge, carrying n-1 unpaired electrons, will be called n-triangulene, in the generalization of the experimentally known structures with n=2 (phenalenyl) and n=3 (triangulene). To be distinguished from the most of previous computational approaches, done by Density Functional Theory (DFT), we challenged the problem in the key of Valence Bond (VB) paradigm in both ab initio and phenomenological manners. The Heisenberg spin Hamiltonian was used to simulate the computed spectrum of VB states for the phenalenyl radical (n=2), predicting with the fitted parameters the effective VB description of the n=3 triangulene and other related systems. The outcome has practical importance in the prospects of spin chemistry, since the VB ab initio calculations are prohibitive beyond the n=2 case. The results are made transparent to the chemical intuition, using the language of resonance structures. The devised methodologies can be applied to related systems obtained by nano-scale tailoring of graphene flakes, acquiring triangular-type protrusions, even with irregular geometries.
Fig. 1 The scheme of structures and spin count in triangular graphene-type molecules.

**Keywords:** Organic Molecular Magnetism, Carbon-based Radicals, Resonance Structures.

**References:**

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**S1 P46**

**FIRST-PRINCIPLE STUDIES OF CHARGE TRANSFER IN MODEL SYSTEMS REPRESENTATIVE FOR DYE-SENSITIZED SOLAR CELLS**

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Although intensively and extensively studied, the dye-sensitized solar cells, still deserve sustained attention, in the key of a new generation of problems, focused in the deep understanding of underlying mechanisms, for the sake of a rational intervention in the engineering of efficient devices, a matter mostly addressed in try-and-error manner. In this view, the conceptual and computational modeling stands as a valuable counterpart to the experimental effort.

Fig. 1 Computed reaction coordinate for charge transfer in the system [Co(terpy)2]2+/3+L0+/1/0.
Continuing our interest in modeling the mechanisms of solar cells,[1] we consider now the issue of redox couples involved in the regeneration of the active dye, as subsequent process to the electron transfer to the TiO\(_2\) substrate. As figure 1 shows, we succeeded to obtain the two-well energy curve, specific to the charge transfer processes, taking a prototypic example based on a cobalt complex with terpyridine (terpy) as tridentate ligand and a colorant customarily called L0, whose formula is 1,4 (Ph\(_2\))C\(_6\)H\(_4\)-CH=C(CN)(COOH). The results of the calculation are further handled by phenomenological Hamiltonians based on two-state models, in the spirit of electron-vibrational coupling and Marcus theory of electron transfer, extracting key parameters. Several computation experiments are settled, giving insight in the reaction mechanisms, as guideline for the desired property-engineering approach.

**Keywords:** Dye Sensitized Solar Cells, Electronic Structure Calculations, Effective Hamiltonian Models

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**References:**

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**S1 P47**

**DFT SIMULATIONS OF ELECTRONIC PROCESSES IN DYE-SENSITIZED SOLAR CELLS WITH OLIGOMETHINE CYANINE DYSES**

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We report density functional theory (DFT) calculations of three oligomethine cyanine-based dyes as well as complex dye-TiO\(_2\) nanoparticle systems, with applications to dye-sensitized solar cells. We perform DFT and time-dependent DFT studies and provide the electronic structure and simulated UV-Vis spectra of the dyes alone and adsorbed to the cluster. We discuss the matching of the absorption spectra with the solar irradiation spectrum. We display the energy level diagrams and the electron density of the key molecular orbitals and analyze the electron transfer from the dye to the oxide. Finally, we compare our theoretical results with the experimental data available and discuss the key issues that influence the device performance.

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**S1 P48**

**ANTHOCYANINS FROM Brassica Oleracea var. Capitata F. Rubra VS. ANTHOCYANINS FROM Hibiscus Sabdariffa L. AS NATURAL PIGMENTS FOR DSSCs**

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We report results of combined experimental and theoretical studies of anthocyanin natural dyes used as sensitizers for TiO\(_2\) dye-sensitized solar cells (DSSCs). We compare and contrast results obtained for cyanidin and delphinidin dyes extracted from *Hibiscus Sabdariffa L.* harvested in the flora of Senegal and similar anthocyanins extracted from red cabbage. To analyze the compliance of the various dyes with the main criteria [1] that should be met by the TiO\(_2\) sensitizer in a DSSC, we performed Density Functional Theory (DFT)
calculations, which provided the optimized geometry, electronic structure and electronic spectrum of the dyes in fully protonated, as well as partially deprotonated forms, in solution. We discuss the adsorption onto the substrate, the matching of the absorption spectrum of the dye with the solar spectrum, the energy level alignment with the semiconductor and the electrolyte, and the charge transfer to the substrate. Based on previous results showing higher efficiency for red cabbage extracts in alkaline medium [2], we prepare solar cells using dye solutions of various pH values in order to identify the conditions for optimal performance of such devices. We notice that the efficiencies of DSSC depend on the pH of solution, varying from 0.23% to 0.13% for pH 3.5 and 5, respectively. A red shift in the UV-Visible absorption spectra is observed upon dye adsorption on substrate and upon increase of pH value in aqueous solutions.

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S1 P49

PHOTOCATALYSIS BASED ON PLATINUM

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Noble metal nanoparticles (e.g., gold and platinum) supported on TiO₂ surfaces are utilized in many technological applications such as heterogeneous catalysts. To fully understand their enhanced catalytic activity, it is essential to unravel the interfacial interaction between the metal atoms and TiO₂ surfaces at the level of atomic dimensions. To directly characterize the atomic-scale structures that result when individual metal atoms are adsorbed on the TiO₂ surfaces, the TEM, STEM and various spectroscopy techniques have been used.
ABSTRACTS

S2 — Laser, Plasma and Radiation Physics and Applications

- Laser Physics and applications
- Plasma Physics and applications
- Optoelectronics and photonics
- Applied and non-linear optics
- Ultrafast phenomena and applications
A STUDY OF THE ELECTRON ENERGY DISTRIBUTION FUNCTION IN A LOW-POWER HALL THRUSTER DISCHARGE AND NEAR-FIELD PLUME

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Electron temperature and plasma density, as well as the electron energy distribution function (EEDF), have been measured inside and outside the dielectric channel of a 200W permanent magnet Hall thruster. Measurements were carried out by means of a cylindrical Langmuir probe. The measured EEDF evidences a high-energy electron population that is superimposed onto the low energy bulk population outside the channel. Inside the channel, however, the EEDF is close to Maxwellian.

The 3D particle-in-cell numerical simulations complement experiments. The model accounts for the crossed electric and magnetic field configuration in a weakly collisional regime where only electrons are magnetized.

Both the experimental and numerical EEDF depart from an equilibrium distribution at the channel exit plane, a region of high magnetic field. The measured high-energy population on the EEDF presumably corresponds to the electrons emitted by the external cathode that reach the thruster discharge without experiencing collision events.

ENGINEERING ACTIVE SITES ON REDUCED GRAPHENE OXIDE BY HYDROGEN PLASMA IRRADIATION: MIMICKING BIFUNCTIONAL METAL/SUPPORTED CATALYSTS IN HYDROGENATION REACTIONS

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Precedents in the literature have shown that hydrogen plasma treatment is a useful technique to produce carbon vacancies and holes on graphene sheets [1,2]. The purpose of the present study was to show that the generation of these holes can increase and tune the catalytic activity of graphene as metal-free hydrogenation catalyst, a reaction of large importance from the synthetic and industrial point of view [3]. The characterization data obtained in the present study agrees with the expected creation of defects and holes by plasma irradiation of graphene and, in accordance with our initial hypothesis, the resulting treated graphenes exhibit higher hydrogen adsorption capacity and higher hydrogenation activity. Notably the observation of some activity typical of bifunctional hydrogenation/acidic catalysts has been observed for the case of 1-octene hydrogenation by the appearance of skeletal isomer. Theoretical calculations with models of mono- and di-vacancies indicate a large difference in their interaction with H2, calculations with the two models still provide an unsatisfactory rationalization of the H2 activation observed in catalysis (Figure 1).

Thus, it seems that the issue of the exact structure of the hydrogenation sites remains still open and could probably involve oxygen atoms. Overall, the present study illustrates the possibility to engineer active sites on graphene by available treatments, tuning their catalytic activity and the need to combine experimental data and theory to gain a deep understanding on the catalytic process.

A relationship between the power of the plasma treatment and the exposure time with the activity of the material was observed for C=C double bond hydrogenation. The activity data in the case of 1-octene, showing skeletal isomerization besides hydrogenation, indicates that H2 plasma treatment can introduce hydrogenating
and acid sites rendering a bifunctional catalyst that is reminiscent of the activity of noble metals supported on acid supports.

**Figure 1.** Generation of the carbon vacancy on the $4 \times 4$ graphene model by removal of the carbon atom indicated in red in part a. Then, the geometry of the resulting model was optimized at PBE0/6-31G(d) level of theory (b). Dissociative $\text{H}_2$ adsorption at a monovacancy hole presented from two different perspectives (c and d) calculated at the same level of theory. Peripheral hydrogen atoms are omitted.

In conclusion, the hydrogen plasma treatment emerges in the very green procedure to modify graphenes. The energetics of this treatment is much favorable to plasma. In the investigated experiments the maximal consume was of 2 W. This consume for the time of the experiments corresponds to 3.78 °C that is complete insignificant. Noteworthy, to produce some non-selective chemical changes in these graphenes in the way have been produced by plasma, temperatures higher than 500 °C are necessary.

**References**

**S2 L3**
**SYNERGIES BETWEEN THERMIONIC VACUUM ARC SYSTEM AND LASER PROCESSES IN THE LTVA METHOD FOR THE SYNTHESIS OF THE TI-BASED NANOSTRUCTURES**

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Titanium has many desirable features such as good excellent in corrosion resistance (even in seawater), lightweight (specific gravity 4.51), high strength (~1800MPa), and high electric resistance. However, it is prone to wear because of its poor tribological properties, low hardness and antifriction characteristics. One possible solution to improving the performance of Titanium is alloying with other elements, especially Ag, Mg, Ni, and Cr are considered among the most promising.

The aim of this paper is to investigate the growth and structure properties of Ti-based composites thin films deposited by Thermionic Vacuum Arc (TVA) technology in one electron gun configuration. TVA method offers convincing advantages for multi-component depositions, such as high rate of deposition, low thermal energy transfer, very stable discharge conditions, no cathode’ impurities, and very good adherence. In order to come closer to applications and technological control, a great interest has been paid to develop a
combination technique to deposit thin films by using laser-induced high current arc which has the advantages of high ion energy and high-density.

The properties of the deposited Ti-based composites were investigated in terms of wettability, morphology, and tribology. The surface free energy was determined by means of Surface Energy Evaluation System and the morphology were determined from BF-TEM image performed by Philips CM 120 ST TEM system. Compositional and topographical analyses were also undertaken by using Scanning Electron Microscopy with Energy-Dispersive X-ray detection (SEM/EDX).

Acknowledgement: This work was supported by a grant of the Romanian National Authority for Scientific Research, CNDI–UEFISCDI, project INOVATECH 70/2017.

S2 L4

CARBON DUST GROWTH IN ATMOSPHERIC PRESSURE PLASMAS

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The dielectric barrier discharge (DBD) represents a method to generate atmospheric pressure plasma in air or various gaseous environments, ensuring a specific range of plasma parameters as against other laboratory methods to produce plasma at atmospheric pressure, i.e. corona discharge, streamers, sparks or arc discharge. This attracted, over the years, a significant research interest, mainly due to the flexibility in designing the electrode assembly, the easy access of the electrical excitation methods, the absence of ion etching processes, high collisionality, low Debye length and low gas temperature. Thus, DBDs have been widely used for long time in various laboratory scale applications or industrial processes, such as surface treatment, liquid waste processing, plasma polymerization, nanocomposite thin films deposition, gas conversion, decontamination, sterilization or inactivation, and life science applications. An extension of these applications was considered and DBD based processes were employed for laboratory astrophysics experiments, e.g. synthesis of interstellar enols, tholins formations or transitory hydrocarbon environments.

Our group has shown recently, that the high power impulse DBD, in helium and hydrocarbon gas mixtures, is a new method for low temperature deposition of carbon dust analogs (Fig. 1). The Earth based experiments aiming to synthesize dust analogues are of high interest for the laboratory astrophysics community, plasma deposition of film analogs, being performed in radiofrequency reactors (PECVD), pulsed laser depositions (PLD) reactors, along with other methods, such as condensation, physical vapour deposition, combustion and pyrolysis methods. We discuss here the DBD synthesis method of carbon dust, while focusing on both plasma diagnosis (i.e. electrical, optical and imaging methods) and dust physico-chemical characterization (i.e. UV-VIS, FTIR, SEM). The astrophysical implications are presented, from both chemical and morphological points of view, in relation with recent results of astrophysics community and astronomical observations.

Fig. 1. From left to right: typical picture of DBD in He + C₆H₁₀ (15%), optical microscopy image emphasising the island growth over the substrate and SEM picture of dust particles.
IRON OXIDE AND IRON SULFIDE FILMS PREPARED FOR DYE-SENSITIZED SOLAR CELLS

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The iron oxide and iron sulfide are materials with interesting properties for photoelectrochemical and photovoltaic applications. Their chemical stability, non-toxicity and earth abundance make them ideal for low cost production of films optimized for their application. The hematite, $\alpha$-Fe$_2$O$_3$, is the n-type semiconductor which can work as the photoanode in the electrochemical cell. The iron pyrite, FeS$_2$, is the indirect band gap semiconductor with the well positioned band gap of about 0.95 eV and high absorption coefficient of $10^5$ cm$^{-1}$ at 1.5 eV. It allows absorption of most light in less than 100 nm of the thin film. During the pyrite synthesis the intermediate phases like FeS or Fe$_{1-x}$S must be avoided [1]. This can be achieved by the sulfurization of the iron oxide films in the sulphur atmosphere at high temperature:

$$\begin{align*}
2 \text{Fe}_2\text{O}_3 (s) + 11 \text{S} & \rightarrow 4 \text{FeS}_2 (s) + 3 \text{SO}_2 (g) \\
\text{Fe}_3\text{O}_4 (s) + 8 \text{S} & \rightarrow 3 \text{FeS}_2 (s) + 2 \text{SO}_2 (g)
\end{align*}$$

In this work the iron sulfide films were created from iron oxide films deposited by the hollow cathode plasma jet [2] or planar magnetron in dc and pulsed dc modes. In both systems the argon with admixture of oxygen was used as the working gas and the pure iron as the target. The sulfurization was performed in the separate externally heated chamber by exposing samples to the sulfur vapors at the temperature of about 300 to 400 ºC.

The films were prepared on FTO, glass and silicon substrates and analysed by the AFM, SEM, EDX, Raman spectroscopy and absorption spectroscopy including the morphology and homogeneity of the films.

**Keywords:** hollow cathode plasma jet, iron oxide, absorption spectroscopy, dye-sensitized solar cell.

**References**


Hollow Cathodes (HC) are used as sources for intensive light, spectroscopic light, clusters, electron beams and as ion thrusters. They are important for the production of metal ions, clusters and in particular for deposition. The most important part of a HC is its annular cathode cylinder. On its inner surface an ion-rich sheath forms due to the cathode fall of the discharge. For the electrons this leads to the formation of a deep potential well in which they perform a pendulum motion strongly enhancing electron density and ionization rate, and thereby the plasma density. This effect is known since long (see e.g. [i]). To be used as sputtering source the HC cylinder has to be manufactured from the material to be sputtered with an operating voltage of up to 1 kV. The ions of the working gas (usually Ar) are then impinging on the inner wall with corresponding kinetic energy.

The experimental setup of an HC can be designed intriguingly simple where even detached plasma structures have been observed [ii] (see Fig. 1).

In this review we report on various experiments with HCs, mainly as sputtering sources. It was found that an additional cavity in the bottom of the HC cylinder enhances the sputtering [iii, iv]. A recent investigation showed that a HC with an assisting magnetic field and high power impulses strongly increases the extraction rate of sputtered material [v].

**Keywords:** Hollow cathode, sputtering, magnetically assisted, pulsed hollow cathode

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**References**


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**S2 L7**

**DEPOSITION PLASMA-POLYMER ORGANOSILICON COMPOSITE THIN FILMS UNDER DUSTY PLASMA CONDITIONS**

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During the past decades nanocomposite polymer coatings have attracted increasing attention because of their unique optical, mechanical, magnetic and optoelectronic properties arising from the combination of...
organic matrix and inorganic nanoparticles. Combinations of the attractive functionalities of both components at the nanolevel acquired from organic polymers and inorganic nanoparticles, are expected to exhibit synergistically improved material properties. Among the numerous nanocomposite preparation methods, the deposition under dusty plasma condition is one of the most attractive tools, which could be successfully applied in many industrial and technological applications, ranging from microelectronic industry to aerospace industry and biomedical applications. In the present work plasma-polymer nanocomposite thin films were prepared under dusty plasma conditions. Due to their nanocomposite structure, the films showed very interesting mechanical properties, for example high elastic recovery resulting in behaviour similar to superelasticity. Variation of the deposition conditions enabled to vary the surface composition and structure of the deposited films. The surface structure of the films influenced their surface free energy in a wide range so it was possible to prepare films with hydrophilic as well as hydrophobic properties. The mechanical properties of the films were studied using nanoindentation technique and the surface structure was studied using atomic force microscopy.

The present work is supported by Czech Science Foundation under project GACR 19-15240S.

S2 L8
SMART TILES PREPARATION AND ANALYSES AFTER WORKING IN A THERMONUCLEAR FUSION ENVIRONMENT

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Since 2011 the JET tokamak has been operated with a metal ITER-like wall (JET-ILW) including castellated beryllium limiters and lamellae-type bulk tungsten tiles in the divertor. This has allowed for a large scale test of castellated plasma-facing components (PFC).

European program concerning nuclear fusion it is the european project with highest longevity in Romania. The European Programme for Fusion is a model of smart and sustainable research that ensured fusion development in our country, significantly improved by National Institute for Laser, Plasma and Radiation Physics (NILPRP). The “smart tiles”, or marker tiles obtaining technology was developed using TVA deposition method (Thermionic Vacuum Arc); nickel films of 2 μm thickness and beryllium films of 8-10 μm were coated on massive bulk beryllium tiles.

After marker production, they were mounted inside JET fusion reactor in Culham, UK and after a 2 years running shift they were extracted and sent to Romania for sectioning and analysis [1,2].

This work presents the fusion plasma influence on the marker tiles and consequently the sustenability of the ITER-Like-Wall to be used on the new fusion machine to be built in Cadarache-France.

This work has brought several important results which have provided insight into deposition phenomena in the large-scale castellated beryllium structures. For the first time ever a comprehensive analyses have been carried out for materials retrieved from all important locations in the machine.

**Keywords:** thermionic vacuum arc plasma, metallic plasma, thin film deposition and analysis

**Acknowledgments.** This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014–2018 and 2019-2020 under grant agreement no. 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

**References:**
[1] M. Rubel el al., Fuel Inventory and Deposition in Castellated Structures in JET-ILW, Nuclear Fusion 57(6), 2017
CARBONITRIDE COATINGS FOR DIFFERENT APPLICATIONS

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The materials used for working in various environments should possess valuable properties for the envisaged applications. For example, materials used in marine service applications, exposed to corrosion, should present high resistance to wear and superior resistance to high levels of humidity and airborne chloride. Another example is referring to materials used for biomedical applications, which should have good biocompatibility and corrosion resistance in body fluids presenting different pH values and compositions. Therefore, in many applications the coatings represent the best solution for improving the performance of the existing materials for a specific application (e.g. corrosive environments, high wear conditions, low or high temperature, alkaline solutions and dilute acids, deep sea or space environments, or other extreme conditions). Transition metal carbonitride coatings have attracted great interest in various applications due to their superior characteristics such as chemical inertness, high hardness and melting point, superior lubricating properties, high wear resistance, corrosion resistance in different environments, providing extended life service of the coated parts and components, such as they represent attractive candidates for a wide variety of applications [1,2].

The characteristics of the transition metal carbonitrides change with the C/N ratio, such as it is possible to obtain a large varieties of carbonitrides with tailored properties, covering various applications [1]. One of the most common transition metal carbonitride coatings is TiCN, which combine the high hardness and the low friction coefficient of TiC with the high toughness and bonding strength of TiN. Considering the proper selection of the C/N ratio, the TiCN coatings provide good tribocorrosion performance in saline solutions [3,4], while display poor tribological performance under dry testing conditions at both room and high temperature.

We report on the deposition and characterisation of various carbonitride coatings with different applications (e.g. industrial and biomedical applications). The effect of C/N ratio on the microstructure, stress, hardness, elastic modulus and adhesion will be also presented.

Keywords: carbide coatings, cathodic arc, wear-corrosion resistance, friction coefficient.

Acknowledgements: The work was supported by the following grants of the UEFISCDI: project no. 60PCCDI/2018 (MedicalMetMat), no.68/2018 (CoatDegraBac), within PNCDI III, as well the Core Program no.18N/2019 and project PROINSTITITIO no. PFE19/2018.

References:

NANOCOMPOSITE HARD COATINGS FOR BIOMEDICAL APPLICATIONS

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Nanotechnology is an extremely powerful emerging technology, which is expected to have a substantial impact on medical technology now and in the future. In this paper, we analyze the types of nanomaterials, methods of production and their properties. Below is an example of an artificial hip, application of new materials.

Nanostructured multilayer coatings exhibit outstanding physical, mechanical, and chemical properties, opening a range of new applications in high technologies.

The nanostructured TiAlSiN coating was deposited from one pair of TiAl and one pair of TiSi segmental targets (dimensions 88 × 500 mm) as shown in Fig. 1a.

![Figure 1a] Tumble Tower TiAl TiSi

![Figure 1b] SEM coating cross-section AC-HSS

Figure 1b. presents SEM cross-sectional images of the AC and nanolayered TiAlSiN coatings. The coatings adhere well to base material, they are uniformly thick and free of structural defects like cracks and voids. Columnar growth is observed in the TiAlN coating. The dense structure indicates that the applied bias was sufficiently high to provide adequate adatom mobility.

From the above facts and the salient materials properties of the hard coating discussed, it can be largely concluded that a thin single or multilayers of hard coatings with nano grains deposited on metal surface implants favorable physicochemical and mechnanochemical characteristics such as corrosion resistance, wear resistance and good adhesion while retaining the durability and structural benefits of the metal. This field of research provides lot of scope for the materials scientists, and biomedical experts, which has large interdisciplinary research future.

Keywords: nanomaterials, hip, thin films, characterization.

Acknowledgments: The authors would like to thank The Provincial Secretariat for Higher Education and Scientific Research of Vojvodina, which supported this work by grant.

S2 L11

AMBIENT PRESSURE LASER DESORPTION/IONIZATION MASS SPECTROMETRY FOR IN-VIVO REAL-TIME DETECTION OF CANCER MOLECULAR MARKERS

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Laser micro-sampling is a promising tool for ambient pressure imaging of biological material by mass spectrometry (MS). Conventional approaches use laser energy coupling into the analyzed sample through electronic (UV, VIS) or vibrational (IR) channels [1, 2]. We have recently developed a new instrument (called SpiderMass [3, 4]) for in vivo and real-time MS molecular analysis using a laser microprobe operating under ambient conditions through resonant IR excitation of endogenous water molecules. This instrument can be used in surgical conditions to define the tumor resection margins and to assess the cancer stage, through fast
retrieval of molecular patterns specific to cell phenotypes [5, 6]. SpiderMass was also successfully demonstrated in other fields, like analysis of human skin, real-time drug metabolism pharmacokinetic (DMPK) analysis, or food safety [7]. SpiderMass is thus the first MS based system designed for in vivo real-time analysis under minimally invasive conditions.

**Keywords:** Ambient Mass Spectrometry, Laser Ablation, Tissue Sampling, Mass Spectrometry Imaging, Cancer Detection

**References**


**S2 L12**

DEUTERIUM RETENTION IN FUSION RELATED MATERIALS

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One of the main areas of research in the nowadays fusion domain is represented by the study of interaction between the physical components of the thermonuclear reactor with the fusion plasma. The understanding of phenomenon’s that occur from this type of interaction is crucial for selecting and developing, existing or new types of materials, with enhanced plasma compatible properties and endurance in extreme conditions. So far, beryllium (Be) and tungsten (W) had already been selected for International Thermonuclear Experimental Reactor (ITER) as materials for main chamber wall (Be) and divertor area (W). During ITER operation, intense bombardment with energetic particles from plasma can lead to erosion of these materials, their transport in plasma and redeposition together with nuclear fuel in remote areas. In EPPA laboratory in NILPRP, we are specialized in obtaining Be and W based layers, using plasma-assisted deposition techniques, which can mimic different types of layers that can occur in a ITER-like fusion reactor and study their behavior in the laboratory.

The results included in this talk are aimed to improve the existing knowledge on nuclear fuel retention, especially in Be/W mixed layers, which were limitedly studied in literature. Both implantation and co-deposition are the main mechanisms responsible for nuclear fuel retention in fusion reactors. So, to account for both processes Be/W layers can be produced with thermionic vacuum arc technology, subsequently being implanted with deuterium ions at a specific energy and fluence or, by using DC or HIPIMS magnetron sputtering regimes to co-deposit the layers together with the nuclear fuel. Subsequently, we will present the main mechanisms responsible for deuterium retention in layers identified through Thermal Desorption
Spectrometry and the influence of microstructure and layer composition on deuterium inventory will be discussed.

**Keywords:** fusion plasma, deuterium retention, Be/W layers

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**S2 O1**

**PLASMONIC PULSE SHAPING IN SLOT WAVEGUIDES**

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We analyze theoretically the propagation of a plasmonic pulse through various geometries of metal-dielectric-metal (MDM) slot waveguides, consisting of a dielectric layer with variable thickness placed between two semi-infinite metal layers. The simulation of pulse propagation is performed by studying the evolution of each Fourier component of the pulse using the analogy with microwave transmission lines, which is valid whenever only one mode is propagating throughout the slot waveguide. The transmission line analogy allows for precise spectrum determination with minimal computing resources and within an acceptable timeframe; the representation of the equivalent transmission circuit is provided for all slot waveguide geometries. Because the transmission coefficient through a slot waveguide depends on frequency, each spectral component of a pulse is modulated differently so that the output pulse has generally a different shape than the input pulse. As an example, we simulated first the propagation of a Gaussian plasmonic pulse and its Fourier transform through different MDM slot waveguide configurations for different geometric parameters. At the output, we find that the shape of the plasmonic pulse is no longer Gaussian and depends on the specific slot waveguide geometry. This result is generalized for an arbitrary plasmonic pulse, which can in general be complex, as its Fourier transform. As such, a plasmonic slot waveguide with a determined configuration can shape an incident pulse to a desired form with no need for additional dispersive elements.

**Keywords:** plasmonics, gaussian, pulse, waveguide

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**S2 O2**

**FABRICATION AND CHARACTERISATION OF BIPLASMONIC SUBSTRATES OBTAINED BY PICOSECOND LASER PULSES**

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Bimetallic nanostuctures have the potential to become the new generation candidates for applications in catalysis, electronics, optoelectronics, biosensors, and surface-enhanced Raman Spectroscopy (SERS) \(^1\). The bimetallic nanocrystals could have additional properties over the single metal components \(^2\).

This work presents the optimization process that was used in the fabrication of large area biplasmonic substrates employing picosecond laser pulses and a digital galvano scanner. Our aim was to achieve large area homogeneous substrates while having a good and predictable signal amplification by SERS effect. Gold thin films with different thickness were deposited on optical polished substrates and then irradiated with \(\lambda=1064\) nm wavelength laser pulses with 8 ps pulse duration and 500 kHz repetition rate. Various laser fluences and laser irradiation speeds were employed in our experiments in order to optimize the Laser-Induced Periodic Surface Structures (LIPSS) which form on the substrate.
The results will be presented comparatively for two fabrication methods. The first method involves nanostructure formation through laser irradiation followed by thin film deposition. The second method is the inverse: thin film deposition followed by laser irradiation. SERS efficiency is calculated based on Raman spectral analysis on a single signal peak of a Rhodamine 6G solution.

**Keywords**: SERS, laser ablation, Raman spectroscopy, bimetallic structures.

**References**


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**S2 O3**

INVESTIGATION OF ZrCN AND ZrCrSiCN PROTECTIVE COATINGS FOR INDUSTRIAL APPLICATIONS

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Ternary transition metal carbonitride coatings containing abundant elements, such as TiCN, CrCN and ZrCN are known as excellent protective coatings against wear, erosion and corrosion [1,2]. This work aims to assess the influence of Cr and Si addition on the tribological characteristics of ZrCN based coating. The ZrCN and ZrCrSiCN coatings (~ 3.7 µm thick) were deposited on C45 steel substrates by the cathodic arc method, in a mixture of C2H2 and N2. The coatings were investigated in terms of elemental composition, microstructure, mechanical properties and tribological performance, and compared to uncoated C45 steel discs.

The addition of Cr and Si to ZrCN coating determined the decrease of the grain size, indicating an amorphisation process, specific for Si addition. The observed hardness enhancement and improved friction and wear performance in dry test conditions was ascribed to the formation of an amorphous silicon carbonitride phase at grain boundaries, as well to the superior friction characteristics of Cr compounds. The obtained results recommend ZrCrSiCN coatings to be used in tribological demanding industrial applications.

**Keywords**: carbide coatings, cathodic arc, wear-corrosion resistance, friction coefficient.

**Acknowledgements**: The work was supported by the following grants of the UEFISCDI: project no. 60PCCDI/2018, within PNCDI III, as well the Core Program no.18N/2019 and project PROINSTITITIO no. PFE19/2018.

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Figure 1 SERS mapping and SEM image of bimetallic Au-Cu laser induced ripples
S2 O4
TWO MODAL FIELD FOR COHERENT RAMAN EXCITATION OF MOLECULAR VIBRATION

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This report is devoted on the applications of the two modal field for coherent Raman excitation of molecular vibration. The non-excitation of molecules needs of high intensity field in the Raman pump. We proposed a new type of coherent Raman field which consist from the coherent two modes in which the coherence is established between the two groups of photons belonging two field Stokes and anti-Stokes. An interesting effect consists in the fact the coherence Stokes and anti-Stokes photon can be very small due to large fluctuations of the field in each mode.

This bimodal field excite coherently biomolecules with high efficiency due to the coherence which are established between this two groups of photons while the coherence of photons in each type of photons remain very small during the generation. Such a field can be applied in diagnostics of lipids.

Keywords: bi-modal field, Stokes and anti-Stokes photon, coherent Raman field.
Acknowledgment: This paper is supported by the projects: NATO EAP SFPP 984890, for young scientists No. 18.80012.50.33A and No. 15.817.02.07F.

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S2 O5
DEVELOPMENT OF A POLYANILINE COATED FIBER OPTIC – SURFACE PLASMON RESONANCE SENSOR FOR pH MONITORING

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Ph measurement is crucial in the fields of biochemistry, clinical medicine and environmental science [1]. In recent years, substantial efforts were invested towards improving the performance of pH sensors while reducing their cost. Fiber optic – surface plasmon resonance (FO-SPR) pH sensors have attracted increasing interests due to their many advantages, such as low-cost production, small size, immunity to electromagnetic interferences, remote sensing capability, and the safety for in vivo measurement [2]. In the FO-SPR
technology, the light is guided through a metal (typically gold)-coated multimode FO to yield propagating plasmonic waves at the interface obtained with the analyzing environment (typically a liquid). Sensitive changes in the refractive index of light are then triggered by any biological interaction or chemical reaction occurring at this interface, which are further processed in a graph [3].

In this work, we report results on the fabrication and characterization of a SPR based pH sensor using coatings of platinum (Pt) and conductive polyaniline (PANI) layers over an unclad core of a FO. The thin platinum layer was coated using a magnetron sputtering technique, while the pH-sensitive polyaniline layer was synthetized using a relatively novel electroless polymerization method. The thicknesses of Pt and PANI layers were optimized to achieve the best performance of the sensor.

The proposed FO-SPR pH sensor exhibits a fast and linear response in either acid or alkali solution (pH operational range 1 to 14).

**Keywords**: Fiber optic-surface plasmon resonance, Platinum, Polyaniline synthesis, pH sensor.

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**References**


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**S2 O6**

**THERMAL DESORPTION SPECTROSCOPY INVESTIGATION OF DBD PLASMA MODIFIED ALUMINIUM OXIDE SUBMICRON POWDERS**

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Our recent work on the activation of fine Al₂O₃ ceramic powders by atmospheric pressure coplanar DBD (dielectric barrier discharge) revealed several benefits which such activation may have for advanced ceramic engineering. The need of dispersant additives for preparing stable water-based ceramic suspensions can be reduced or even completely removed [1]. Slip casted Al₂O₃ samples from DBD activated powders exhibited finer pore size distribution and higher sinterability. Final microstructure of sintered samples had the grain size reduced by a factor of 1.7 [2]. The performance of electrophoretic deposition (EPD) reduced significantly the deposited layer surface roughness, due to the reduced deposition rate and reversed deposition polarity from cathodic to anodic [3].

To address the nature of underlying physico-chemical processes, DBD plasma activated Al₂O₃ as well as yttria stabilized ZrO₂ powders were thoroughly investigated by means of thermal desorption spectroscopy. We have found that plasma treated powders contains additional oxygen, nitrogen monoxide, nitrogen dioxide and carbon dioxide functional groups. Performed experiments pointed out the important role of plasma originated molecular gasses physisorbed on the ceramic particles surface.

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INFLUENCE OF SURFACE MODIFIED CELLULOSE ON THE PROPERTIES OF BIO MEDICAL POLYESTER SCAFFOLDS

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Among aliphatic polyesters, poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) copolymer is increasingly studied for biomedical applications because it shows biodegradability and biocompatibility, lack of immunogenic or carcinogenic effects and lack of toxicity [1-2]. Micro- and nano-celluloses are often used to improve the properties of biopolymers. However, cellulose is very hydrophilic and surface modification is necessary to enhance its effect in PHBV and other hydrophobic biopolymers.

In this work, cellulose was surface modified using two approaches, a physical one (plasma treatment) and a chemical one (TEMPO oxidation). Plasma treatment of cellulose has been intensively studied for different purposes like cleaning, sterilization, activation, increased hydrophilicity or hydrophobicity [3]. In this work, plasma treatments were applied directly in the suspension of cellulose in water under oxygen flow leading to efficient surface functionalization. TEMPO-mediated oxidation is an effective method to convert the hydroxyl groups of cellulose into carboxylic groups using TEMPO as a catalyst and sodium hypochloride as oxidant. The birefringence of cellulose suspension in water after TEMPO oxidation was highlighted in Fig. 1.

 Plasma and TEMPO modified celluloses were incorporated in a PHBV matrix and the influence of differently modified celluloses on the morphology, thermal and mechanical properties of this biopolyester was studied. Both treatments were found efficient to improve the fiber-polymer interface and the properties of PHBV for biomedical application.

Keywords: surface properties; cellulose; plasma treatment; biopolyester

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References:

THOMSON SCATTERING OF HELICAL BEAMS

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We study in the classical formalism the radiation scattering on free electrons (Thomson scattering) of helical beams. For a laser field modeled by a Laguerre-Gauss [1] solution of the wave equation interacting with a free electron, we study the electron trajectory and then the radiation emitted by it during the interaction with the laser. For the emitted radiation we calculate the frequency spectrum, and the angular momentum. We compare our results with those corresponding to the case of scattering of a plane wave pulse of arbitrary length of circular polarization [2], respectively of a wave described by a Gaussian mode.

References.

S2 O9

PROTON NIEL CALCULATION FOR GAAS USING GEANT4 MONTE CARLO CODE

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The space radiation environment includes high energy particles such as photons and charged particles. These energetic particles typically degrade the electrical and optical properties of semiconductor and device performance, when these energetic particles pass through it. In particular, the devices that are used in space applications. Laboratory sources of energetic particles have been used historically to simulate the radiation damage from space environment. Numerous investigations have been made on the correlation of displacement damage produced by various particle types and energies [1-6]. The results of these studies are demonstrated that the experimental degradation measurements can be estimated reasonably well by using the Non-Ionizing Energy Loss (NIEL) approach, which gives the amount of energy deposited by an incident particle that can lead to displacement damage. However, some discrepancies are still observed in the case of gallium arsenide (GaAs) irradiated with protons having energies greater than 20 MeV.

In this work, we present the calculations of proton NIEL for GaAs by employing the Monte Carlo transport code GEANT4, to estimate the damage induced by the protons irradiation in GaAs-devices. The obtained results show a good agreement with NIEL calculations given by other authors[2, 7, 8]. In order to validate our NIEL calculations, the experimental measurements of damage coefficient for a variety of GaAs devices (e.g., LEDs, solar cells and resistors) irradiated with protons of energies going from 1 MeV up to 1000 MeV, is used to investigate the relevance of the NIEL scaling law for protons [1, 3, 4]. A reasonable agreement is found between our NIEL calculations and experimental data for protons (< 20 MeV). However, a discrepancy can be observed for high-energy protons. These discrepancies are attributed to many different causes that have been discussed in detail in this work.

Keywords: Displacement Damage, NIEL, Proton, GaAs.

References:
LASER ION SOURCE BASED ON THE Nd-YAG LASER FOR THE COMMISSIONING OF THE HEAVY IONS LINEAR ACCELERATOR IN FRAMEWORK OF NICA PROJECT

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NICA facility is aimed to perform at JINR wide program of fundamental and applied researches with the ion beams from p to Au at energy from a few hundred MeV/u up to a few GeV/u. The new accelerator facility Nuclotron-based Ion Collider fAcility (NICA) is assumed to operate using two injectors based on the KONUS-type linacs: Light Ions Linear Accelerator (LILAC) as injector for light ions, polarized protons and deuterons and a Heavy Ions Linear Accelerator HILAC for the heavy ions. In 2016 HILAC consisting of three accelerating sections: RFQ and two DTL sections based on IH cavities had been assembled. To produce the ions that have ratio \(Z/A=1/6\), Laser Ion Source (LIS) based on commercial available Nd-YAG laser had been developed and constructed. Experimental setup for investigation of ion's spectrum of the LIS is described. Charge states spectrum for carbon and Fe plasma are presented. The results of the acceleration in HILAC of the ions C\textsuperscript{2+} are described.

COMPARISON OF THE PROPERTIES OF IZO AND AZO THIN FILMS DEPOSITED BY RF MAGNETRON SPUTTERING

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Transparent conductive oxides (TCO’s), based on undoped and doped zinc oxide (ZnO), have become increasingly important by recent developments of transparent electronics and optoelectronic devices [1].

In this study we compare the properties of doped ZnO, like aluminium zinc oxide (AZO) and indium zinc oxide (IZO), thin films deposited by RF magnetron sputtering. Both architectures were deposited on glass substrates, using argon atmosphere of 6.0 purity, and commercial available targets of AZO and IZO respectively, at different values of the applied RF power (from 40W up to 100W, with steps of 20W). The other working parameters were kept constant: the pressure in the deposition chamber was 0.5 Pa and the target-substrate distance was 10 cm for every deposition. During each deposition process high resolution optical emission spectra were recorded.
The structural characterization of the deposited thin films was carried out by X-ray diffraction (XRD) and X-ray reflectometry (XRR). The atomic force microscopy (AFM) and scanning electron microscopy (SEM) methods were used for morphological investigations.

The optical properties were analysed by spectroscopic ellipsometry, UV-VIS spectroscopy, and Fourier–transform infrared spectroscopy (FTIR). First results show that all deposited layers present a transparency larger than 80% in the spectral domain of 400 nm – 800 nm.

This study was performed in order to identify the optimal conditions which will be used for producing thin films as constitutive of a transparent field effect transistor and/or other optoelectronic devices like organic photovoltaic cells.

**Keywords:** plasma physics, transparent conductive oxide, materials science

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### S2 P1

SCATTERING MATRIX MAPLE APPLICATION FOR PROPAGATION OF ELECTROMAGNETIC RADIATION IN STRATIFIED MEDIA

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A recurrent scattering matrix formalism for electromagnetic wave propagation modeling in stratified media structures. The python procedure is computationally efficient and stable. For a case study, it is applied successfully to the modeling of total attenuated reflection in nematic liquid crystals.

The modes of a planar multilayer waveguide can readily be determined by using an algorithm that exploits the analyticity of the waveguide dispersion relation. No prior knowledge of the number of solutions or their approximate locations is required; the algorithms finds all the solutions within the region of interest.

The application could be used for structures of transparent and lossy materials.

**Keywords:** scattering matrix formalism, stratified media structures

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### S2 P2

LASER-BASED SPECTROMETER FOR THE DETERMINATION OF THE DISSOCIATED CO\(_2\) GAS FROM A PLASMA GENERATOR

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In this paper we present a type of trace gas detection system based on a continuous wave (cw) CO\(_2\) laser in combination with photoacoustic spectroscopy [1].

The present research is included to expose the suitability of CO\(_2\) laser system to monitor in real time CO\(_2\) emission from various dynamic processes in a plasma generator [1-3].

Recent applications on a laser-based spectrometer using a cw CO\(_2\) laser are presented and a comparison is made to an Optical Emission Spectroscopy (OES) investigation for the determination of the dissociated CO\(_2\) gas from plasma generator [2]. Relationships between the photoacoustic signal and gas pressure, laser power and gas concentration were measured and discussed in detail, respectively [1-3].
The combination of photoacoustic spectroscopy and the CO₂ laser has resulted in simple, robust and easy to maintain designs which are giving photoacoustic spectroscopy a competitive advantage over other sensitive techniques [1, 3].

**Keywords**: laser photoacoustic spectroscopy system, plasma generator, CO₂ gas.

**Acknowledgements** We acknowledge the financial support of the Space Technology and Advanced Research - ESA, projects (project No. 161/2017, project No. 173/2017 and project No. 153/2017).

**References**
processing [2]. Therefore, the development of reversible and highly sensitive ammonia sensor is highly required.

In this work, a conductometric ammonia gas sensor has been designed and fabricated using polyaniline (PANI) as sensing element. The sensor is fabricated by coating an alumina substrate with a platinum film using a magnetron sputtering technique and an in-house fabricated shadow mask, while the conductive polyaniline layer was synthesized using a relatively novel electroless polymerization method. Structural and morphological characterizations of PANI layer were carried out using X-Ray Difractometer (XRD) and Scanning Electron Microscope (SEM), respectively. The detection of ammonia gas has been carried out at room temperature and using an in-house built setup for testing electrical gas sensors.

The proposed sensor is highly sensitive for concentrations of ammonia gas below 1ppm and has small response as well as recovery time.

**Keywords:** Polyaniline, Electroless polymerization, Ammonia gas, Conductometric sensor.

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**S2 P5**

**STRECHING AND COMPRESSION OF DOUBLE PLASMA VORTEX**

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The interest for complex plasmas is increasing due to the multiple applications [1] they are targeting (astrophysics, plasma fusion, industry etc). In this paper we report a Kelvin-Helmholtz instability obtained in a laboratory plasma. Micrometric particles with a diameter of 14.45 µm immersed in rf plasma behave like probes that collect electrons and ions. We obtain a crystal under low pressure (250 mT in CO2) that levitate between two electrodes. The electric power fed into the discharge is 2W. The particles are illuminated by a He-Ne laser beam passed through a cylindrical lens.

![Figure 1](image)

**Figure 1.** Dusty plasma with vortexes obtained at 250mT and 2W.

The particularity of this crystal is the presence of two symmetrical vortexes in the crystal extremities. In Figure 1 we can see the two phases of the crystal, in the middle zone the particles are static and in the extremities the particles move continuously in ellipsoidal shapes. After introducing more gas (CO2) into the vacuum chamber at constant speed through the gas valve, we observe a collective displacement of the particles in the crystal in the direction of gas flow. Crystal shift also involves a change of his shape, especially at the level of the two vortexes. One vortex was stretched and the other was compressed. The presence of vortex in dusty plasma is a great opportunity to investigate turbulent flow and instabilities. In the community of dusty
plasma physics there are several ideas to explain the nature of vortexes, from non-conservative force [2] to gradient temperature [3] between the two electrodes or the fact that the gradient of dust-charge is not parallel to non-electrostatic force (gravitational force and ion drag force) [4].

**Keywords:** plasma physics, dusty plasma.

**Acknowledgement:** This work was supported by the by Romanian Space Agency (ROSA) under contract DUSTEXSPACE nr. 123 Competition C3- 2016 and PN 18 13 01 01

**References:**

S2 P6

**CAN WET IMPREGNATION BE A Viable ALTERNATIVE TO BULK DOPING?**

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We show that wet impregnation is a viable alternative to bulk synthesis of various doped nanosized tetravalent metal oxides(Sn, Ce, Zr). Regarding the chosen dopant doped by wet impregnation, rational design includes, in the case of CeO₂ divalent(Ca), trivalent(Yb) and tetravalent(Zr) with concentrations up to 30%. For ZrO₂ trivalent Eu in concentration of up to 20%[1] and finally, for lanthanide(1% Pr, Sm, Eu, Tb, Dy and Er) doped SnO₂, monovalent Li+ with concentration of up to 15% were added by wet impregnation. The homogeneity of the solid solutions is confirmed down to atomic scale by a complex characterization toolbox with both long and short-range sensitivity based on in situ/ex situ XRD, Raman, DRIFT, TEM, XPS and luminescence techniques. Luminescence is exploited as a probe tool for the atomic homogeneity or represents a desired functionality optimized by simple wet impregnation. For CeO₂, the homogeneity of the solid solution emission at various stages of thermal treatment was monitored using up-conversion[2]. For, ZrO₂, wet impregnation with Eu stabilizes the tetragonal phase with local homogeneity being confirmed using Eu luminescence as local probe. For lanthanide doped SnO₂, wet impregnation with Li induces modifications in the structural properties of the host and gives new perspective on the actual mechanism of emission enhancement in the tetravalent host. The mechanism of emission enhancement, which can be as high as 70, discards the local symmetry distortion and assumes only a small contribution from improved crystallization induced by Li.

Collectively, our findings offer a significant advance into doping behavior for several technologically relevant tetravalent oxides and propose a viable alternative for traditional synthesis methods while maintaining the homogeneity down to atomic scale. By use of wet impregnation, the same batch of preformed nanoparticles can be doped with different metal concentrations or with various metals at a fixed concentration, allowing a systematic and reliable investigation of the effect of doping, metal type and concentration on the various functionalities of these technologically relevant oxides.

**Keywords:** Wet impregnation, Rational design, Luminescence, Homogeneity.

**Acknowledgements:** The authors acknowledge CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2016-0305 for the financial support

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Rotation of plasma crystals induced by the torque exerted by an electron beam slightly off-axis was investigated. The crystal was made of melamine formaldehyde microparticles with a diameter 11.8 µm and was levitated in a radiofrequency discharge at 13.56 MHz. A beam of electrons with energies from 8 to 14 keV determined the rotation of the whole crystal. Depending on the energy and beam frequency the crystal rotated with variable speed and kept its hexagonal symmetry. However, above a threshold, the symmetry was broken and the crystal lost its particle arrangement. The particle tracking velocimetry (PTV) technique was used to determine the individual trajectories of the microparticles and their velocities. Small crystals of 8 to 10 microparticles and wider crystals of 40 to 50 particles were used. The particles moved on circular trajectories with the highest mean velocity on the largest radius.

**Figure 1.** Rotation of two plasma crystals: a) a crystal with 43 particles irradiated by a 10 keV electron beam keeps its symmetry; b) symmetry breaking in a plasma crystal with 9 particles at 13 keV

**Keywords:** plasma physics, electron beam, PTV, dusty plasma

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**S2 P8**

**NUMERICAL INVESTIGATIONS INTO LASER-PLASMA INTERACTIONS BY MEANS OF PARTICLE-IN-CELL SIMULATIONS**

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We present a series of preliminary numerical results on laser-plasma interactions by means of particle-in-cell (PIC) simulations using in silico setups which are relevant for the CETAL and ELI-NP laser facilities in Măgurele. We survey the major PIC codes focusing on the physical regime they cover, the type of processing (GPU vs. CPU), and the scalability on large clusters. We present numerical result which pertain to high- and ultra-high power lasers interacting with gaseous and solid targets and discuss possible future experiments at CETAL and ELI-NP.

S2 P9
AGEING EFFECT OF DBD ACTIVATED CERAMIC POWDERS: THE IMPACT OF STORAGE HUMIDITY ON THE ELECTROPHORETIC DEPOSITION RATE

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Electrophoretic deposition (EPD) of plasma pre-treated Al2O3 powders results in ceramic layers of substantially improved deposit homogeneity [1]. To evaluate the practical applicability of this phenomenon, we report on the magnitude and dynamics of undesired gradual deterioration on plasma treatment – the ageing effect. Powder samples were treated by diffuse coplanar dielectric barrier discharge (DBD) and sequentially evaluated for their EPD performance for the time span of 30 days. Two sets of powder samples were evaluated. The first was stored in arid environment of 23% RH, the second one in a humid air of 86% RH. The storage in the arid environment resulted in a slow but gradual decline of deposition rate (Fig. 1L). However, the uniformity of deposited layers remained unaffected. The samples stored in the humid environment exhibited a substantially more complex behavior (Fig. 1R). Already after one week the effect of plasma treatment had disappeared, and the deposition polarity had to be changed from anodic to cathodic. Afterwards gradual increase of deposition rate was observed until the final recurrent decline at fourth week. The results point out the importance of water molecules controlled secondary processes on the treated powder surface.

Fig. 1. EPD deposition rate for DBD plasma activated Al2O3 powders stored in air of low (left) and high (right) relative humidity level.

Keywords: ageing effect, activated ceramic powders, humidity

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References
S2 P10

INVESTIGATION OF THE INFLUENCE OF VARIOUS DOPANT MATERIAL ON A DIELECTRIC BARRIER LAYER OF DIELECTRIC BARRIER DISCHARGE

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New and promising alumina-based ceramic materials are of great importance to the scientific community in fields of plasma physics and material sciences for their widespread useability. In the presented research, we study the influence of various elements (Mg, Cr, and Fe) on electric properties of ceramic-based dielectric barrier materials as well as discharge properties such as ignition and quenching voltages of dielectric barrier discharge (DBD) in coplanar geometry. The investigation was carried out with respect to different electrode gaps between 0.3 - 1.0mm for fixed ceramic thickness of 0.3mm. We have complemented this study with basic morphology investigation with the use of a scanning electron microscope (SEM) and profilometer.

Keywords: Dielectric barrier material, alumina-based ceramics, ignition voltage, coplanar dielectric barrier discharge.

S2 P11

EFFECTS OF CARBON AND SILVER ON THE NANOSTRUCTURE AND MORPHOLOGICAL BEHAVIOR OF TITANIUM BASED FILMS

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Titanium (Ti) and its alloy are widely used due to his high strength, light weight, corrosion resistance. The purpose of this study is to achieve the controlled synthesis of Ti based thin films, with compact structure and extremely smooth surface, made by Thermionic Vacuum Arc (TVA) technology. The obtained thin films were characterized using scanning electron microscope (SEM) accompanied with energy dispersive spectrometer and transmission electron microscope (TEM). The films are composed of nanoparticles very smoothly distributed embedded in amorphous matrix film. We measured by contact angle method the wetting charcatcer of the surfaces and the results showed suitable results for biomaterials applications. We desired to develop a correlation between the parameters of the film deposition and the wetting properties. This will be used to analize the potential correlation between the surface properties and the biological reactions and applicability.

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S2 P12
CHARACTERIZATION OF PLATINUM BASED THIN FILMS DEPOSITED BY THERMIONIC VACUUM ARC (TVA) METHOD

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Due to its excellent electrical properties, high chemical stability and catalytic activity, the noble metal platinum (Pt) is used in many important industrial and scientific applications, ranging from high-temperature chemical sensors for microelectromechanical systems (MEMS)¹ and thin-film strain gauges² to counter-electrodes for dye-sensitized TiO₂ solar cells³ and catalysts for purification of exhaust gases from automobiles⁴. The morphological properties of Pt thin films fabricated via reactive DC magnetron sputtering and Atomic Layer Deposition (ALD) were extensively studied in scientific literature.

The current work aims to characterize the morphology, chemical and mechanical properties of Pt and PtTi thin films deposited via Thermionic Vacuum Arc (TVA) method on glass and silicon substrates and were characterized by means of Electron Microscopy techniques (SEM and TEM). The quantitative elemental microanalysis was done by using X-Ray Photoelectron Spectroscopy (XPS) and Energy-dispersive X-ray spectroscopy (EDS). The tribological properties were studied by ball-on-disc tribometer.

The purpose of our study is to find potential applications of Pt based thin films in fields such as nanoelectronics, fuel cells, medicine and materials science.

Keywords: Pt thin films, TVA, morphological properties.

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S2 P13
THIN FILM DEPOSITION USING MICROWAVE GENERATOR FOR NANOMATERIALS APPLICATIONS

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This research presents a new method that can be used in metallic thin film deposition, based on the microwave absorption by the metallic wires. Thin films were grown on Si substrate at room temperature from pure wires using the innovative microwave technique. During growth, the ambient atmosphere was CO₂ and air.

For the vaporization and ionization process of the metallic wires we used a microwave generator with a 2.45 GHz frequency at 800 W. Briefly, the microwave generator arrangement is composed of a power supply, a microwave source and a cylindrical cavity having the TM₀₁₁ propagation mode.
In this experiment, we vaporized and ionized the metallic wires that are made of W, Zn and Mo, Pb and In with 0.5 mm diameter, by direct interaction with the microwave field from the cylindrical cavity. The electron temperature regarding metallic plasma produced was estimated using the ratio of atomic emission lines acquired by a high definition optical multichannel spectrometer.

The structure and morphology of the deposited films were investigated using profilometry, SEM and XRD techniques.

The results showed that the atmosphere could change the chemical composition of the deposited films. The properties of the deposited films were correlated with their structure, surface morphology and chemical composition.

**Keywords**: microwave waveguide, magnetron, metallic plasma, metallic wires

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**S2 P14**

**PROBE MEASUREMENTS OF TVA PLASMAS PARAMETERS**

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The thin film depositions are of tremendous importance in nowadays technologies, having wide applications in every day’s life.

Knowing the plasma characteristics is essential in thin film depositions, especially when the ion bombardment of film surface has a significant influence on the resulting quality; therefore, ion energy distribution function (IEDF) is an important parameter that needs to be determined. Although the TVA system was intensively used in the last decade to deposit thin films for nuclear application, the influence of the processing parameters on the films’ structure and properties needs further investigations. Plasma diagnosis helps us to understand the correlation between the processing parameters, ion energies and ion fluxes, and the corresponding structure and properties of the films obtained in a TVA system. It is also necessary to determine if the energetic ions are favourable or not in obtaining high-quality coatings.

One of the simplest devices capable of obtaining the ion energy distribution function (IEDF) is the retarding field analyzer (RFA). The basic principle of an RFA is the measurement of an electrical current given by electrically charged plasma species against a retarding voltage. The ion energy distribution function is obtained from the first derivative of the current-voltage characteristic I-V.

In this work are shown the results of ion energy analysis of the TVA plasma ignited in different materials vapors. One of the most promising deposition method is the TVA technology. In TVA, the plasma is generated by electrons-metal atom collisions. The atoms are evaporated from the anode by its intense electron bombardment. These evaporated atoms are deposited on different substrates mounted in the vacuum chamber. Usually, the plasma potential is raised to a high positive voltage and this allows the metal positive ions to acquire high energy (order of hundred eV) and to deposit it on the substrate. Due to a low background pressure \((9\times10^{-4}\text{Pa})\) the energy of ions is directly proportional to this potential difference. This is an important feature of the method, as the ion energy can be directly controlled by the operating plasma parameters. As a result the forming deposition layer obtain a very regular, dense and pure structure.

**Keywords**: TVA, RFA, ion energy distribution function
S2 P15

DEVELOPMENT OF NEUTRON BEAM DIAGNOSTIC AT THE "QUINTA" SETUP

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Accelerator Driven Systems (ADS) are the subcritical fast reactors with external source of neutrons considered now as tool for the transmutation of the long-lived components of radioactive wastes (RAW) and for the solution of global energy problems. The idea of Nuclear Relativistic Technology is to use extremely hard spectrum of neutrons formed by beams of the relativistic particles in deeply subcritical quasy-infinite (at the negligible leakage of neutrons) Active Zone consisting of the depleted (natural) uranium, thorium and spent nuclear fuel. "Energy and Transmutation of RAW" project will provide fundamentally new data and numerical methods necessary for design of demonstration experimental-industrial setups based on the proposed scheme. In framework of the project that started in JINR in 2010 QUINTA setup was constructed for the development and testing methods and systems for measuring parameters of nuclear-physical processes and over the years had been used for data acquisition in accelerating runs of synchrotron Nucleotron of Laboratory of High Energy Physics of JINR. QUINTA was limited modelling central part of Big URANium Target (BURAN) target setup, which is realistic prototype of quasy infinite Active Zone in the Nuclear Relativistic Technology. Measuring the hardness of the neutron spectrum using of TFBC-detector, the measurements of the neutron spectrum using the activation technique and the measurements of neutron leakage from the set-up “Quinta” by passive silicon detectors and scintillation detector DEMON are described. The plans of the full-scale experiment at the BURAN setup in JINR are presented.

S2 P16

DISSOCIATION OF THE CARBON DIOXIDE USING MICROWAVE PLASMA GENERATOR

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We present a new method of carbon dioxide dissociation using a microwave plasma generator (MPG). MPG is based on direct interaction between microwave field and metallic wires such W,Mo and Cu. Briefly, the microwave generator arrangement is composed of a power supply, a microwave source with a 2.45 GHz frequency at 800 W, and a cylindrical cavity having the $TM_{011}$ propagation mode. The metallic wires having 0.5 mm diameter are vaporized and ionized in direct interaction with the microwave field from the cylindrical cavity.

Dimensions of the metallic nanoparticles was analyzed using SEM technique. The metallic plasma was diagnosed by optical emission spectroscopy (OES) method. The experiment was conducted in carbon dioxide at normal atmospheric pressure and room temperature.

During of conversion of the metallic wires to metallic nanoparticles, the carbon dioxide was dissociated in monoxide of carbon and oxygen.

**Keywords**: microwave, metallic wires, carbon dioxide dissociation, carbon monoxide

**Acknowledgements** This work was supported by the Romanian Space Agency through (STAR) Space Technology and Advanced Research Programme (project No. 161/2017, project No. 173/2017 and project No. 153/2017).

**References**
APPLICATIONS OF PLASMA IN DENTISTRY

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This article highlights the fact that lately, plasma has more and more applications in medicine. The plasma generation can be realized at low, atmospheric and high air pressure and their temperature could be different. Biomedical application of plasma technology has become very popular in various fields today but it is not clear when it was first used in the field of dentistry. Plasma produces both morphological and chemical changes of the surface and free radicals on the polymers surface. By using various treatments with plasma changes occur on the surface of some polymer type materials in terms of physical and chemical properties, without affecting their properties as a whole. Plasma applications, in dentistry, were classified into two categories, surface treatment and direct applications, and were reviewed, respectively according to the approach. The current paper discussed modification of dental implant surface, enhancing of adhesive qualities, enhancing of polymerization, surface coating and plasma cleaning under the topics of surface treatment. Decontamination, microbicidal activities, root canal disinfection and tooth bleaching were reviewed as direct applications. Non-thermal atmospheric pressure plasma was of particular focus since it is possibility for its use in living tissues. Restorative treatment using dental implants has become a standard procedure in contemporary dentistry. Future perspectives have also been discussed briefly. Some researchers reported that for enamel, dentin and composite,a super-hydrophilic surface could be easily obtained by plasma brush treatment without affecting the bulk properties regardless of the original hydrophilicity. Although it is still not popular among dentists, plasma has shown promises in several areas of dentistry and is now opening a new era of plasma dentistry.

Keywords: Dentistry, plasma, technology, treatment

ATMOSPHERIC PRESSURE PLASMA ASSISTED CALCINATION BY PREPARATION OF INORGANIC SUBMICRON FIBERS

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Inorganic ceramic fibers (Al₂O₃, SiO₂, TiO₂, ZnO, etc.) are one of the most studied materials in the submicron region. They are usually prepared by thermal treatment of composite metal-organic fibers prepared from solution of polymer material - base polymer and precursor serving as a source of inorganic material using standard spinning techniques [1]–[3]. Then, the composite fibers are exposed to the high temperatures (500-1000°C) for several hours (5-10 hrs) in the process of thermal calcination. Thermal calcination is used for removing the organic base polymer by the preparation of inorganic submicron fibers. Due to the high temperature approach and long treatment times, conventional thermal calcination needed by the processing of inorganic submicron fibers is significantly time- and energy-consuming process.

In this work we study the plasma assisted calcination of fibers consist of Al(NO₃)₃/PAN by using Diffuse Coplanar Surface Barrier Discharge (DCSBD) [4]–[6]. The effect of plasma on the composite fibers was examined in terms of the organic polymer removal using Fourier Transform Infrared Spectroscopy (FTIR) and Energy-dispersive X-ray spectrometry (EDX). The influence of plasma on the morphology of the fibers was investigated by Scanning Electron Microscopy (SEM).

Effect of plasma treatment has been studied at different plasma treatment time (in the range 1-30 minutes), working gas (ambient air, oxygen, nitrogen, synthetic air and synthetic air with water vapour) and two different power supply parameter (frequency and input power). Also the influence of increased temperature during plasma treatment was studied.

The chemical composition and structure of resulted fibers prepared by conventional thermal calcination, plasma calcination and combined calcination were compared. The fibers pre-treatment by DCSBD plasma led to shortening of thermal treatment and decrease the temperature required for removal of polymer and precursor residues.

**Acknowledgement:** This work was supported by the Slovak grant agency Vega, project No. 1/0782/19.

**Keywords:** inorganic nanofibers, plasma assisted calcination, low-temperature plasma.

**References**


ABSTRACTS

S3 – Nuclear and sub-Nuclear Physics and Applications

- Nuclear and subnuclear sciences and Engineering
- Advanced detection systems
- Accelerated particle beams
- Nuclear Techniques and applications
- Nuclear Safety and Radiation Protection
**S3 L1**

**DEVELOPMENT OF NEUTRON SONDE MICROSCOPY**

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Conventional neutron beams for the investigations of bulk materials have a width 0.1 - 10 mm. For the investigations of local microstructures with high spatial resolution we need the neutron beams of the width from 0.1 to 10 mkm. Planar waveguides are tri-layer focusing devices which transform the conventional neutron beams into very narrow and slightly divergent microbeams. In [1,2] the polarized neutron microbeam of the width of 2.6 mkm and the angular divergence of 0.14\(^\circ\) was used for the investigation of a magnetic amorphous microwire. This method is termed as Neutron Sonde Microscopy. Recently we have investigated the angular divergence of the neutron microbeam as a function of the neutron wavelength and the waveguiding channel width. The time-of-flight [3] and fixed wavelength [4] reflectometers was used. Experimental data were described by Fraunhofer diffraction on a narrow slit which was the waveguiding channel. In this review we report the obtained results.

**Keywords:** planar waveguide, neutron microbeam, Fraunhofer diffraction, magnetic microstructure.

This work was supported by the scientific project JINR-Romania in 2019.

**References**


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**S3 L2**

**FIRST EXPERIMENTAL TEST OF TIME-GRADIENT MAGNETIC FIELD SESANS DIFFRACTOMETER AT PULSED REACTOR IBR-2**

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The Q-resolution of the conventional small angle neutron scattering (SANS) diffractometers is practically limited at 1x10\(^{-3}\) Å\(^{-1}\), that doesn’t allow for studies of large-scale structures. Focusing [1] and spin-echo based [2] SANS techniques developed to complement the conventional SANS are allowing to overcome this limit.

In this work we describe the implementation of a new spin-echo SANS technique based on the use of time-gradient magnetic fields (TGF NSE) [3] aiming to extend the possibilities of the REFLEX reflectometer [4] at the pulsed reactor IBR-2 (Dubna, Russia).
This technique requires the use of the linearly increasing magnetic field in the form of the sequence of sawtooth pulses, that suites very well to pulsed structure of neutron beam at IBR-2. A wide range of neutron wavelengths employed in the time-of-flight operation mode allows for the simultaneous coverage of a wide range of spin-echo lengths (corresponding to a wide Q-range in conventional SANS), as the latter is proportional to the cube of the neutron wavelength, and therefore for SANS studies over a wide length scale.

In this work, the last experimental results obtained using the prototype of the TGF-NSE setup at the pulsed beam of IBR-2 reactor are presented. Some technical problems and their solutions are discussed.

References:

S3 L3

TOWARDS MANIPULATION OF QUANTUM GAMMA PHOTONS

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The first quantum revolution took place a hundred years ago and allowed understanding quantum systems. Nowadays we speak about the ongoing second quantum revolution, which is about making use of quantum systems, meaning developing quantum technologies. The latter have already proven superior from quantum key distribution to quantum computing or imaging. The most frequently used particles are photons, particularly visible ones. During the last years appeared a growing interest for higher energy photons, reaching now X rays. Our goal is to extend the applications to the gamma range. The benefits for technology are straightforward, as gamma rays can penetrate media which are inaccessible to lower energy quanta. Implications cover a wide range of activities, from medical imaging to military applications. However gamma rays are ionizing radiation, meaning the first thing to be solved is the radiation safety issue, physically and also legally. They are also hard to handle, as the optical elements used for low energy photons are useless in this case. We have to adapt and develop new tools in order to benefit from the quantum correlations entangled gamma photons offer us. Nevertheless it is this quantum correlation that provides a strong advantage, knowing that, at least for an annihilation source, all emitted quanta are maximally entangled, in a single state (for a BBO downconversion with visible light one obtains one entangled pair out of 10 million). Between preparation (radioactive decay) and measurement (detection), we need a quantum channel for those gamma photons. Naturally, the first quantum channel we have to study is the Compton scatter.

Keywords: quantum correlated gamma quanta

S3 L4

NUCLEAR CORE EXCITATION
IN THE DYNAMICS OF PYGMY DIPOLE RESONANCE

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The nature of Pygmy Dipole Resonance in nuclear systems is still under debate and is one of the motions expected to be explored at ELI-NP experimental facility in Magurele, Romania, that will shortly enter its operational regime. We present microscopic approaches able to predict this state and discuss the role of the core excitation on the isoscalar-like nature of this mode. The self-consistent transport simulations performed with the Vlasov equation, considered as the semiclassical limit of Time-Dependent Hartree-Fock approximation, indicate an isovector motion of more isospin symmetric nuclear core when Pygmy Dipole mode is excited.

References:

ADVANCES IN BIO-MEDICAL APPLICATION OF IONIZING RADIATION AT IFIN-HH & ELI-NP

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The research in the radiobiology of ionizing photon beams at IFIN-HH was fathomed and diversified during the last years. The preparative phase for the near opening of ELI-NP infrastructure provides the opportunity to address other types of radiation sources as proton beams and the specific conditions of high dose rate of irradiation.

The bystander effect of ionizing radiation has been investigated in connection with mitochondria stress [1]. The interplay between mitochondria and nucleus has been analyzed, the key role of mitochondria stress in the cellular response of fibroblast to ionizing radiation or radiomimetic drugs being revealed [2]. In the same context, the influence of physiological state on the UV induced response of cells has been investigated, the differentiated SH-SY5Y cells showing a higher level of DNA damage comparing with the proliferative ones [3].

In the context of the large expectance from the radiotherapy techniques rely on accelerated ion beams, two of the particles accelerators from IFIN-HH have been adapted to irradiate biological samples in therapeutic range of doses (0.1-5 Gy) with proton beams. A robust dosimetry protocol was implemented using various standard detectors for this range of doses. As a first application, the generation of radical oxygen species in cells irradiated with protons was monitored, proving an increasing ROS level with dose and time after irradiation.

The gold nanoparticles are promising platforms for carrying the genotoxic drugs. The arrest of cells in G2/M cell cycle phase by a prior irradiation (1 Gy) increases the uptake of cytostatic functionalized nanoparticles, the combination of radiation with functionalized nanoparticles proving a higher efficiency against the cancer cells.

The applications of specific biomolecules labeled with appropriate radioisotopes (radiopharmaceutics) in nuclear medicine represent an established research field in IFIN-HH. The recent development of the Center of Radiotherapeutics Research by adding a new irradiation exit line and chamber for Cu64 radioisotope enlarge the range of radiolabeled compounds could be designed and tested in this facility.

All this expertise will be used for proper design of bio-medical oriented experiments in the next future at ELI-NP according to the IFIN-HH research strategy [4]. Procedures for monitoring of molecular biomarkers by NMR spectroscopy in biological samples after the irradiation pulse are designed in order to optimize the radiotherapy protocols at ultrahigh dose rate [5].
Keywords: radiobiology, proton beams, nanoparticles, radiopharmaceuticals.

References

S3 L6
A NOVEL APPROACH IN NUCLEAR STRUCTURE – GAMMA SPECTROSCOPY IN SUB-BARRIER TRANSFER WITH HEAVY IONS USING ROSPHERE

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The transfer reactions were associated for a long time with charged particles spectroscopy following direct reactions induced by light projectiles (like proton, deuteron, tritium, etc.) at energies well above the Coulomb barrier. The mechanism of similar few-nucleon transfer reactions with heavier projectiles like $^{13}$C or $^{18}$O was well understood, but their spectroscopic use was rather limited.

During the last years potential for gamma spectroscopy of the one or two nucleon transfer reactions with $^{13}$C, $^{18}$O and $^{11}$B was systematically explored using the ROSPHERE gamma spectroscopy array at IFIN-HH in Bucharest. At incident energies slightly below the Coulomb barrier on targets heavier than the projectile, the kinematics of the projectile-like product is restricted to the backward angles, thus the target-like products recoil in the forward direction. This is ideal for DSAM or plunger experiments and opens the possibility to measure the lifetime of many low-spin states that are hardly accessible with other reaction mechanisms. Consequently, the use of sub-barrier transfer reactions with moderately heavy ions for gamma spectroscopy with HPGe arrays provide an excellent complementary approach for fusion-evaporation, deep inelastic or neutron capture experiments and might also become an useful technique at the future radioactive beam facilities.

Keywords: experimental nuclear physics, nuclear spectroscopy.

S3 O1
DETERMINATION OF RADON LEVELS IN ISTANBUL UNDERGROUND TRANSPORTATION SYSTEMS

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Radon is a colorless, odorless, tasteless and a radioactive gas that is the product of degradation of Uranium. As Radon is declared as a carcinogenic substance by international organizations and which is impossible to be sensed by people, the studies on the detection of Radon are continues commonly. Studies are carried out to determine the amount of Radon in homes, in tunnels, caves, metro stations and underground working areas. In this study we determine the Radon levels in offices, ticket gates, platforms and drivers rooms at the Metro underground stations in Istanbul province. Measurements were done at 6 subway lines, in total for 67 stations for one period time between February-March 2018. Both AlphaGUARD active measurement technique and LR-115 passive technique was used to achieve the results. Radon concentration values were found between 39.47 Bq/m$^3$ and 382.02 Bq/m$^3$ for the platforms. The average radon value of all station platforms was found to be 112.80 Bq/m$^3$. The values are below the limit values determined for Turkey (limit
value is 1000 Bq/m³ for the indoor). The data obtained were compared with the international standards and studies.

S3 O2
LHC MINIMUM BIAS MEASUREMENTS IN THE FORWARD REGION FROM PROTON-PROTON COLLISIONS AND PREDICTIONS OF MONTE CARLO EVENT GENERATORS

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In this work we present a study of the predictions obtained with a set of event generators for observables measured in proton-proton collisions at √s=7 TeV at the LHCb and TOTEM experiments. The versions of the event generators chosen for the study namely, PYTHIA, EPOS, QGSJET and SIBYLL are all tuned to measurements from the LHC experiments in the central pseudorapidity region and are based on various implementations of perturbative QCD calculations and effective field theories. The observables used are: charged energy flow, charged-particle distributions, charged-hadron production ratios and V^0 ratios. The tunes improve the predictions even in the forward region and in general, the observed differences seem to be an effect of the extrapolation from the central pseudorapidity region.

Keywords: LHCb, proton-proton collisions, minimum bias, event generators.

S3 O3
PROGRESSES IN THE IMPLEMENTATION OF RADON NATIONAL ACTION PLAN IN ROMANIA

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The exposure due to radon is the biggest concern for public exposure, therefore the risks associated with radon exposure should be careful considered by countries. Based on the provisions of the Council Directive 2013/59/Euratom [1], has been issued an issued a Radon National Action Plan approved by a governmental decision.

The Radon National Action Plan describes the individual actions and strategic directions in order to comply with the provisions of the European Council Directive. Radon National Action Plan is structured on seven strategic directions covering: development of regulatory framework, measurements of indoor radon and development of radon map, identification of indoor workplaces and other workplaces with high exposure radon risk, implementation of prevention action in new buildings, information and awareness of public, minimisation of lung cancer risk due to radon, training and education of professionals who could be affected by exposure to radon[2].

The paper describes the progresses in the implementation of Radon National Action Plan performed for each strategic direction by CNCAN[2].

References
[1] 2013/59/Euratom of 5 December 2013 laying down basic safety standards for protection against the dangers arising from exposure to ionising radiation, and repealing Directives 89/618/Euratom,
S3 O4

POSITRON ANNIHILATION SPECTROSCOPY STUDIES ON POLYETHYLENE IMPLANTED WITH CU IONS USING AN ECR ION SOURCE

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Positron annihilation spectroscopy (PAS) has proven to be a powerful tool for characterizing microstructure of different materials especially the free volume properties in polymers. When positrons emitted from a $^{22}$Na isotope are injected into materials, they lose energy through ionization and excitation. After thermalization, positrons will diffuse in the media and finally they will be annihilated with electrons, emitting two 511 keV gamma-rays. In polymers, positrons will form positronium (Ps), which prefers to be localized in free volume holes. The ortho-positronium (o-Ps), one state of Ps, provides information about free volume properties.

Positron Annihilation Lifetime Spectroscopy (PALS) and Coincidence Doppler Broadening Spectroscopy (CDBS) were performed on polymer membranes. The combination of CDBS and PALS offers coherent information on both the size of free voids in polymers and on the chemical surroundings of the annihilation sites. In particular, the coincidence Doppler broadening of the 511 keV radiation produced by various molecules can be related to the annihilation at specific sites within molecules.

For the experiment we implanted samples of polyethylene with Cu$^{5+}$ ions at fluences on the order of $10^{17}$ ions/cm$^2$ using an Electron Cyclotron Resonance (ECR) ion source. After several surface implantations with energies of 90 keV, the samples were studied using the positron annihilation digital spectrometer.

The o-Ps lifetime is related to the free volume size, while the o-Ps intensity contains information about the number of free volume holes and crystallinity. A decrease in o-Ps lifetime and intensity was observed, due to the formation of ions clusters in the free volumes of the polymer.

**Keywords:** positron spectroscopy, polyethylene, ECR, Cu$^{5+}$ ions

S3 O5

THE STUDY OF ARCHAEOLOGICAL OBJECTS USING X-RAY COMPUTED TOMOGRAPHY

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Computed tomography is an imaging technique increasingly used in recent years to study archaeological objects. It combines outstanding advances in two areas, X-ray imaging and computational techniques. Basically, the technique is based on targeting an X-ray beam to the subject and measuring the effects of multiple orientations. The function of interest in X-ray tomography is the absorption coefficient, i.e. the tendency of a material to absorb X rays. The distribution of these coefficients is transformed by means of a specialized algorithm into a 3D image of an object, thus providing the opportunity to visualize the inside of the objects in a non-destructive manner.

Our investigations focused on a significant set of prehistoric objects made of clay (whole vessels and vessels fragments, anthropomorphic statuettes) and metal (copper, bronze, iron, silver, but also bimetallic - copper / bronze and iron). The Nikon XT H 225 computerized tomography system was used. Provided with a powerful micro-focus X-ray source and a high-resolution flat panel detector, this equipment provides a high speed image acquisition at high quality. With the powerful software VGStudio MAX 3.0, the data collected by the tomograph is then analyzed and processed. In the case of ceramics, the thickness of the vessel walls could be determined when their interior was not accessible (either the vessels were long and narrow or containing soil or other materials), observations were made on the structure of the paste, especially on the particle density of the paste, cracks, orientation of the voids left by the organic matter, and even the way of joining different segments of clay. Good results have also been obtained as a result of the examination of the metal objects, the identification of the shape of the corroded pieces, the cracks and the casting defects.

**Keywords:** computer tomography, archaeology, pottery

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**S3 O6**

**A DIGITAL POSITRON ANNIHILATION LIFETIME SPECTROMETER**

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Positron annihilation lifetime spectroscopy (PALS) provides a very powerful technique for non-destructive microstructure investigations in a broad field of material classes such as metals, semiconductors, polymers or porous glasses. Even though this method is well established for more than five decades, no proper standardization for the used setup configuration and subsequent data processing exists. Eventually, this could lead to an insufficiency of data reproducibility and avoidable deviations.

Based on V1742 CAEN fast digitizer, a digital positron lifetime spectrometer has been developed and tested in this work. It includes two ORTEC BaF₂ scintillation detectors, a CAEN VME controller and a CAEN VME rack together with a computer. The design includes a custom written C/C++ software application to interface with the hardware and process the data efficiently. Tests reveal a 240 ps time resolution and a 220 ps positron lifetime in silicon, comparable with conventional analog lifetime spectrometers using the same type of detector. To measure the time resolution, a ⁶⁰Co radioactive source was used. The analog section consists of nuclear instrument modules (NIM). The pulse processing part of the spectrometer is able to analyze and store in real-time several thousands of events per second, which is an order of magnitude more than the count rates in typical positron lifetime experiments. These improvements makes this digital spectrometer more simple and convenient in comparison with other spectrometers, and it can be applied to the other scintillation timing measurements with picosecond accuracy.

In particular, with this spectrometer we are planning to study polymers.

**Keywords:** digital lifetime spectrometer, timing, waveform sampling, DRS4 chip.
S3 O7

IMAGING WITH THERMAL NEUTRONS AND GAMMA RADIATIONS FOR GEOLOGICAL SAMPLES

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Some multi mineral rocks (Fig. 1) were selected for investigation by neutron and gamma imaging at imaging facility (INUS) placed at tangential channel of the TRIGA Annular Core Pulsing Reactor (ACPR) from the Institute for Nuclear Research (INR). ACPR is a nuclear research reactor designed to be operated in steady state with a maximum power of 500 kW and in pulsing mode with a peak power of 20000 MW. For investigations presented in this paper ACPR was operated in steady state mode.

Images with Lanex Regular scintillator, LiFZnS:Cu scintillator and EMCCD Hamamatsu C-9100-02 camera were acquired for these three rocks in a mixed collimated beam. For rocks 2) and 3) were performed tomography reconstructions. 213 image projections on 190.8° rotation of the samples were obtained along with 11 dark images and 11 flat fields as inputs to Octopus Reconstruction version 8.9.3.4. On LiFZnS:Cu scintillator image is formed only by thermal neutrons, but on Lanex Regular scintillator the image is formed in a majority by gamma radiations and in a minority by thermal neutrons in a proportion about 2:1. Scintillations from scintillators were captured with EM-CCD Hamamatsu C9100-02 camera.

For rock number 2 with mammal teeth there is no difference between images obtained on the two types of scintillators. A difference is observed for rock with sulfur that presents better contrast among mineral components on image obtained with thermal neutrons on LiFZnS:Cu scintillator than on image obtained on Lanex Regular scintillator.

Fig. 1 Three multi mineral rocks with a big content of galena (1, 17.5 cm x 12 cm x 5 cm), calcite with embedded prehistoric mammal teeth (2, 15 cm x 12 cm x 9.5 cm) and with sulfur content (3, 12 cm x 11 cm x 6.5 cm)

Keywords: neutron and gamma imaging, geological samples

S3 O8

QUARKONIA PRODUCTION AT LHC IN PROTON-PROTON COLLISIONS FOR THE FORWARD RAPIDITY REGION

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Studies of quarkonium production at Large Hadron Collider (LHC) aim for a better understanding of the hadronization of heavy quark pairs into meson states in the frame of the non-relativistic QCD (NRQCD) and color-singlet (CSM) models.

Here a review for J/ψ and Υ meson production measurements [1-3] performed by LHCb in the forward rapidity region in pp collisions at centre-of-mass energies of 8 and 13 TeV is presented. The two mesons were reconstructed in the dimuon decay channel. Single and double differential cross-sections were measured in the fiducial phase-space defined by the rapidity (y) and transverse momentum (p_T) ranges of 2.0 < y < 4.5 and p_T < 14 (15) GeV/c for J/ψ (Υ) at \( \sqrt{s} = 8 \) TeV and p_T < 30 GeV/c for Υ at \( \sqrt{s} = 13 \) TeV. Both prompt J/ψ and J/ψ from b-hadron decays were considered and measured individually. In the case of Υ, the dimuon branching fraction times the differential cross-section was measured as a function of p_T and y. The results of the measurements were compared to theoretical approximations [4].

For the LHCb measurements previously introduced, RIVET [5] analysis modules are developed to reproduce in a generator-independent way most of the associated distributions and spectra available through the HepData portal (www.hepdata.net). The RIVET plugin implementation in C++ code was used in a data versus MC comparison with simulated quarkonia produced with a special setup of PYTHIA 8 event generator [6].

**Keywords:** LHC, heavy flavour quarkonium, event generator, QCD

**References**


S3 O9

**MODERN FACILITY FOR NEUTRON RADIOGRAPHY AND TOMOGRAPHY FOR APPLIED RESEARCH ON THE BASE OF THE WWR-K REACTOR**

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At the basin-type reactor on thermal neutrons WWR-K, an experimental facility is setting up to conduct researches using neutron radiography and tomography. A neutron beam with a cross section of 20 x 20 cm forms a system collimator, for which the value of the characteristic parameter L / D can vary from 350 to 2000. The neutron radiography method consists in obtaining neutron images of the investigated objects. Due to the different degree of attenuation of the neutron beam during the passage through materials of different chemical composition, density and thickness of the components of the investigated sample, the information on the internal structure of the materials with spatial resolution at the micron level is provided. This method of
nondestructive control is characterized by a deeper penetration into the thickness of the material compared with complement x-ray introscopy method and is advantageous in studying samples with both light (for example, hydrogen or lithium) and heavy elements.

All modern and newly created neutron sources are equipped with neutron radiography and tomography facilities. Methods of neutron radiography now is widely applied for material investigations and products for nuclear technologies, paleontological and geophysical objects, unique objects of cultural heritage. It should be noted that now, much attention is also paid to unique research of physical and chemical processes in fuel cells and batteries, processes associated with the penetration of hydrogen or water into the thickness of various materials. Functional development of the invention of neutron radiography is made by neutron tomography. In this method the volumetric reconstruction of the internal structure of the investigated object is performed from a set of individual radiographic projections, i.e. for different angular positions of the sample relative to the direction of the neutron beam.

The presented work describes in detail the design and main parameters of the new experimental facility for investigations using neutron radiography and tomography, created on the 1st channel of the WWR-K reactor.

**BASIC PARAMETERS OF THE EXPERIMENTAL FACILITY FOR RESEARCHES USING NEUTRON RADIOGRAPHY AND TOMOGRAPHY**

Figure 1. 1 - detector system and goniometers for positioning of beam; 2 - evacuated casing of a neutron beam; 3 - vacuum station of the collimator system; 4 - bismuth filter for a neutron beam; a system of rotary and inclined investigated sample in a neutron system of collimators forming a for evacuating air from the casing location of a single-crystal and a collimator;

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**S3 O10**

**SIMULATIONS USED FOR THE DESING AND INTERPRETATION OF CYCLOTRON EXPERIMENTS**

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At at TR-19 cyclotron from IFIN-HH several experiments are conducted. In order to achieve the optimal experimental conditions different computer codes and Monte Carlo simulation codes are used in advance. One of the main interests of the research center is obtaining various radioactive isotopes of medical interest. Before irradiating the chosen target estimations of the production cross sections for the isotope which is of interest, as well as other possible impurities. In this purpose, Talys computer code is used and this way, the most optimal irradiation energy can be chosen. This kind of estimations were done for the production of $^{48}$V, $^{64}$Cu, $^{56}$Co, $^{52}$Mn and others.

Another type of experiments that are conducted at the TR-19 cyclotron are radiobiology experiments. The main purpose of these experiments is studying the radiation effect on different types of living cells. Since a PET cyclotron is delivering high current proton beams, the main challenge was reducing the beam current at the order of pA. For this an extension line was build and Monte Carlo simulations using the FLUKA code were performed in order to predict the cell irradiation parameters and being able to adjust them. This contribution will present and discuss the results obtained for the computer code calculations and the Monte Carlo simulations for the cases presented above.
Keywords: Monte Carlo simulation, cyclotron, radiobiology, cross section estimations.

References:

S3 O11
INSTALLATION AND COMMISSIONING OF A NEW SOLID TARGET STATION AT CYCLOTRON FACILITY IN IFIN-HH

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The desire to utilize long-lived PET isotopes in the Radiopharmaceuticals Research Center (CCR) of IFIN-HH has significantly increased over the years related to high importance of a few emerging PET isotopes: $^{64}$Cu, $^{124}$I and $^{89}$Zr. Because of low positron energy, low abundance of gamma radiation, suitable half-life and favourable coordination chemistry, these radionuclides are attracting widespread interest. The main equipment of CCR is represented by a TR19 cyclotron (Advanced Cyclotron Systems Inc.), a versatile, fully automated and computer controlled machine. It can provide protons with variable energy in the range 14-19 MeV and currents up to 300 µA.

Following the commissioning in 2014 of a new beam line positioned below the main external 6 m long beam line, we are able to implement a fully automated solid targetry facility for the production of $^{64}$Cu and upgradable to $^{124}$I and $^{89}$Zr. The objective of our work was the implementation of a safe and cost effective system utilizing commercial equipment from manufacturers who were able to demonstrate convincing data for the production of the intended radionuclides. Following an auction procedure a commercial solid target systems were readily available to plug onto our secondary short beam line: Comencey ALCEO Solid Target (Figure 1)
Critical issues will be presented of the equipment installation and Site Acceptance Test.

**Keywords**: solid target, cyclotron, $^{64}$Cu

**References**:

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**S3 O12**

**METAL REMOVAL FROM CHROMIUM CONTAINING EFFLUENTS BY SACCHAROMYCES CEREVISIAE**

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Yeast *Saccharomyces cerevisiae*, was applied to remove metal ions from four complex effluents containing Cr(VI) ions. The characterization of the biomass surface was investigated by Scanning Electron Microscopy and Fourier-transform Infrared Spectroscopy. The adsorption behavior of *Saccharomyces cerevisiae* for metal ions present in solution was studied as a function of pH, initial Cr(VI) concentration, contact time, and temperature. Langmuir, Freundlich, Temkin and Dubinin–Radushkevich equilibrium models have been used to describe the experimental sorption equilibrium profile. The kinetics of the sorption was explained by pseudo-first order, pseudo-second order, Elovich and the intra-particle diffusion models. Maximum biosorption capacities have been calculated from the Langmuir adsorption isotherm, while mean free sorption energies through the Dubinin-Radushkevich model. The negative $\Delta G^\circ$ values confirm spontaneous sorption dominated by physisorption. *Saccharomyces cerevisiae* can be successfully applied for complex wastewater treatment.

**Acknowledgments.** This work was supported by the Russian Foundation for Basic Research (RFBR) [grant numbers 18-29-25023 мк].
DESIGN AND PERFORMANCE STUDIES OF THE LUMINOMETERS FOR FUTURE LINEAR COLLIDER EXPERIMENTS

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Precision luminosity and hermeticity are important components of a detector system optimized to fully exploit the reach and precision of proposed electron-positron colliders. The electromagnetic sampling calorimeters projected for the forward region of the future linear collider are presently being designed by the FCAL Collaboration. The LumiCal and BeamCal detectors are dedicated systems for luminosity measurements at the ILC[1]/CLIC[2] experiments. The LumiCal detector provides a precise measurement of the integrated luminosity, while the BeamCal is designed for instantaneous luminosity measurement and beam-tuning when included in a fast feedback system, as well as for tagging beam particles scattered through low angles. The LumiCal is positioned in a circular hole of the end-cap electromagnetic calorimeter ECAL. The BeamCal is placed just in front of the final focus quadrupole. A sketch of the forward region layout is shown in Fig. 1.

To achieve the stringent ILC performance requirements, it is necessary for the calorimeter designs to be as compact as possible and to identify radiation tolerant sensors and readout technologies. The performance of a prototype LumiCal was studied in an electron beam at DESY with a momenta in the range of 5 GeV. We’ll present the design of this prototype as well as the result of this test beam study.

In addition, efforts are underway to develop a multi-channel ultra-low power ASIC for the LumiCal readout as well as an ASIC with a dual readout scheme for the BeamCal.

Fig. 1: The very forward region of the ILD detector. LumiCal, BeamCal and LHCAL are carried by the support tube for the final focusing quadrupole and the beam-pipe. TPC denotes the central tracking chamber, ECAL the electromagnetic and HCAL the hadron calorimeter.

Keywords: Calorimeters; LumiCal; BeamCal; ILC/CLIC.

Acknowledgments: The measurements leading to these results have been performed at the Test Beam Facility at DESY Hamburg (Germany), a member of the Helmholtz Association (HGF). This work was partially supported by the Romanian UEFISCDI agency under 18PCCDI 2018 project and Romanian Space Agency (ROSA) under grant STAR-168.

References:
S3 O14

TARGET PREPARATION AND CHARACTERIZATION FOR NUCLEAR PHYSICS EXPERIMENTS

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Target preparation techniques are continuously under development. In the particular case of nuclear physics experiments, target composition and quality are crucial for obtaining reliable data. Target characteristics are considered individually for matching specific parameters of each experiment.

The target laboratory in IFIN-HH is endowed with high quality equipment for evaporation-condensation, cold rolling and electron gun methods [1]. In order to fulfill characterization requirements, methods as XRD, AFM, SEM/EDX, RBS are applied. Manufacturing processes combined with the characterization techniques lead to a strong perspective for improving target preparation [2-4].

Detailed and specific information about the aforementioned methods is given and our recent results regarding target manufacturing and characterization are presented for various target types.

Keywords: target preparation, characterization techniques, nuclear physics experiments, deposition techniques

References

S3 P1

PSS FOR THE TARLA ACCELERATOR FACILITY

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Turkish Accelerator and Radiation Laboratory (TARLA) facility which is an important accelerator based research facility in Turkey is under construction at Institute of Accelerator Technologies of Ankara University. The accelerator will mainly consist of an injector that provides high current continuous wave (CW) electron beam at 250 keV energy, two SC accelerating modules separated by a bunch compressor in order to accelerate beam up to 40 MeV energy. TARLA is a state-of-art superconducting accelerator based on light source radiation. TARLA facility is proposed as a user-oriented facility with different types of secondary particles or radiations. TARLA will produce IR-FEL between 3.2-390 µm wavelengths and Bremsstrahlung radiation in the energy range of 5-30 MeV to serve researchers in Turkey. In this study, we will describe the architecture, functions and some technical features of personnel safety system (PSS) and current status of the TARLA facility. All accelerator and experimental areas surrounded by 2.25 m radiation shielded walls. A detailed hazards and risks assessment was carried out accordance with IEC EN 61511, where the safety functions were formulated and their safety implementation level (SIL) was derived by taking into account the organizational measures. In addition, this work includes hardware implementation and PSS software implementation about TARLA radiation safety.
INVESTIGATION OF SUBMICRON SI-GE BICMOS TECHNOLOGY NODE BEHAVIOUR FOR TWO ASIC UNDER PROTON BEAM IRRADIATION

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Current study aims to highlight the radiation hardness tolerance of MAROC3 and SPACIROC2 Application-Specific Integrated Circuit (ASIC) implemented in 0.35 µm Si-Ge BiCMOS technology node [1, 2]. Having a mixed-signal architecture both chips are used to readout multi-anode photomultiplier tubes (MaPMTs) or similar photodetection devices in single-photon counting mode. Mainstream applications of these ASICs are in detectors for high energy physics experiments: accelerators and space. Therefore, in either environment the ASICs must withstand excessive ionizing radiation.

An in-house made automated test bench was designed and implemented [3] to accommodate the online monitoring requirements of MAROC3 and SPACIROC2, together with a well-defined testing strategy. Tolerance against the total ionizing dose (TID) was measured and changes in the chips normal operation mode were recorded for later analysis. Three SPACIROC2 samples have been irradiated up to 100 krad (Si) with a 200 MeV proton beam and flux of $1.089 \times 10^9$ protons/cm²/s at the Proton Irradiation Facility (PIF) from Paul Scherrer Institute (PSI), Switzerland. Whilst the MAROC3 was tested with 35 MeV proton beam, cumulated dose 400 krad TID (Si) and fluence of $2 \times 10^{11}$protons/cm²/s delivered by the JULIC cyclotron at the COSY facility, Juelich, Germany.

Data analysis revealed a leakage current increasing with TID especially within the digital part of the ASICs, however their functionality was recovered through annealing process at the room temperature without any permanent effects. Other malfunctions in the devices operation were pinpointed and investated such as: loss of the internal DAC linearity, trigger efficiency, perturbation or singular effects in normal running.

Keywords: radiation hardness, ASIC, leakage current, TID.

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shell and "one-body" models) to available data proves the very important role of nuclear shell structure in stability of superheavy elements. The spectroscopic information on α-decay results from the ratio between the calculated rates with the microscopic (shell model) and one-body resonance (asymptotic) formation amplitudes. Recent advances in locating a possible center of a new island of stability at the closed shells $Z=120$ and $N=172$ or 184 are also reviewed.

**Keywords:** α-half lives, decay properties, competition α-fission.

**References**


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**S3 P4**

**ESTIMATION OF RADON CONCENTRATION IN WORKPLACES OF RADIOACTIVE WASTE STORAGE FACILITY**

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One of the main contributors to the human exposure is Rn-222, a decay product of Ra-224, which can be found in soil and construction materials. The radon problem was assumed in Romania at national level by responsible authorities through the design and the development of a National Radon Action Plan, as required by national legislation into the Governmental Decision 526/25.07.2018 as a consequence of the European Council Directive 2013/59/EURATOM (EU-BSS) implementation.

The paper presents the results of radon concentration measurements conducted in the workplaces of the radioactive waste storage facility which belongs to Horia Hulubei National Institute for Physics and Nuclear Engineering.

A number of 11 rooms were the subject of radon concentration measurements. After a period of accumulation, about 7 days, the ventilation system was started in order to evacuate the radon indoor and to decrease its concentration. The measurements revealed that a specific ventilation time is needed in order to decrease the radon concentration in such way that the radioprotection criteria are met.

**Keywords:** Radon, ventilation, exposure.

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**S3 P5**

**INVESTIGATION OF PHYSICO-CHEMICAL AND MECHANICAL PROPERTIES OF COMPOSITE SORBENTS EMBEDDING IN CEMENTITIOUS MATERIALS**

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The use of nuclear techniques and applications as top methods in different areas generated a special waste, the radioactive waste. To improve the safety of disposal, it would be necessary to
immobilize these wastes to produce a long term stable solid waste form. The embedding of radioactive waste in Portland cement matrix is the most used method, applied in the world, but not all the radioactive waste are compatible with the normal cement matrix because of negative effects of some chemical reactions developed during the hydrolysis and curing steps of cement paste. The composite sorbents used for the low and intermediate aqueous radioactive waste treatment must be conditioned in a long term stable matrix.

For assess if the composite sorbents have harmful effects on the conditioning cement matrix stability were prepared samples based on the Portland cement with different quantity of sorbents.

The purpose of this paper is to obtain the structural and mechanical information on these samples at different period of time, necessary to evaluate the safety and performance of waste packages.

**Keywords**: Composite sorbents, cement, XRD and mechanical tests.

**S3 P6**

**MULTIFUNCTION RACK CONTROL UNIT USED TO CONTROL ELECTRONIC DETECTOR SYSTEMS FROM PHYSICS EXPERIMENTS**

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It is well known the fact that all physics experiments have need for an Electronic Detector System [1], of which role is to amplify and measure all signals which are coming from particle detectors. Measured signals are processed and converted into data which can be analyzed by researchers. All this apparatus which form the Electronic Detector System are placed in a large metallic rack and connected with the detectors through some cables (signal cables, supply cables). In case of a malfunction these apparatuses, which can be a power supply or a data acquisition system, must be reset or decoupled from the grid (power cycled) by the engineers or technicians. In many cases, these procedures must be done manually, which implies that a technician or an engineer to be permanently nearby the accelerator.

We developed a custom system, called Multifunction Rack Control Unit (MRCU), with which we can monitor and control the equipment’s related to a detector or subdetector. The first version of this system has been tested with very good results for nearly two years on the hadronic sampling calorimeter (HASC) sub-detector from NA62 experiment [2] at CERN. With the MRCU we could reset and/or power cycle different equipment’s that were placed in the rack, monitor the consumed currents by these and also monitor the temperature and humidity in different places of the rack. The MRCU have also implemented a circuit for temperature measurement by using 9 Resistance Temperature Detectors (RTD) [3] to monitor the temperature of HASC front-end electronics.

The MRCU can be accessed and controlled remote using Ethernet connection which means that the presence of a technician or engineer on the experimental area is not mandatory.

**Keywords**: MRCU, NA62, HASC detector, power management.

**Acknowledgements.** The work and the cost of all materials and laboratory tools used for design, assembly and testing the MRCU system were supported by Ministry of National Education (MEN) and the Institute of Atomic Physics Bucharest (IFA) through grants Nr. 1/16.03.2016, and national project "NUCLEU" number PN 16 42 01 03.

**References**


THE XRD STUDIES AND MECHANICAL BEHAVIOUR IN TIME OF ALUMINIUM IMMOBILIZED IN MAGNESIUM POTASSIUM PHOSPHATE CEMENT

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The radioactive aluminium waste generated by the decommissioning of research nuclear reactor as VVR-S, or other nuclear techniques applications, is a type of radioactive waste which cannot be conditioned in Cement Portland based matrix and must be conditioned in a long term stable matrix. Generally, the most common matrix is based on cementing systems which develop in the hydration and setting steps a pore solution with a pH higher than the passivation (4.5 ÷ 8.5) domain for metallic aluminium. The stability of matrices is an essential condition to assure the radiological safety during the final disposal and is directly connected with physico-chemical reaction between the system components and structural modifications which lead to performance parameters imposed by the waste acceptance.

This paper reports results obtained by investigation of aluminium immobilised in magnesium potassium phosphate cement which, according with the experimental works developed up to now, seems to be a promising solution for conditioning of these types of wastes. Characterizations performed on the magnesium phosphate formulations were compressive strength and X-ray diffraction. Structural and mechanical changes are compared for samples kept in laboratory simulating and real disposal conditions at different period of time.

Keywords: Aluminium metallic, conditioning matrix, XRD, mechanical tests.

RESEARCH REGARDING THE RADON LEVEL IN THE WORKSPACE OF THE “HORIA HULUBEI” NATIONAL INSTITUTE FOR R&D IN PHYSICS AND NUCLEAR ENGINEERING

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The paper presents studies regarding the concentration of radon activity in the working spaces [1]of the Department of Life and Environment Physics from the IFIN-HH. The department conducts activities of radiobiology research, environmental physics, radioecology, radiological monitoring of the environment and occupational dosimetry. The offices and the laboratories dedicated to research, sample conditioning and measuring are located at the ground and the two levels of the building, where approximately 50 people conduct their activities. Radon is an alpha radioactive gas with: i) a halving time of 3.823 days, ii) the maximum radiation energy of 5.48 MeV and a penetration depth of 4.12 cm in the air; iii) the density of 9.73 kg·m⁻³. It is the only radioactive element in a gaseous state and is obtained from the direct disintegration of radium. From the three isotopes of radon, only Rn-222 is of importance for the environment. Due to the fact that radon is colorless, odorless and without taste, it cannot be detected by the human senses, even though the exposure to this element and its descendants represents half of the dose of radiation absorbed by a person. The present
research tackles the measurements of the concentration of radon activity in 30 workspaces with one to four persons, with an eight-hour work day. To conduct the measurements, the Radon Monitor of SARAD type, model RTM 1699-2 [4] was used. The quantification of the concentration of activity of radon is based on a continuous sampling of the air, which is assured by the internal pump of the Radon Monitor. The detection is made with a semiconductor detector in a small volume enclosure of 130 ml. The Monitor was placed in the offices and the laboratories for periods between three and 23 hours. The values of the activity concentration were in the range 10±19,2% Bq·m⁻³ and 120±6,2% Bq·m⁻³. The maximum value allowed by the current legislation is of 300 Bq·m⁻³. The personnel concerned in this study was monitored for external exposure as well and the absorbed dose did not exceed 0,2 mSv/month. In conclusion, the level of radon in the monitored workspaces is considerably lower than the maximum permissible value, which proves that they are airy and the building materials are adequate. It also took into account the influence of the soil, meaning that the ground floor spaces are more airy than those at levels 1 and 2.

**Keywords:** radioactivity, radon, workspace

**References**

**S3 P9**

**RADIATION SPECTRUM OF ELECTRONS MOVING IN SPIRAL IN TRANSPARENT MEDIUM**

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The time-averaged radiation power $\overline{P}^{rad}$ of system of electrons moving one by one along a spiral in transparent medium can be calculated by the instrumentality of spectral distribution $W(\omega)$ [1, 2]

$$\overline{P}^{rad} = \int_0^\infty W(\omega) d\omega,$$

$$W(\omega) = \frac{2e^2}{\pi c^2} \int_0^\infty dx \mu(\omega)S_N(\omega)\omega \sin\left[\frac{n(\omega)\omega \eta(x)}{c}\right] \cos\left[V^2_0 \cos(\omega_0 x)+V^2_\parallel - \frac{c^2}{n^2(\omega)}\right],$$

where $\eta(x) = \sqrt{V^2_0 x^2 + \frac{4V^2_\parallel}{\omega_0^2} \sin^2\left(\frac{\omega_0 x}{2}\right)}$, $\omega$ is the cyclic frequency, $r_0 = V_\perp \omega_0^{-1}$, $\omega_0 = e^2 B^{ext} \tilde{E}^{-1}$,

$\tilde{E} = c \sqrt{p^2 + m_0^2 c^2}$, the magnetic induction vector $\tilde{B}^{ext}||0Z$, $V_\perp$ and $V_\parallel$ are the components of the velocity, $\tilde{p}$ and $\tilde{E}$ are the momentum and energy of the electron, $e$ and $m_0$ are its charge and rest mass, respectively, $\Delta t$ is the time shift of the $l$th electron, $c$ is the velocity of light in vacuum.

In the case of system of electrons moving one by one along a spiral the coherence factor $S_N(\omega)$ takes the form:
$$S_N(\omega) = \sum_{j=1}^{N} \cos[\omega(\Delta t_j - \Delta t_j')]$$.

The structure of spectral distribution of the radiation power of the synchrotron-Cherenkov radiation of one, two, three and four electrons moving in a spiral in a transparent medium with relativistic longitudinal velocity component (the component parallel to the magnetic induction vector) is investigated. The method of direct numerical calculation of the function of spectral distribution of the radiation power $W(\omega)$ is used to establish and investigate the effect of hopping in synchrotron-Cherenkov spectral distribution of radiation power of one, two, three, and four electrons, moving along a spiral in transparent medium. The effect of hopping caused by appearance of the anomalous Doppler effect at harmonic $m = -1$ is obtained for the case when the longitudinal component of velocity (parallel to the magnetic induction vector) is bigger than the light phase velocity ($V_l > c/n(\omega)$) in transparent medium [1, 2].

The obtained results in this study are in good agreement to those obtained in [1, 2].

**Keywords:** synchrotron-Cherenkov radiation, effect of hopping, anomalous Doppler effect.

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**S3 P10**

**GAMMA-RADIATION BEHAVIOUR OF SOME CONDUCTIVE CARBON COMPOSITES EXHIBITING SELF-REGULATION TEMPERATURE PROPERTIES**

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Composite materials containing different types of carbon materials are used in temperature self-regulating devices based on their electrical percolation at room temperature and suddenly increasing of their resistivity at elevated temperatures, i.e. PTC effect - Positive Temperature Coefficient of resistivity [1, 2]. Conductive composites containing either carbon black (CB), graphite or both and high-density polyethylene (HDPE) matrix were prepared by a simple procedure based on dry mixing of the components, followed by warm molding into disc samples of 50 mm and 0.7 mm thickness. The influences of the $\gamma$-irradiation treatment and $\gamma$-irradiation exposure (at lower dose rate) on the degradation state of the polymer matrix and the temperature self-regulating properties of the composite materials were studied. Two irradiation scenarios were applied, namely: one consisted in $^{60}$Co exposure of the samples in wrapped state in aluminum foils within the range of $0 - 350$ kGy at a dose rate of 1.1 kGy/h, followed by a thermal treatment at 80 °C for 4 hours; another one consisted in a supplementary irradiation at a lower dose rate ($^{137}$Cs, dose rate 365 Gy/h, $D = 75$ kGy) of the samples prepared according to the first procedure. The first irradiation scenario was applied to impart adequate PTC properties to the composite, while the second one is intended to study the behavior of the material in radiation field conditions. The beneic effect of $\gamma$-irradiation (at high dose-rate and in limited presence of air, on temperature self-regulating properties is discussed comparatively, on non-irradiated and irradiated materials, proving that irradiation significantly enhances these properties of a composite material with polymer matrix. On the other hand, radiation exposure at lower dose rate resulted in ageing of the polymer matrix.

Differential scanning calorimetry (DSC) and infrared spectroscopy (ATR-FTIR) were used for diagnosis of the irradiation effects. Oxidation induction temperature was the main kinetic parameter derived form the
DSC thermograms which was used for calculations of activation energies of oxidation, isothermal oxidation induction periods and durability estimation [3]. From infrared spectroscopy data, the radiooxidation effects were assessed through the evolution of carbonyl (~1700 cm\(^{-1}\)) H-O (~3400 cm\(^{-1}\)) and C-O (~1200 cm\(^{-1}\)). DSC and FTIR data and were correlated with the information inferred by Raman spectroscopy and SEM.

**Keywords**: composites, radiation processing, radiation-induced degradation

**Acknowledgements**: The financial support of Romanian Ministry of Research and Innovation through the projects: PN19310101-46N and 04-4-1122-2015/2020 is acknowledged by the authors.

**References**

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**S3 P11**

**GAMMA ASSISTED SYNTHESIS OF COLLOIDAL COPPER BASED NANOPARTICLES**

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Radiochemical synthesis of metallic nanoparticles is an eco-friendly method that allows the obtaining of controlled size, well dispersed, fully reduced, highly stable particles at very mild conditions.

Colloidal Cu\(^0\) and Au (core)/Cu (shell) nanoparticles were synthesized in a one-step process, in an aqueous system of Cu\(^{2+}\)/PVP/Isopropyl alcohol and Cu\(^{2+}\)/Au\(^{3+}\)/Sodium Dodecyl Sulfate (SDS)/Ethylene Glycol, respectively, using high energy ionizing radiations (\(\gamma\)-rays) up to a dose of 100 kGy.

The synthesized Cu based NPs were characterized by UV-Vis spectroscopy, Dynamic Light Scattering (DLS), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and FTIR spectroscopy. After irradiation, the change of color to red-wine was a first indicator for the formation of Cu based nanoparticles. Moreover, the UV-Vis spectra showed a maximum absorption peaks in the range of 570-610 nm, specific to Cu\(^0\) NPs, and 510-560 nm, respectively, specific to gold nanoparticles (Fig. 1). The SEM analysis revealed the formation of Au (core)/Cu(shell) nanoparticle structures.

The antibacterial properties of radio-synthesized Cu based nanoparticles were assessed against *Staphylococcus aureus* and *Pseudomonas aeruginosa*, respectively (Fig. 2).

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**Fig. 1** – UV-Vis spectra of synthesized Cu-based nanoparticles

**Fig. 2** – The antimicrobial efficiency of synthesized CuNps: a) against Staphylococcus aureus; b) *Pseudomonas aeruginosa*
The size of nanoparticles and their stability in air is influenced by certain parameters such as the choice of stabilizer, pH during synthesis, the Cu²⁺/stabilizer ratio and absorbed dose.

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S3 P12
THE CALIBRATION OF A DOSIMETRIC SYSTEM WITH THERMOLUMINESCENT DETECTORS

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The monitoring of staff who works in radioactive field (radiotherapy, nuclear medicine, RX diagnostics, industrial appliances who use radioisotopes etc) is mainly done with thermoluminescent dosimeters. The calibration is done at gamma radiation (137Cs) and X radiation. All radiation qualities shall be in accordance to ISO 4037-1. [1] The traceability of the measurement unit is done using the secondary standard UNIDOS Webline, type T10021 with ionization chamber Hp(10) type T34035. This is calibrated at PTB Germany with an expanded uncertainty of 3% for a 95% confidence level. The chamber set includes a phantom slab of 31 mm thickness with chamber assembly and an additional phantom slab of 120 mm thickness. The slab phantom is composed of tissue-equivalent acrylic material (PMMA). The total external dimensions are 300 mm x 300 mm x 151 mm.

Figura 2. TLDcube dosimetry system

The TL system used consists of: CUBE thermoluminescent reader and DIT-MF dosimeters equipped with GR 200A TL detectors (LiF: Mg, Cu, P). TL detector irradiation was done on the ICRU phantom with the following dimensions 300 mm x 300 mm x 150 mm. The doses used for calibration are 1 mSv and 0.5 mSv.

The response of GR 200A detectors in DIT-MF type cassettes for S-Cs and N-60 quality, the reproducibility and stability of the dosimetry system was studied.

Keywords: personal dosimetry, thermoluminescent dosemeter,
References
S3 P13
DETERMINATION OF DECONTAMINATION EFFICIENCY OF POLYMERIC GELS IN THE SPECIFIC CASE OF THE TRITIUM LABORATORIES

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The purpose of the present paper consists in finding a more efficient and less expensive decontamination method for surfaces contaminated with Tritium-labelled compounds. This paper studies the polymeric hydrogel DeconGel, presenting the methods and facilities used, as well as the obtained results and their interpretation. All the experiments were conducted within Tritium Laboratory (TRITIULAB) from Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH). Because the results were more than satisfying, this paper concludes by recommending the implementation of this new method.

The decontamination factor of Decongel type 1108 for the analysed surfaces (contaminated with a mixture of tritium labelled compounds) can take values in the range of 76%-93%, while in the case of Decongel type 1102 the values of the decontamination factor for the analysed surfaces (contaminated with tritiated oil) can vary between 76% and 98%, results far greater then the ones obtained with the classical method of wet wiping.

Keywords: polymeric hydrogel, decontamination, tritium, radiochemistry, radioisotope

S3 P14
HIGH GAIN AMPLIFIER FOR MEASURING THE PROTON BEAM CURRENT AT VERY LOW VALUES IN NUCLEAR APPLICATIONS

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The latest studies regarding the Relative Biological Effectiveness (RBE) involves the use of low doses of 1.2 Gy to 1.8 Gy. Using a variable energy cyclotron (14 MeV- 19 MeV) we obtained proton currents in the range of pico-amps to hundreds of pico-amps with energy of less then 3 MeV. To obtain a 1Gy/min dose rate it is necessary to use a proton current of about 11.2 pA. The measurement of ultra low current beams in pico-amps range is performed by using precision instrumentation operational amplifiers with a very small input bias current (femtoamps). A transimpedance amplifier (TIA) converts the beam current (I_b) into a DC voltage (V_o) to be applied to the data acquisition system. The negative feedback circuit is made by three resistors (R₁=R₂).

Considering a non-ideal operational amplifier, the transimpedance gain of the circuit is:

\[ A_z = \frac{V_o}{I_b} = -\left( R_1 + R_3 + \frac{R_1 \cdot R_3}{R_2} \right) - \left( 1 + \frac{R_1}{R_2} \right) \frac{V_{OS}}{I_b} + \left( R_1 + R_3 + \frac{R_1 \cdot R_3}{R_2} \right) \frac{I_b}{I_b} \]

, where \( V_{OS} \) is the input offset voltage, and \( I_b \) is the input bias current of the inverting input.

The equation is formed by three terms: the first term has the largest share and it is defined by a ratio of resistors, the second and the third terms count the error due to the offset voltage, respectively the influence of the input bias current. The last two terms decrease inversely proportional to the beam current, and they show that the response of the circuit is not linear.
By using a 3fA input bias current precision amplifier and precision metal film resistors with tight tolerance (0.1%) and low temperature coefficient (below 10ppm/°C), the gain of the proposed circuit can be maintained almost constantly.

**Keywords:** current beam, pico-amps, transimpedance amplifier, high gain.

**S3 P15**

**ON-SURFACE NANOSTRUCTURES PRODUCED BY 6 MEV ELECTRON BEAM IRRADIATION OF MULTI-LAYERED TUNGSTEN**

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Multi-layer samples containing W and an alloy of W with K produced by fast spark plasma sintering (SPS) were exposed to a pulsed electron beam (EB) with energy 6 MeV [1]. Morphological changes were observed under a SEM such as the appearance of different nanostructures (ripples or nanoparticles) on the surface of the samples and surface exfoliation, depending on the sample type and the electron beam fluency, as shown in Fig. 1. The irradiation was carried out in vacuum at a pressure of 2.4 × 10⁻² torr. An EDS analysis revealed that the nanostructures observed on the sample surfaces are made of W and are likely to be formed due to electron beam heating and vaporization of the surface followed by rapid vapor condensation. The EB fluence was measured with a Faraday Cup Radiabeam FARC-04-2M. The LINAC delivered EB pulses at a frequency of 53 Hz and pulse duration of 4 µs. The electron fluence for 10 minutes of irradiation was ~5.0×10¹⁵ el/cm².

Figure 1. High resolution image of a W irradiated sample for a duration of 10 minutes by an electron beam with energy 6 MeV.
**Keywords:** tungsten, nanoparticles, electron beam, irradiation.

**Acknowledgement:** Support from EUROfusion - WPMAT-RO project is acknowledged.

**References**


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**S3 P16**

**MONITORING THE LEVEL OF RADIOACTIVITY INDUCED IN THE ENVIRONMENT BY THE CONTROLLED DISCHARGE OF LIQUID EFFLUENTS CONTAINING POTENTIALLY POLLUTANT RADIOISOTOPES**

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Liquid and gaseous wastes as well as solid wastes resulting from activities carried out in a nuclear installation contain radioactive isotopes that are potential radioactive pollutants for the environment.

The Romanian legislation allows the discharge of liquid and gaseous radioactive effluents into the environment only in compliance with the non-prescriptive release conditions (Norms on limitation of releases of radioactive effluents into the environment - NDR-04/2005 – issued by the National Commission for Nuclear Activities Control).

In this paper, we present the case of liquid effluents in which the composition consists of radioisotopes $^{192}\text{Ir}$, $^{60}\text{Co}$, $^{241}\text{Am}$, $^{137}\text{Cs}$, $^{3}\text{H}$. We have analyzed relevant samples from the contents of liquid effluent tanks. The samples were analyzed by gamma spectrometry for the gamma emitting radioisotopes ($^{192}\text{Ir}$, $^{60}\text{Co}$, $^{241}\text{Am}$, $^{137}\text{Cs}$) and using a tritium ($^{3}\text{H}$) liquid scintillator installation ($^{3}\text{H}$).

The calculation algorithm starts from the activity of each radioisotope (Bq), those representing the product of the discharged volume and isotope concentration at the time of discharge $A_{\text{discharge}} = C_{\text{rad}} \times V$. The variation of the activity of each radioisotope disintegration decay was calculated with the law of the time of discharged into the environment, until the next discharged. Considering that each new release introduces into the environment another quantity of radioactivity that accumulates with the existing one, the relationship was used $A_n = A_{n-1} \cdot e^{-\lambda t} + A_{\text{discharge}}$. The current legislation provides for emission limits (annual) for each radioisotope, the novelty of this paper being the monitoring of the activity of the five radioisotopes over a period of 5.5 years.

**Keywords:** pollutants, environment, liquid effluent, radioactivity

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**S3 P17**

**EXPERIMENTAL APPLICATION OF POLYMERIC HYDROGEL METHOD (STRIPPABLE COATINGS) FOR CLEANING AND DECONTAMINATING SURFACES IN HOT CELLS**

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**Abstract.** This paper aims to test a new method of decontamination using a polymeric hydrogel for radioactive clean-up of surfaces found in a hot cell. In this experiment our team studied a decontamination method with strippable coatings, using Decongel. Depending on the results, more than one application of the gel might be
necessary. The classic process of decontamination of hot cells is realised with the wet-wiping method which involves the successive wiping with a smear which is afterwards measured until no radioisotope can be detected, being then able to conclude that the unfixed contamination was removed. But it depends on the type of contaminants, type, pH and structure of surfaces, uses a significant amount of materials in its process and results in a great amount of waste, all of them rendering it inconvenient. Another problem that appears during the classic decontamination process is the spreading of contamination to the workers involved or to other surfaces.

But the new proposed method manages to eliminate these risks, minimizing, at the same time, the exposure of workers to radiation and lowering both the volume of radioactive waste and the costs involved. The paper describes the experiments performed for the removal and cleaning of radioactive contaminants from the surfaces of a hot cell and compares their results with those of the classic method. The radioactive contamination of the hot cells was due to the handling of metallic powder which could not be omitted in the preparation process of sealed sources (Ir-192, Co-60), though it can also be the result of other processes. For measuring the activity and type of contaminant (radioisotope) the gamma spectrometry was used in both the case of smears and dried gel. The hot cell used in the experiments were part of DRMR (Department of Radioisotopes and Radiation Metrology), a department of IFIN-HH (NIPNE) which includes research laboratories and facilities specifically designed and equipped for radiochemical experiments. This hot cell had been used for a variety of irradiation operations and for the handling of Co-60 sources over many years. The results of this study are going to be presented in the extenso-paper.

Keywords: polymeric hydrogel, strippable coatings, decontamination, Co-60, Ir-192

Acknowledgement: The costs of this experiment are supported by the Romanian National Project-PN 09 37 02 06

Reference:

S3 P18

LITHIUM AND FLUORINE ACCUMULATION BY CYANOBACTERIA SPIRULINA PLATENSIS

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The process of lithium and fluorine accumulation in Spirulina platensis biomass during cyanobacteria growth was studied. These elements were separately added in the nutrient medium at the first and third days of biomass cultivation. Metal uptake by biomass was traced using Proton Induced Gamma Emission (PIGE)
technique at 3 MV Tandetron particle accelerator of the Horia Hulubei National Institute for Physics and Nuclear Engineering (IFIN-HH) in Romania. Obtained results showed continuous accumulation of both elements in biomass with the increase of their concentration in cultivation medium. Addition of lithium in the cultivation medium did not affect biomass productivity and proteins content, while content of chlorophyll and carotenoid was significantly reduced. Lithium influenced phycobilins content just at its addition in medium on the third day of biomass growth. Addition of fluorine affected biomass growth at its addition in medium on the third day on biomass growth. Increase of proteins and phycobilins content was observed at low fluorine concentrations, while content of chlorophyll and carotenoid increased significantly (up to 80%). Increase of carbohydrates content was noticed at the addition of both elements in the cultivation medium. *Spirulina platensis* can be applied for lithium and fluorine removal from wastewater.

S3 P19

**90SR AND NATURAL URANIUM DETERMINATION BY CHERENKOV COUNTING**

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Cherenkov radiation, when produced at significant levels, can be employed for the efficient measurement of radioactivity. Although the production of Cherenkov radiation does not involve the scintillation phenomenon, a conventional liquid scintillation counter can detect and count Cherenkov photons emitted from a given sample in a standard counting vial. Cherenkov counting technique has become well established for the rapid assay of certain relatively high-energy beta emitting nuclides, such as $^{32}$P, $^{89}$Sr, $^{90}$Sr/$^{90}$Y, $^{234m}$Pa etc.

Cherenkov radiation is produced by charged particles moving through a transparent medium with a speed greater than the speed of light in that medium. The threshold energy of a particle for producing Cherenkov radiation in water is 263 keV. Among the advantages of this technique are: (i) extreme simplicity of sample preparation, (ii) the ability to count in aqueous systems without use of any organic fluors or reagents that could destroy the sample leaving the sample suitable for further tests and (iii) no interference caused by other radionuclides in the sample with decay emissions that cannot produce the Cherenkov effect, such as $^3$H, $^{14}$C, $^{35}$S, etc. Another important consideration is that conventional liquid scintillation counting equipment can be used without modification.

$^{90}$Sr is one of the most important anthropogenic radionuclides from the radiation protection point of view due to rather long residence time in the biosphere, bio-availability for certain dietary products and high dose contribution after ingestion due to preferential fixation into the skeleton. For this reason, is important that $^{90}$Sr to be monitored regularly in many types of environmental samples related to the human food chain. Even that the radiostrontium is released in insignificant amounts during normal operations of nuclear reactors, its presence in effluents should be continuously monitored to verify the conformance with the limits included in the operation license. Also, determination of uranium is required in any program of uranium mining and ore processing and is also important in environmental safety monitoring.

Institute for Nuclear Research Pitesti has a research reactor in operation, so determination of uranium and $^{90}$Sr content in different types of samples are carried out frequently in Radiation Protection Laboratory. We studied the reliability of activity determination of natural uranium and $^{90}$Sr by Cherenkov counting of their high energy beta-emitter descendants, $^{234m}$Pa and $^{90}$Y respectively (both with $E_{\beta_{\text{max}}} = 2.28$ MeV), using a TriCarb 2100TR Liquid Scintillation Analyzer. Experimental tests using aqueous samples spiked with known quantities of standard solution showed that the Cherenkov counting could be used for quantification of natural uranium and $^{90}$Sr/$^{90}$Y respectively, being a robust and reliable rapid counting method.

**Keywords:** Cherenkov counting.
S3 P20

TWISTED PHOTONS IN INTERACTION WITH MESOSCOPIC SYSTEMS

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Based on the investigation of the connection between twisted photons and spherical photons we present a method devoted to describe the interaction between helical beams and some mesoscopic physical systems. We present some analytical and numerical results for the case of fullerenes as well as for nuclear systems in the appropriate energy regimes.

References:

S3 P21

A PRECISION CURRENT MONITOR ARCHITECTURE IN NUCLEAR APPLICATIONS

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The main magnet of the TR19 cyclotron commissioned in 2012 in IFIN-HH must produce up to 2T magnetic field. The stability of the magnetic field is critical to the beam quality provided by the cyclotron. The magnet power supply has to deliver a regulated current regulated up to 600Amps with a stability of ±10⁻⁵. Unfortunately, the original system proved to be unreliable. The proposed circuit (Fig.1) is designed to bias with a precise programmable current the electromagnetic coil of the main magnet inside a particle accelerator in a range between zero and a few hundred amperes. The supply voltage (Vₜ) is provided by an external power rectifier. A controller monitors the supply current (Iₛ) and it drives a series pass circuit (SPC). The current through the electromagnetic coil (LOAD) and the output voltage are measured and monitored by using a current sensor (CS) and a negative feedback circuit formed by 2 resistors (R₊₁, R₊₂). The SPC block is formed by n bipolar junction transistors (Q₁÷Qₙ) to divide the output current and implicitly the power dissipated to values that are permissible for each device (less than 20A). Some series shunt resistors (Rₛ₁÷Rₛₙ) are mounted in the emitters of BJT’s to balance the output currents (Iₑ₁÷Iₑₙ). A high side current monitor (HSCM₁÷HSCMₙ) designed to work with a wide range os supply voltages (10V÷ 200V) measures the current through each transistor and it outputs a voltage (V₊₁÷V₊ₙ) proportional to that current. The signals from the high side current monitors are sent to a hysteresis comparator made by an operational amplifier (HCOA). If one of the emitter currents ((Iₑ₁÷Iₑₙ) exceeds a threshold, the HCOA circuit outputs an error signal (OCPT) and the controller decrease to zero the output current.
Keywords: particle accelerator, main magnet, current monitor, protection circuit.

S3 P22

STUDY OF DIFFERENT TYPES OF CLAYS FOR USAGE IN NUCLEAR FIELD

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Clay represents the common name for hydrated laminar magnesium-aluminum-ironsilicate and is a material used in a wide range of fields and sectors; from the building industry to pharmaceuticals industry, cosmetics and even gardening. But this study aims to study them for usage in the nuclear and chemical field. In many countries, clays are already part of large application, manly for the study of radioactive wastes found in the clays layers of the ground. This paper presents a chemical and radiological characterisation of some types of clays from Romania, which is available on the market. The samples were both purified and unpurified and have different geographical origins. The importance of their characterisation comes from their high capacity of retaining cations, anions and water. The final purpose is to use clays as radioactive decontaminants, but the study is still ongoing, this paper presenting only the partial results, meaning the characterisation of clays.

Keywords: radioactivity, clays, nuclear, heavy metals
S3 P23
DECONTAMINATION METHOD FOR SOLID WASTES RESULTED FROM THE PROCESS OF MODERNISATION OF TRITIUM LABORATORY

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The problem that this study tries to solve is the radioactive decontamination process that needs to be done quite often within a tritium laboratory. In order to improve the safety and efficiency of the decontamination in a tritium laboratory, solutions have been researched. This paper presents the results of testing a method of decontamination using a strippable coating method applied on surfaces resulted from the modernization of the laboratory's structure and their interpretation. A polymeric gel was used for this work, (for decontamination), which is a fast, efficient and easy method.

Keywords: polymeric gel, decontamination, tritium

S3 P24
RADIATION HARDNESS ASSURANCE OF FIELD PROGRAMMABLE GATE ARRAYS IN LHC EXPERIMENTS

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Scheduled for 2019-2020, the LHCb Upgrade Program Phase I [1] will enhance the performances of its previous architecture to allow operation at an instantaneous luminosity up to $2 \cdot 10^{33}$ cm$^{-2}$ s$^{-1}$, which will be 5 times higher compared with previous luminosity. A triggerless readout together with a fully software trigger architecture are proposed to replace the present hardware trigger systems in order to archive an increase in the readout rate from 1 MHz to the LHC bunch crossing rate of 40 MHz. The LHCb Ring Imaging Cherenkov (RICH) sub-detectors will be upgraded [2]. The RICH photo-detection system will use multi-anode photomultiplier tubes (MaPMT) and the digital readout will be handled by an SRAM-based Field Programmable Gate Array (FPGA) from Xilinx KINTEX-7 family, with a backup solution being the antifuse FPGA from Microsemi Xcelerator family. The LHCb radiation environment has upper limits: 200 krad (Si) total ionising dose (TID) and $1.2 \cdot 10^{12}$ HEH/cm$^2$ [2]. The two FPGAs need to withstand these harsh conditions and operate flawlessly at high radiation hadronic fluxes. The experiments performed so far on these two devices gave negligible TID cumulative effects in the antifuse FPGA, and high single event effects rates for the KINTEX-7 FPGA: $\sigma \sim 10^{-7}$ cm$^2$/device ($\sim 19$ Mb configuration) at 20 – 200 MeV protons[3-4]. Following the changes in the firmware ($\sim 12$ kb critical bits), the KINTEX-7 FPGA was keep for the LHCb upgrade phase 1, whereas the antifuse FPGA was proven suitable for the second upgrade phase (TID larger than 2 Mrad).

Keywords: LHC, radiation effects, FPGA, RICH detectors.

Acknowledgements. The work and the cost of all materials and laboratory tools used for design and assembly the test setup and to perform the irradiation tests were supported by Ministry of National Education (MEN) and the Institute of Atomic Physics Bucharest (IFA) through grants 7/16.03.2016, and national project ”NUCLEU” number PN 16 42 01 03.

References

S3 P25

**2D IMAGING IN HIGH RATE ENVIRONMENT WITH HPD-TRD FOR CBM@FAIR**

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The Compressed Baryonic Matter (CBM) experiment @ FAIR is going to start taking data at unprecedented interaction rates (10 MHz) in 2024. A major sub-system of the experiment is the Transition Radiation Detector (TRD) used for particle identification and tracking. The most challenging part of the TRD wall is the inner zone, composed of 4 layers, 10 chambers per layer (40 chambers in total for SIS-100 setup). These chambers are designed and will be produced and tested by the Romanian group in Hadron Physics Department (HPD) of IFIN-HH. They will be equipped with a Front End Electronics (FEE) ready to perform up to 1 MHz data rate/cm² also developed in HPD.

A summary of R&D activities and the results related to our solutions is presented.

**Keywords:** FAIR, mCBM, TRD
ABSTRACTS

S4 – Cross-disciplinary Applications of Physics

- Nonlinear dynamics, complex systems and applications
- Biological complexity and genetics, Biophysics and bioengineering
- Econophysics
- Physics of Social Systems
TEXTURE ANALYSIS OF MODERN, SUBFOSSIL AND FOSSIL BIVALVE MOLLUSK SHELLS

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One of the actual research topics of the modern paleontology is the study of fossilization processes. The changes can occur with the mineral matter of shells and bones over the million years. During the life of an animal, the stability of the mineral skeleton component is controlled by the cellular matrix, but after the death of the cells, various processes take place, up to complete destruction of shells and bones. But primary minerals that were a part of the shells and bones may be preserved. Phase changes also occur, for example, a transformation of aragonite to calcite. In addition to the original crystals of the mineral, another phase also grow, filling the space between original crystals, but these crystals already have an abiogenic origin. Fossil objects are replaced by other minerals, while maintaining the original form of fossil. It is important to understand whether a change in the orientation of the crystals of the same mineral occurs after the death of the stabilizing matrix. How strong these changes are? For this purpose, the shells of modern, subfossil (semi-fossil, geological age about 40 and 600 years) and fossil bivalve mollusks need to be studied. In particular, studies will be conducted on the shells of the same mollusk species, but belonging to different geological epochs. In parallel, questions of the influence of habitat conditions on the texture of shell mineral crystals, the strong taxonomic affiliation of texture to a particular genus or family of bivalve mollusks will be determined. According to previous studies, the characteristic texture of the calcite crystals for shells of modern mollusks of the genus *Mytilus* was revealed using neutron diffraction (Nikolayev D et al 2019).

In the present work we focused on the study of the Bivalvia mollusks shells. The spectra of the shells were measured at SKAT (Keppler R et al 2014) spectrometer at pulsed reactor IBR-2 (Dubna, Russia). We measured modern and 30 000 years old *Mytilus galloprovincialis* and *Ostreidae edulis*. Investigated samples exhibited different phase content. All *Mytiluses* possess both calcite and aragonite phases of different content. The crystallographic texture of all *Mytilus* samples demonstrated very sharp texture of the calcite phase. Other samples do not show sharp crystallographic texture.

The JINR – Romania scientific cooperation program 2018-2019 as well as JINR – Poland scientific cooperation program 2018 -2020 are acknowledged.

**Keywords**: Bivalvia mollusks shells, crystallographic texture, fossil object, neutron diffraction.

**References**

Keppler R et al 2014 Potential of full pattern fit methods for the texture analysis of geological materials: implications from texture measurements at the recently upgraded neutron time-of-flight diffractometer SKAT *Journal of Applied Crystallography* 47 1520

SP L2

GRAPHENE/ HfO₂ FERROELECTRIC NANOLECTRONIC DEVICES

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HfO₂–based ferroelectrics such as HfO₂ doped with Zr (termed as HfZrO) or Al fabricated using atomic layer deposition method (ALD) on Si, are among the best substrates for graphene monolayer transfer since their root mean square (rms) surface roughness is very small, around 0.2 nm [1], smaller than the corresponding parameter of SiO₂, which ranges between 1 nm and 3 nm depending on the deposition technique and even smaller or comparable with the rms surface roughness of hexagonal boron nitride (h-BN), which is about 0.4–0.6 nm. Thus, we have transferred graphene monolayers at 4 inch wafers consisting in 6 nm HfZrO/Si and we have experimentally demonstrated memories with enhanced capabilities [2], harvesting of high frequency electromagnetic fields [3], and transistors that are able to reconfigure their transport horizontal or vertical depending on the polarity of the applied gate voltages, and ballistic transistors which are switching on and off with a switching time of 2 ps.

We acknowledge the financial support of the GRAPHENEFERRO grant of Ministry of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCCF-2016-0033.

References

SP L3

COMPLEX STRUCTURAL INVESTIGATIONS OF COFE2O4 FERROFLUID-BASED LOW VISCOSITY SODIUM ALGINATE MEMBRANES

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Alginate is a biomaterial with different biomedical and engineering applications. It is well known that alginate hydrogels have been particularly successful used in wound healing, drug delivery, and tissue
engineering applications, due to the fact that these substances hold structural resemblance to the extracellular matrices in tissues [1].

CoFe$_2$O$_4$ ferrofluid-based sodium alginate membranes were prepared [2,3]. Complex structural investigations of sodium alginate membranes doped with CoFe2O4 nanoparticles and the effect of their cross-linking with CaCl$_2$H$_2$O, by means of small-angle X-ray scattering (SAXS), atomic force microscopy (AFM), scanning electron microscopy (SEM), X-ray diffraction (XRD) are reported.

Acknowledgment: The work was accomplished with the financial support of the 2019 RO-JINR Projects, Theme 04-4-1121-2015/2020.

Keywords: ferrofluids, sodium alginate, SAXS, AFM, SEM, XRD

References

S4 L4

GREEN PRODUCTION OF BIOETHANOL

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Conventional bioethanol for transportation fuel typically consumes agricultural feedstocks also suitable for human consumption and requires large amounts of energy for conversion of feedstock to fuel. Alternative feedstocks, optimally those not also in demand for human consumption, and off-grid energy sources for processing, would both contribute to making bioethanol far more sustainable than current practices. Cellulosic bioethanol production involves three steps: the extraction of sugars from cellulosic feedstock, the fermentation of sugars to produce ethanol, and the purification of ethanol through distillation. Traditional production methods for extraction and distillation are energy intensive and therefore costly, limiting the advancement of this approach. Here we report an initial demonstration of the conversion of cellulosic feedstock into ethanol by completely off-grid solar processing steps. Our approach is based on nanoparticle-enabled solar steam generation, where high-efficiency steam can be produced by illuminating light-absorbing nanoparticles dispersed in H$_2$O with sunlight. We used solar-generated steam to successfully hydrolyze feedstock into sugars, then used solar steam distillation to purify ethanol in the final processing step. Coastal hay, a grass grown for livestock feed across the southern U. S., and sugar cane as a control, are successfully converted to ethanol in this proof-of-concept study. This entirely off-grid solar production method has the potential to realize the long-dreamed-of goal of sustainable cellulosic bioethanol production.

S4 L5

NEUTRON STUDIES OF STRUCTURE AND DYNAMICS OF MOLECULAR AND POLYMER SELF-ASSEMBLED SYSTEMS

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Review of recent studies of self-assembled molecular and polymeric systems and composites by Small Angle Neutron Scattering and Neutron Spin-Echo has been presented. These powerful techniques allow discover very subtle mechanisms of formation of supramolecular structures, e.g. composed of star-shaped macromolecules with single or doubled fullerene centers, monomers-surfactants creating micelles to be polymerized to fix conformations and size of precursors. Complementary quasi-elastic scattering experiments has enabled to examine the dynamics of such complicated structures at segmental and macromolecular scales in solutions. Along with this, effective approaches are developed to create new polymeric membranes having fine channels for proton diffusion [1]. These materials ordered at molecular level were modified by nanodiamonds to improve the functional properties (mechanical, thermal, conductive) (Fig.1). For these purposes there were improved water-emulsion synthesis methods for perflourinated polymers and the technologies for preparing diamond single crystals ~ 4-5 nm in size. The diamonds’ surfaces were modified by grafting hydrophilic groups to regulate the electrostatic interactions of particles in aqueous media. As a result, the necessary prerequisites are provided for the production of polymer membranes reinforced with diamonds to increase their conductivity and stability in the required operating conditions. In general various molecular, polymer and composite systems’ subtle structural features and the mechanisms of their short-range ordering have been evaluated by advanced neutron scattering techniques. It makes possible to achieve preset structures and functional properties in materials designing.

Fig.1 Assembled nanodiamonds in polymeric matrix of proton conducting membrane.

Keywords: polymer, structure, neutron, scattering

The work was supported by Russian Foundation for Basic Research (grant No 19-03-00249).

References

THE MAGNETIC ANISOTROPY IN SIMPLE LANTHANIDE UNITS

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The magnetic anisotropy is the basic ingredient that determines the formation of magnetization axis that drives a spin-carrier molecule into a nominal magnet.[1] The attention on Single Molecule Magnet class was progressively shifted towards smaller species such as binuclear or even mononuclears, namely Single Ion Magnet cases. The molecular simplicity allows insight into structure-property relationships. In this spirit, we deliberately consider simple mononuclear unit, the $[\text{Ln(NO}_3\text{)}_5]^2^-$ units (Ln=Sm, Eu, Gd, Tb, Dy, Ho, Er) from a newly synthesized series of systems having complex counterions. Using computational tools with care (e.g. routine DFT methods are not working),[2] we are able to analyze and even predict the magnetic properties of the units The magnetic anisotropy is suggestively accounted by our methodological invention,[3] namely the drawing of the polar maps for response of states (all spectral terms) with respect of magnetic field, scanned at all 3D orientations around the given site. The resulting lobes identify the easy magnetization axis and the magnitude of the carried magnetic moment, as illustrated in the Figure 1 for the Tb and Dy congeners.
Keywords: magnetic anisotropy, single ion magnet, lanthanide

References:

**S4 O1**

A NON-CONVENTIONAL OPTICAL PROCEDURE FOR ESTIMATING LIVING CELLS CONCENTRATION IN AQUEOUS SUSPENSIONS

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When coherent light is incident on a fluid that contains scattering centers (SCs) randomly distributed in suspension, light is scattered by SCs and the far field interference has the aspect of a speckled image, more precisely a dynamic speckle image, as the SCs undergo Brownian motion. The unconventional method proposed in this work involves recording the scattered light and computing the contrast of each frame, followed by averaging it on a certain number of consecutive frames, followed by finding an analytical function that links the contrast with the SCs concentration.

A coherent light scattering experiment on an aqueous suspension of Saccharomyces cerevisiae yeast with a concentration that covers five orders of magnitude was carried on. The scattered far field was recorded using a CCD. A computer code for image processing was used to calculate the far interference field speckle contrast (SPK). The results reveal that the average contrast presents an increasing trend in the very small concentration range, up to $4.8 \cdot 10^{-2}$ g/l. From $4.8 \cdot 10^{-2}$ g/l to 10 g/l the contrast exhibits a decreasing trend.

The non-conventional method presented here and the results found on testing it on yeast cells stand as a proof of concept for this alternative method. A simple calibration method and an analytical function that can...
be used in assessing the cells concentration in an aqueous suspension is suggested in the extended paper. The method can be used in monitoring the number or concentration of different cell types, like bacteria in a suspension cell culture, a technique currently used in biomedical laboratories.

**Keywords:** Light Scattering, Speckle Contrast, Cell Concentration

**References**


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**S4 O2**

**EXTERNAL MAGNETIC FIELD INFLUENCE ON THE VISCOSITY OF Fe3O4-WATER MAGNETIC NANOFLUID**

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Magnetic nanofluids are colloids which comprise of ferromagnetic nanoparticles and a carrier liquid such as water, oil, ethylene glycol etc. Generally, the nano-sized ferromagnetic particles are maghemite ($\gamma$-Fe$_2$O$_3$), magnetite (Fe$_3$O$_4$) or cobalt-ferrite (CoFe$_2$O$_4$) etc [1]. They have many potential application area such as electrical, mechanical and optical systems. Magnetic nanofluids can be actuated under the influence of the external magnetic field. Moreover, their thermophysical properties can be tuned with varying magnetic field. These make them attractive for microfluidics such as micro sized heat sinks, micro operations, pumping and mixing [2]. Therefore, it is important to investigate their thermophysical properties in the presence of the external magnetic field. In this experimental study, the viscosity of the Fe$_3$O$_4$-water magnetic nanofluids with different volumetric concentrations of 1 to 4.8% was measured by vibrational type viscometer in the absence and presence of the external magnetic field. In order to generate external magnetic field, a NdFeB permanent magnet couple was used. The external magnetic field strength was altered in the range of 0-250 G by adjusting the distance between magnets. The results indicated that, in the absence of the external magnetic field, the relative viscosity of the Fe$_3$O$_4$-water magnetic nanofluid increases up to 2.6 for the highest concentrated sample. In the presence of the external magnetic field, it is observed that the relative viscosity further increases. Moreover, increment in the relative viscosity is more remarkable with increasing particle concentration. The maximum relative viscosity was observed as almost 17 for the sample with 4.8% vol. concentration at 250 G.

**Keywords:** magnetic nanofluid; magnetic field; viscosity; magnetic actuation.

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**References**


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S4 O3

ANOMALOUS SEISMO-LAI VARIATIONS POTENTIALLY ASSOCIATED WITH SOME MODERATE VRANCEA EARTHQUAKES

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During last decade, due to fast progress of geospatial technology development, all weather, high-resolution and high-dynamic range, a huge time-series data base is available for earthquake precursors anomalies monitoring in active geotectonic areas. Pre-earthquake spatio-temporal developed geodetical, geophysical, and geochemical anomalies are controlled by various factors like as earthquake moment magnitude and its focal depth, geological setting, topography, land covers as well as climate and atmospheric conditions. Multi-precursors analysis has an important role to acknowledge the seismo-LAI (Lithospheric-Atmospheric-Ionospheric) anomalies associated to moderate and strong earthquakes. In this paper, changes before and after the Vrancea earthquakes in the crustal dynamics as well as in the land and atmospheric parameters (surface latent heat flux -SLHF, and air surface temperature- AT anomalies, have been investigated on the basis of time-series geospatial (NOAA AVHRR and MODIS Terra/Aqua) and field data analysis for 2012-2018 period. Ground surface deformations have been detected through analysis of Synthetic Aperture Radar Interferometry (InSAR) radar satellite Sentinel 1 and high quality in-situ GPS monitoring data. The detected changes show strong evidence of coupling between lithosphere-land surface-atmosphere-ionosphere associated with the Vrancea’s earthquakes For some analyzed earthquakes, starting with ten days up to one week prior to a moderate or earthquakes a transient thermal infrared rise appeared in SLHF (tens of W/m²) and AT (2-10°C) values higher than the normal, function of the magnitude and focal depth, which disappeared after the main shock. Ground vertical surface displacements presented on interferometric deformation map are in the range of 4 cm for uplifts and subsidence. The joint analysis of geospatial, geophysical, and geological information is revealing new insights for Vrancea zone seismicity understanding in Romania. Since the variations of the solar and geomagnetic indices follow a normal behavior during the whole period of the observed anomalies between 3 and 10 days before the earthquake, it can be concluded that multi-precursors analysis is very important to detect the possible Lithosphere Atmosphere Ionosphere Coupling (LAIC) effects.

Keywords: Earthquake presignals; geospatial and in-situ data; lithosphere–surfacesphere-atmosphere-ionosphere coupling model, Vrancea, Romania.

Acknowledgements: This work was supported by Romanian Ministry of Research and Innovation project Contract PCCDI 18/2018 VESS-3-PIMS.

S4 O4

ANALYSIS OF THE SCALE FREE BEHAVIOR OF WAITINGTIME DISTRIBUTIONS FOR EARTHQUAKES

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Whether we talk about earthquakes, solar flares or the financial market, all highly complex dynamical systems present the same scale-free behavior for their waiting time distributions [1]. Our work is motivated by the similar nature of these time series dynamics, which we explore in depth by focusing on earthquakes and compared with the known results for the logistic map and the Dow Jones Industrial Average. Expanding on our previous results [2], where we computed the waiting time distributions of earthquake magnitudes (see Fig.1), now we perform the same analysis for earthquake depths. The distributions obtained for earthquakes in Romania, Japan, Italy, and California have the same scale-free nature for waiting times. Moreover, for the
Vrancea region in Romania, our preliminary analysis shows some interesting results for the depth values in the transition zone between surface and deep earthquakes.

Figure 1: Waiting time distribution for earthquakes in Romania. The waiting time, measured in days, represents the time span between an earthquake of magnitude M and the first event of magnitude M + ρ. With ρ = 0.25, 0.5, 0.75, 1

Keywords— waiting time, scale free distribution, earthquake dynamics, Romania

References

S4 P1

THE STUDY OF HEAVY METALS IN WHEAT GROWN ON SEWAGE SLUDGE-TREATED FERTILE SOIL

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There are four categories of emission sources: stationary (industrial processes, industrial and domestic burning), mobile (car traffic), natural (spills, industrial fire). Sludges are wastes resulting from the treatment of waste water of domestic or industrial origin. Knowing the characteristics and content of sludge generated in sewage treatment plants of urban waste water is very important in taking recovery decisions or disposal of waste. Traditional solutions, such as landfills and incineration, have several disadvantages: the landfill may represent a risk of underground water contamination, just like burning, which is the source of air pollution [1,2]. The use of sludge in agriculture or for the growth of forest soils is considered acceptable ways of using the medium and long term in the European Union [3]. The sludges are made of water and dry matter, which provide macronutrients (nitrogen, phosphorus) and organic matter. In this paper are presents the concentration
of heavy metals (Cd, Cr, Cu, Fe, Mn, Pb and Zn) obtained by Atomic Absorption Spectrometry (AAS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) on wheat samples. These cultures were grown under laboratory conditions at different soil treatment concentrations (0/100, 25/75, 50/50, 75/25, 100/0) and aimed at observing the potential impact on the environment. Analyzes were performed at different stages of grain growth.

Keywords: heavy metals, sewage sludge, ICP-MS, AAS.

References

S4 P2

PHYSICAL METHODS FOR THE STRUCTURAL AND COMPOSITIONAL CHARACTERIZATION OF PREHISTORIC ARTEFACTS

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In the last 15 years, Romania has seen a significant increase of the interest in archaeometric investigations, due to endowments with state-of-the-art equipment of specialized laboratories [1]. We present preliminary results, of a complex study on prehistoric ceramic fragments, obtained using a wide range of physical characterization methods: structural (XRD analysis), morphological (SEM microscopy elemental and optical analysis), magnetic (EPR magnetic resonance), optical (FTIR, thermoluminescence) and thermal analysis (DTA / TG).

The ceramic fragments studied were gathered from several archaeological sites of the early Neolithic (Vădastra), the Eneolithic (Vădastra, Cruşovu, Radovanu) and the Bronze Age (Verbita, Cârna and Chitila). Fragments of bricks from the early Latene Fortress of Băzdâna were also analyzed.

The data acquired will be integrated into a wider context that will allow to expand the knowledge and understanding regarding the evolution, constants and peculiarities of the technological processes of ceramics and some clay structures.

(The research was carried out within the framework of the scientific collaboration between INCDFM and IAB.)

References
S4 P3
THE 1991 SEISMIC CRISIS IN THE WEST OF ROMANIA AND ITS IMPACT ON THE SEISMIC RISK AND HAZARD MANAGEMENT

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We present here a detailed spatial and temporal analysis of the greatest crustal earthquakes sequence occurred in the West of Romania in order to get useful information about zone seismicity and structural models for understanding and knowledge the seismogenic processes within a complex tectonic setting, as a first step in the realistic assessment of seismic risk and hazard. The 1991 seismic sequence was recorded within the most active crustal seismogenic zone of Romania since July 12, when an Mw5.6 strike-slip event occurred on NE-SW oriented fault. It produced heavy damages in the epicentral area (Io = VII MM degrees) and was followed by a strong aftershock on 19 July (Mw = 5.0). It seems like this quake triggered a high seismic activity at about 100 km in the Herculane – Mehadia area (Mw = 5.7, Io = VII – VIII MM, normal faulting un NW-SE fault system), where another significant seismogenic zone develops. After less than six months (02.12.1991) a second strong earthquake occurred 10 km North-East of the epicentre of the July 12 main event, having also significant macroseismic effects (Mw = 5.5, Io = VIII MM) and strike-slip faulting on an EW oriented structure. The seismic activity which lasted several years being marked by a lot of smaller sequences (Mw = 4.8, Io = VI MM degrees). Our results pointed out a clear migration of the seismic activity towards NE and the reactivation, during the two phases of the sequence, of two orthogonal faults systems accompanied by the rotation of SH max to the same direction, a rotation that could be an effect of the complex reactivation or a cause. Large variations of b values in time and space correlate with fractal dimensions of seismicity and stress tensor variations emphasizing some details on the 3D geometry of reactivated geological structures, clustered activity, identification of possible asperities and directivity of the main rupture and, thus, the real dimensions of the seismogenic structure and the most likely mechanism thereof and finally to estimate the reactivation potential of the faults system. Our results allow redefinition of the Banat seismogenic source with significant effects on the local seismic hazard model.

Keywords: b value, stress field, tectonic regime, seismic hazard.
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S4 P4
IRON OXIDE NANOPARTICLES GENOTOXIC IMPACT OF ROOT TIP CELLS OF ZEA MAYS EMBRYOS

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The environmental impact of manufactured nanoparticles increase concern regarding consists in the possible effects that these may have on the environment components. Plants could provide the potential way for nanoparticles accumulation into the food chain, leading to possible effects of these on the human health. The study of genotoxic effects of nanoparticles is one of the actual research topics, which could contribute to the knowledge and understanding of the nanoparticles influences on the environment. The aim of the present work was to investigate the genotoxic influence of iron oxide nanoparticles coated with aspartic acid and having 9.17nm physical diameter, on the Zea mays seeds. The experimental study focused on the cell proliferation in the root tips tissue, during the seeds germination under the iron oxide nanoparticles presence,
by addition into the germination substrate of the aqueous solutions of nanoparticles with different volume fractions ranging between 20 and 400μ/l. The iron oxide nanoparticles genetic impact in the root tip cells was qualitatively and quantitatively analyzed. For all samples (controls and the ones under iron oxide nanoparticles presence) the mitotic- and chromosomal aberrations indexes were determined. Cytophenetic tests were carried out by optical microscopy providing data about of the abnormal cells presence due to the iron oxide nanoparticles influence during the seeds germination. The process of the mitotic division appears to be stimulated under iron oxide nanoparticles influence and their presence leads to the chromosomal aberrations occur. The chromosome fragments, inter-chromatidian bridges or micronuclei are some of the abnormal cell types appeared in most analyzed samples under the iron oxide nanoparticles presence.

**Keywords:** iron oxide nanoparticles, mitotic division, genetic impact, chromosomal aberrations.

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**S4 P5**

CHARACTERIZATION OF FOLIC ACID IN INTERACTION WITH BOVINE SERUM ALBUMIN THROUGH MOLECULAR APPROACHES

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Folic acid (FA) or B9 vitamine is a bioactive food component whose deficiency can lead to a variety of health problems, while a high intake of FA can reduce the cytotoxicity of natural killer cells. Therefore, monitoring of FA levels in the human body lacks a simple, selective detection tool. It is known that FA binds to albumin [1-4], hence, in this work, a simple, rapid and reliable detection mechanism for the FA binding to bovine serum albumin (BSA) was optimized using spectroscopic and electrochemical techniques. The binding mechanism of FA to BSA was studied both in solution and adsorbed on gold substrate. The quenching mechanism of the fluorescence emission of free BSA in solution, was monitored in the presence of FA in increasing concentrations and it was found to have a static character. The affinity and kinetics of biomolecular interactions between BSA and FA, based on refractive index changes, which are sensitive to the adsorption of molecules on a gold coated chip was assessed by surface plasmon resonance technique. The adsorption of BSA and BSA-FA complex on gold substrate in increasing concentrations of FA was also studied by cyclic voltammetry and electrochemical impedance spectroscopy. Changes in redox current and corresponding parameters of equivalent electric circuit at gold-solution interface were used to evidentiate and interpret the biomolecular interaction. In order to characterize the FA-BSA interaction, the affinity constant and the thermodynamic parameters of the interaction were determined. The values of these parameters put in evidence that the binding of FA to BSA is moderate and is dominated by both by electrostatic and hydrophobic forces.

**Keywords:** folic acid, quenching mechanism, kinetics of biomolecular interactions, affinity constant, thermodynamic parameters.

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**References:**


S4 P6
FERRIHYDRITE NANOPARTICLES EFFECTS ON THE CONFORMATION AND THERMAL STABILITY OF HUMAN SERUM ALBUMIN

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In the last years, a great attention has been given to nanoparticles research due to their physicochemical properties that allow their used in analytical instruments or in promising imaging applications on biological systems. The use of ferrihydrite nanoparticles (Fh-NPs) in practical applications implies a particular control of magnetic properties, stability, biocompatibility, interaction with the surface of the target, and toxicity. In this study, the formation and organization of human serum albumin (HSA) in a corona around the simple Fh-NPs and Fh-NPs doped Cu and Co was examined by Atomic Force Microscopy (AFM). The topology of all Fh-NPs shows organized areas of HSA around each type of Fh-NPs. Thermal stability of these nanohybrids was further investigated by fluorometry, using 214-Trp residue from HSA structure as spectral sensor. The denaturation temperature, T_m, was determined and stabilization of the HSA structure in the presence of Fh-NPs was discussed. This study can be used to our advantage in the development of various applications that target the structure stability of protein - Fh-NPs complexes.

Keywords: ferrihydrite nanoparticles, human serum albumin corona, stability.
Acknowledgment: The work was accomplished with the financial support of the RO-JINR Project No. 54/2019, Investigation of biogenic and chemically synthesized systems in interaction with biostructures for applied research, Theme 02-1-1107-2011/2019.
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S4 P7
STRUCTURAL, FERROELECTRIC AND CYTOTOXIC PROPERTIES OF BARIUM TITANATE-HYDROXYAPATITE COMPOSITE CERAMICS

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Composite ceramic materials obtained by mixing of barium titanate (BT) and hydroxyapatite (HA) are known to stimulate bone regeneration [1-5] by direct piezoelectric effect. Electric dipoles generated by mechanical stress attract positive calcium ions and negative phosphate ions of hydroxyapatite accelerating bone growth. Barium titanate submicron powder (200-400 nm) was obtained by solid state reaction of the raw materials, previously homogenized by ball milling. BT powders were then mixed with 5, 10, 15 and 20 wt. % hydroxyapatite powder. Disc samples of 13 mm diameter and 2 mm height were obtained by uniaxially pressing of BT-HA powder. The compacted samples were then sintered at temperatures between 800-1300 °C. XRD diagrams show BT and HA peaks for sample sintered at 800 °C. Calcium titanates and barium phosphates phases are present for samples sintered at higher temperatures, proving that HA reacts with BT and partially decomposes. Density of BT-HA ceramic sintered samples decreases with increasing of HA amount and increases with temperature. Powder morphology was studied by SEM and micronic grains were attributed to BT and nanometric grains to HA. Polarisation decreases with increasing of HA content from 3.3 μC/cm² to 0.8 μC/cm² (at 30 kV/cm). Considering that the value for polarization of BT is 8 μC/cm² one may observe that the hydroxyapatite presence dramatically alters the ferroelectric properties. Preliminary results for cytotoxicity were obtained for BT and BT-HA samples. Evaluation was made for 24 hour of incubation of NIH3T3 cells for all disks samples by MTS method. Simple barium titanate disks sintered at 1300 °C are biocompatible. BT-HA samples toxicity was evidenced due to the presence of secondary phases.

**Keywords:** composite, barium titanate, hydroxyapatite, osteogenesis.

**Acknowledgements:** This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0062

**References:**

**S4 P8**

**CLUSTERING OF SEISMICITY IN THE VRANCEA REGION AT THE SOUTH-EASTERN CARPATHIANS ARC BEND**

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The Vrancea region is a particularly complex seismic zone of continental convergence characterized by at least three tectonic units in contact: East European plate, Intra-Alpine and Moesian subplates. The strongest seismic activity of Romania concentrates here at intermediate depths (60–200 km) in an old, almost vertical high-velocity lithospheric slab. The purpose of the present paper is to investigate source parameters and clustering properties for a time interval starting on 2016 to the present applying spectral ratios technique and empirical Green’s function deconvolution. The probability to find clusters of earthquakes (including main and empirical Green co-located events) within the seismic active volume is relatively high taking into account the increased density of foci. We selected a set of earthquakes (main events) located at different depths as templates for different co-located groups of events. The source parameters for an enlarged data set combining the present results with previous ones are investigated in order to determine scaling laws characterizing the Vrancea subcrustal activity. The source scaling properties are essential elements to understand and model the tectonic processes responsible for generating earthquakes in such a confined lithospheric volume. The scaling laws appear to be self-similar over the entire magnitude range spanned by the whole database (Mw ~ 2.8 to Mw 7.7).
At the same time, the source time function and source spectrum for the most of moderate-magnitude earthquakes are relatively simple, compatible with a circular source model with homogeneous rupture process. Particular high stress drop values, for moderate and large events, indicate fast and efficient rupture processes at different scales, possibly explained by fast running shear melting processes.

**Keywords**: Vrancea source, spectral ratios, empirical Green’s function, seismicity clustering

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**S4 P9**

**COOPERATIVE THREE-PARTICLE RESONANCE AND ITS REPRESENTATION BY MASTER EQUATIONS**

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Much attention is paid to the issue of coherence that occurs not only between individual photons but also between quantum groups. Generation of the non-classical electromagnetic field (CEM) in multi-photon emission and the coherent radiation interaction with matter (nuclei, atoms and solids) has been the subject of several theoretical and experimental studies in recent years. Examples include high - degree coherence in multi-photon light generation of two - photon micro-mask emission, two - photon reverse - conversion laser, blending of four waves and other effects in the optical range, and the possibility of coherently generating photons in spectral regions x and gamma. The cooperative emission of a photoconductor of the radiator system proposed by Dicke is experimentally observed in single photon transitions and spreading processes. Recently, this phenomenon has been studied in the multi - level system and in the multi - photon interaction of EMC radiators. Considering that the phenomenon of cooperation between radiators opens new experimental possibilities, the super fluorescence of the nonlinear interaction of the vacuum field radiators remains the focus of many theoretical models proposed lately. For example, using classical and quantum methods, a quantitative description of two-color super fluorescence can be provided. The problem of cooperative exchange integrals between several atoms identical to two levels located at distance r is investigated in works [1] - [4]. The authors of the paper [1], using the on-shell approximation, obtained the new solution for different probability amplitudes as infinite series containing all the delay times. At short distances, when the delay time is neglected, they have achieved well-known results in the literature. For two atoms, limited by a region less than the wavelength of the motor field, the authors of the article [4] predict significant deviations of the power spectrum from the resonance fluorescence of an atom due to the dipole - dipole interaction between atoms. The correlations between the radiation rate, the angular distribution, the spectrum and the radiation intensity of a two-atom pumped system are calculated in the paper [3] using the Lehmburg master equation and the fluctuation-regression theorem. Considering that the exact solution of two loaded harmonic oscillators interacting with the quantified EMF [5], the authors of the article [6] have shown that the situation found for two atoms is exceptional and comes from the geometric simplicity of the system. All these strict solutions take into account the effects of photon cooperation between the small number of radiators and contribute to the understanding of the cooperative phenomenon of EMC vacuum. In this chapter we will investigate the cooperative emission of the inverse radiator system, taking into account the resonance between cooperative transitions of one and two photons of three atomic subsystems. Since the co-operative phenomenon of two photons has a low co-operative rate of two quanta, we propose to expand our attention to the new type of cooperative resonance interaction between three radiators, where the transition of a single photon of two radiators enters resonance two quantum’s with the forbidden dipole transition of the third atom. These co-operative effects between the three particles take place in the EMC vacuum fluctuations and can amplify or reduce the spontaneous emission rate of each atomic subsystem as a function of the distance between them. In order to obtain stronger pulses of bound photons, it is proposed that cooperative interaction in each of the three subsystems of radiators be reversed relative to the dipole transition prohibited by the hydrogen or helium atoms type. The large number of experimental and theoretical classical descriptions of the decomposition of two
photon relative to the transition $2^3S_{1/2} \rightarrow 1^2S_{1/2}$ and $2^3S_0 \rightarrow 1^2S_0$ gives us a large number of possibilities in the experimental realization of such resonance types.

**Keywords:** Quantum optical phenomena in absorbing; Nonlinear optics; Stimulated Raman scattering; Cooperative phenomena in quantum optical systems

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**S4 P10**

**SIGNATURES OF CLASSICAL CHAOS IN QUANTUM SYSTEMS**

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Starting from a well-known model based on two coupled fourth-order oscillators that describes the intrinsic quadrupole vibrations of atomic nuclear surface we investigate the correspondences between classical and quantum chaos. The role of the classical phase-space structure upon the statistical properties of energy levels distribution of the associated quantum system is discussed in detail by means of extensive numerical simulations. Our analysis focuses on a distribution function that encodes two possible mechanisms for energy levels generation and we explore the correlations between the relative weight of the regular and irregular volumes in the classical phase-space.

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**S4 P11**

**DISCRETE NONLINEAR SCHRODINGER EQUATIONS FOR HIGH DENSITY BOSE-EINSTEIN CONDENSATES LOADED INTO OPTICAL LATTICES**

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We derive by analytical means a new set of discrete nonlinear Schrödinger (DNLS) equations using the Gross-Pitaevskii 0 K equation for the dynamics of a high-density Bose-Einstein condensates loaded into a deep optical lattice [1]. The derived equations take into account the changes in the density profile of the wave function in each well of the potential through the versatile $q$-Gaussian local ansatz of the condensate wave function. The $q$-parameter of the ansatz allows a description of the entire density regime of the condensate, from low- to high-densities [2]. We compare our equation with those previously used for low-density condensates loaded into optical lattices [3].

References:

S4 P12

EFFECTIVE EQUATION FOR HIGHLY OBLATE BOSE-EINSTEIN CONDENSATES

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We study by variational means within the Gross-Pitaevskii 0 K formalism the dynamics of highly oblate Bose-Einstein condensates [1] and derive an effective two-dimensional equation which has a nonpolynomial nonlinearity. The derived equation describes the high-density (also known as Thomas-Fermi) regime of the condensate and relies on a $q$-Gaussian ansatz which accounts correctly both for the bulk of the condensate and its surface [2]. We compare our equation with its known one-dimensional version [3] derived for high-density condensates and the one- and two-dimensional equations derived for low-density condensates [4].

References:

S4 P13

PERMEABLE SEGMENTED THERMOELECTRIC ELEMENT

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A promising line of increasing thermoelectric elements efficiency is to use the legs of two or more materials – segments the thermoelectric properties of which are selected on condition of maximum figure of merit parameter. The elaborated numerical methods for calculation of such thermoelements were used for
designing of patented in segmented thermoelements of materials based on $\text{Bi}_2\text{Te}_3$ and skutterudites. It was shown theoretically that the efficiency value equal to 15% should be expected at the temperature difference about 670 K.

Another promising line of increasing energy conversion efficiency is to use permeable legs for heat carrier fluxes. Owing to the presence of heat exchange between heat carrier and “cold” parts of legs, this enables to give more thermal energy to material and convert it into electric energy. Computer calculations of permeable thermoelement models confirmed the possibility of improving the efficiency of energy conversion by 25%.

The first results of theoretical research on permeable generator thermoelements of segmented legs were obtained for materials based on $\text{Bi}_2\text{Te}_3$. A method for calculation and optimization of thermoelement operation in maximum efficiency mode under optimal pumping velocity of heat carriers and electric current density was described. The influence of structural factors (the height of legs, the diameter of channels and their number) on the efficiency and electric power was studied. The results pointed to the possibility of further efficiency increase. However, the problem of finding the optimal segmented legs of various materials was not solved. The materials based on $\text{Bi}_2\text{Te}_3$, $\text{PbTe}$, $\text{PbTeG}$ the effect of structural parameters under optimal operating conditions on the energy characteristics of thermoelement was calculated. The rational values of such parameters that enable determination of the necessary material research requirements for creation of segmented thermoelement.

**Keywords**: segmented materials, thermoelectric element.

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**S4 P14**

**DEVELOPMENT AND PHARMACEUTICAL VALIDATION OF BACTERIAL ENDOTOXINS TEST**

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[18F]sodium fluoride and [18F]fluorodeoxyglucose are radiopharmaceuticals produced as sterile solution suitable for intravenous administration, which must contain no more than 175EU/V Endotoxin, where V is the maximum administrated total dose at the expiration time. Endotoxins are potentially toxic natural compounds of the cell wall of gram negative bacteria. The absence of bacterial endotoxins implies the absence of a pyrogenic component.

The aim of this work was to established the optimal dilution of [18F]sodium fluoride and [18F]fluorodeoxyglucose for bacterial endotoxins test. The bacterial endotoxin test was performed using Endosafe Portable Test System (PTS) and applied as a quality control for release criteria of all [18F]radiopharmaceuticals manufactured in Radiopharmaceutical Research Centre, IFIN-HH.

For the PTS System the sample should be diluted to give a satisfactory Spike Recovery reading and % Coefficient of Variance readings. Four different dilution factors were checked: 1:10, 1:50, 1:100 and 1:175. Three batches for each radiopharmaceutical was run on the Endosafe PTS System.

The results from the series of dilution show that 1:50 is the minimum dilution volume to carry out the test and therefore the recommended dilution volume. No inhibition of the product positive control was found in the recommended dilution range.

**Keywords**: validation, endotoxins, radiopharmaceuticals, recovery.
**S4 P15**

**BACTERIAL CULTIVATION LIGHT EXPOSITION EFFECTS ON BIOGENIC PARTICLES PROPERTIES**

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The development of nanoparticles synthesis techniques using microorganisms is an important area of research at the present time for biomedical applications\textsuperscript{[1,2]}. As a result of variation of the cultivation period for the microorganisms, \textsuperscript{8} and respectively \textsuperscript{21} days, bacterium Klebsiella Oxytoca creates, as it was established earlier\textsuperscript{[3–6]}, two types of ferrihydrite nanoparticles (Fe\textsubscript{12} and Fe\textsubscript{34}), identified by means of Mössbauer spectroscopy\textsuperscript{[3]}, static magnetic measurements analysis\textsuperscript{[4]}, scanning electron microscopy\textsuperscript{[5]}, small angle X-ray scattering\textsuperscript{[5]} and ion beam analysis\textsuperscript{[6]} methods.

In the present work, SEM, SAXS and IBA methods are applied to the investigation of ferrihydrite particles obtained from the Klebsiella Oxyrca metabolic cycles different in light exposition.

**Keywords:** Klebsiella Oxytoca, ferrihydrite, SAXS, SEM, IBA

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**S4 P16**

**TIME SERIES SATELLITE REMOTE SENSING DATA FOR MONITORING OF CLIMATE CHANGES IMPACTS ON URBAN GREEN LAND COVER**

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Urban vegetation land cover change is a direct measure of quantitative increase or decrease in sources of urban pollution and the dimension of climate and extreme climate events and changes that determine environment quality. Satellite Earth observation data in the visible (VIS) and near-infrared
VNIR wavelengths represent a useful source of information for urban vegetation land cover systems monitoring through derived biogeophysical parameters (vegetation index, leaf area index, canopy cover, fraction of absorbed photosynthetically active radiation, chlorophyll content, net primary production, vegetation water stressed.). Use of satellite remote sensing data to assess urban green spatio-temporal changes due to climatic or anthropogenic stressors is an excellent example of the value of multispectral and multitemporal observations. This study addresses climate changes effects and anthropogenic impacts due to urban growth on urban green biophysical variables based on time series satellite data in synergy with in-situ data and new analytical methods. This paper explored the use of time-series MODIS Terra/Aqua Normalized Difference Vegetation Index (NDVI/EVI), Land Surface Temperature (LST) and Leaf Area Index (LAI), land surface albedo data to provide land cover vegetation change detection information for Bucharest test area during investigated 2000 - 2018 period. Training and validation are based on a reference dataset collected from Landsat OLI remote sensing data. The mean detection accuracy for investigated period was 89%, with a reasonable balance between change commission errors (19.87%), change omission errors (23.63%), and Kappa coefficient of 0.76. Annual change detection rates across the urban/periurban green areas over the study period were estimated at 0.78% per annum in the range of 0.45% (2000) to 0.79% (2018). Vegetation dynamics in urban areas at seasonal and longer timescales reflect large-scale interactions between the terrestrial biosphere and the climate system. Research on spatial and temporal variations of vegetation land covers in urban areas is an essential issue for understanding the city heat energy balance and thermal flux dynamics in relation with microclimate and climate impacts, useful for development of city heat transfer models, water resource management, and environmental studies. This paper investigated also the influences of urban growth and green land cover decrease on metropolitan climate of Bucharest in Romania.

**Keywords**: urban green land cover, urban growth, city climate, time-series satellite data, biogeophysical parameters, Bucharest.

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**S4 P17**

**HIGH PRESSURE SANS INVESTIGATION OF STRUCTURAL CHANGES IN MODEL LIPID MEMBRANES**

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Changes in the structural parameters of 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC) model lipid membranes occurring under the influence of increasing external hydrostatic pressure were studied. The dependences of the thickness of the lipid bilayer, the aqueous layer and the size of the multilayer vesicles on the external pressure were obtained.

Dispersion of multilayer DMPC vesicles in heavy water with a lipid concentration of 17.5% wt/wt was studied by small-angle neutron scattering method (SANS) at YuMO spectrometer (IBR-2, JINR, FLNP, Dubna, Russia) [1] in the pressure range from 1750 to 2400 bar. During the experiment, the sample was
maintained at a temperature of 60 °C by a Lauda thermostat with an accuracy of 0.03 °C. Thus, the DMPC membrane initially was in the liquid phase, and the process of pressure change was considered to be isothermal.

The primary TOF small-angle spectra were treated by specialized SAS program. [2] The obtained neutron scattering curves were processed using ATSAS Primus and SasView small-angle scattering data treatment software. The positions of the diffraction peaks observed on the scattering curves reveal the changes in the repeat distance of the multilayer lipid membrane with increasing pressure. It is shown that with an increase in pressure from 1750 to 2400 bar, the repeat distance changes nonlinearly. A minimum is observed near the pressure point of 2200 bar, that allows to make an assumption about the possibility of a phase transition of the lipid membrane under the indicated external conditions. Using the Kratky-Porod approximation [3], the thickness of the lipid bilayer and the aqueous layer between the bilayers are determined. The obtained parameters are refined in the SasView program by the method of approximation of experimental curves with model functions.

References

S4 P18
PULSED MAGNETIC FIELDS AFFECT THE ULTRASTRUCTURE OF LIVING CELLS CONTAINING ENDOGENOUS MAGNETOSOME CHAINS

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The aim of present study was to reveal the effect of pulsed magnetic field with different parameters on the cells of bacteria Magnetospirillum gryphiswaldense analyzed by scanning-transmission electron microscopy (STEM) and by Fourier Transform Infrared Spectroscopy (FTIR).

Magnetotactic bacteria produce biogenic magnetite (Fe3O4) nanoparticles inside the cells, which present themselves in the form of chains of magnetosomes (nanoparticles enveloped in a membrane and aligned by means of cytoskeletal filaments). Such cells received much attention in the last years, due to significant biomedical uses in theranostics and in imaging.

Since application of magnetic pulses to such bacteria cells is still insufficiently researched, we were interested to quantify the effects of pulse trains and bursts of magnetic field with peak flux density of up to 0.92 T, on the cells ultrastructure. Each pulse had a duration of 400 µs, while three types of magnetic stimuli were prepared, analyzed - in time and in frequency, and applied to the cell suspensions (one type of pulse train and two types of bursts). The applicator was a transcranial magnetic stimulation (TMS) coil connected to the Magstim Rapid2 instrument. Magnetic field strengths was measured and recorded by a small magnetic field probe connected to a real-time spectrum analyzer.

The bacterial cells at stationary growth phase were suspended in culture medium at a concentration of 1.96 × 10^9 cell/ml, and identical samples, in a volume of 2 ml each, were exposed to the different stimuli applied by the TMS coil.

Cellular appearance of the magnetotactic bacterial cells analyzed by STEM showed mild cellular integrity damaging, apparition of cyst-like cells (spheroplasts / coccoid cells, with or without magnetosome chains inside) and abnormal magnetosome chains presence.
Modifications appeared in some of the FTIR spectra of magnetic-pulses treated suspensions when compared to the control, both with trains of pulses and with bursts, indicating the possibility that some proteins may be affected.

Collapsing of magnetosome chains has been also observed in some situations, and may be due to cytoskeleton (filaments) damage thru modification in conformation of actin-like protein of these filaments.

Keywords: magnetotactic bacteria, magnetic field, Fourier-transform infrared spectroscopy, transmission electron microscopy

S4 P19

STUDY OF BIOMATERIALS FROM NATURAL RESOURCES

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Biomaterials are used in the medical field due to their properties. The experiment consisted of pulsed laser deposition of BHA doped with clinoptilolite (CLIN) and alumina (Al2O3) structures were synthesized by the substrates of Ti or Si with a KrF* excimer laser source. Antibacterial properties of these materials have been investigated. Antibacterial activity indicating a superior cytocompatibility recommend these structures. The complex stoichiometry of targets was analysed SEM and XRD. The thin films consisted of closely aggregated/fused round-shaped micrometric particulates within the range of (0.2 – 4) µm.

S4 P20

STRUCTURE INVESTIGATIONS OF COBALT FERRITE/LAURIC ACID/SODIUM DODECYL SULPHATE/WATER FERROFLUIDS USING SMALL-ANGLE NEUTRON SCATTERING

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Investigations of the structure, morphology and properties of the magnetic nanoparticles of water-based ferrofluids is an important issue due to an increasing interest for biomedical applications. Using the small angle neutron scattering (SANS) we performed experimental study on different concentrations samples of CoFe2O4/lauric acid/DDS-Na/H2O ferrofluid. The ferrofluid was prepared by the coprecipitation method of Fe(OH)3 and Co(OH)2 and stabilized by the adsorption of lauric acid on ferrite particles and peptisation of hydrophobic precipitate in aqueous solution with sodium n-dodecyl sulphate.

The experimental data were processed using specialized programs. FITTER, and also PRIMUS, Gnom, DAMMIF and DAMAVER programs from the ATSAS Package were used for data analyzing in order to find the effect of concentration on spatial arrangement and morphology of nanoparticles.
Specific values of the parameters computed from the experimental curves (i.e. gyration radius, fractal dimension) are considered as good descriptors for differentiating the effect of increasing concentration in each sample spatial arrangement.

**Keywords**: ferrofluids, cobalt ferrite nanoparticles, SANS

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**S4 P21**

**COMPOSITE MATERIALS BASED ON NANOBIO SILVER AND CALCIUM CARBONATE FOR TOPICAL APPLICATIONS**

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Two new composite materials based on nanobio silver and calcium carbonate (Ag-CaCO$_3$) were obtained in green seaweed (Ulva lactuca) extracts. The composite materials were characterized by XRD, SEM, EDX, UV-vis and FTIR spectroscopy. The chemical composition of composites, determined by EDX, revealed Ag/Ca molar ratios of 1/155 and 1/55.

The morphology of composites was analyzed by SEM and demonstrated the influence of the polysaccharides from green seaweeds in calcium carbonate synthesis. At higher amounts of polysaccharides, the calcium carbonate precipitates as beads-like aggregates, obtained by agglomeration of calcite nanoparticles. With the decrease of polysaccharides concentration, the CaCO$_3$ aggregates are almost cubic. A similar dependence has been demonstrated for other vegetal extracts too [1]. The decrease of polysaccharides concentration can be correlated with the consumption of phytochemicals in the silver synthesis. The presence of polysaccharides as capping agents was demonstrated by FTIR spectra.

The dermatological properties of composites were tested *in vivo* in the treatment of second-degree thermal skin burns induced to the laboratory animals [2]. A better healing effect was identified for a higher amount of silver, but good healing properties were observed for both Ag-CaCO$_3$ composites. The oxidative activity of composite materials was also tested *in vivo* by analyzing the rats’ tissue, demonstrating that higher silver content induces the oxidative stress. The experimental results recommend the utilization of composites in topical treatment of burns.

**Keywords**: nanobio silver, calcite, Ag-CaCO$_3$ composite.

**Acknowledgements**: This work has been performed in the frame of Project No. 10 from Order No. 397/27.05.2019 of JINR-VBLHEP, Dubna, Russia.

**References**

INACTIVATION OF SALMONELLA ENTERITIDIS AND ESCHERICHIA COLI ON SOYA SPROUTS

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In the present study, the inactivation of Salmonella Enteritidis and Escherichia coli inoculated on soya sprouts by low-temperature plasma were evaluated. Plasma was generated by Diffuse Coplanar Surface Barrier Discharge (DCSBD) at atmospheric pressure in ambient air for 0; 2; 4; 6; 8; 10 min. Plasma treatment reduced the number of S. Enteritidis (6 min) and E. coli (8 min) to below detection level (1.0 log₁₀ CFU/g) from the initial population of 6.78 log₁₀ CFU/g and 7.36 log₁₀ CFU/g, respectively (Fig. 1). Decimal reduction times (D-value) obtained from modeling of the inactivation kinetics by Weibull model for S. Enteritidis and E. coli were determined as 1.13 min and 1.38 min, respectively. DCSBD treatment time of 10 min caused a decrease of the antioxidant potential of soya sprouts measured by ABTS, DPPH and FRAP test. Additionally, after being treated with DCSBD (10 min), the total polyphenols, flavonoid and reducing sugar content was also decreased.

Fig. 1 Effect of DCSBD on the inactivation kinetics of S. Enteritidis and E. coli inoculated on the surface of soya sprouts modeled using the Weibull model

Keywords: Devitalisation; DCSBD; Soya sprouts

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ABSTRACTS

S5 – Engineering and Industrial Physics

- Physics of energy transfer, conversion and storage
- Environmental Physics
- Sensors and Device Physics
- Micro- and Nanoelectronics
- Microelectromechanical systems
- Instrumentation and Metrology
- Imagining, Microscopy and Spectroscopy and their applications
- Instrumentation, processing, fabrication and measurement technologies
- Applications of fluid mechanics and microfluidics
THE NEUTRON IMAGING STUDIES OF CULTURAL HERITAGE

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One of the most important tasks of archeology and other history-related sciences is the comprehensive study of cultural heritage items. The results of these studies have a significant application value, because they provide a way to penetrate into the far past and allow us to understand the formation and evolution of civilizations and ethnic groups.

The experimental methods applied to characterize archeological and cultural heritage items are used to obtain detailed data regarding the phase analysis, assembly of inner parts and design items, the evolution of cracks and defects, and the traces of corrosion propagation. Valuable and irreplaceable archaeological items are part of the cultural heritage of nations, requiring innovative approaches to their study in order to ensure their physical preservation for future generations. It is desirable to investigate them by modern non-destructive methods. The fundamental difference in the nature of neutron interactions with matter compared to X-rays provides additional benefits to neutron methods, including sensitivity to light elements, a notable difference in contrast between different metals, and high penetration ability. The non-destructive character of the neutron radiography and tomography method has prompted the rising interest in studying rare archaeological items and museum rarities, especially metallic artifacts, weapons and ancient jewelry.

Recently, there has been a significant increase in successful cooperation between the Joint Institute for Nuclear Research and the Institute of Archeology of the Russian Academy of Sciences. The complementary archaeological and physical research makes it possible to study a large number of valuable objects from various large-scale archaeological excavations in the territory of the Russian Federation. Examples of the scientific achievements resulting from this cooperation, as well as a demonstration of the opportunities provided by neutron radiography and tomography methods, are given in the talk. We present several interesting results of neutron studies of the historical and cultural heritage objects dating to different periods of the history. The obtained neutron tomography results demonstrate the opportunities offered by the neutron tomography method for non-destructive testing of large cultural heritage artefacts. Morphological calculations based on the experimental tomography data were used to analyze the spatial arrangement of different components of the studied objects. The obtained characteristics of the internal structures of the studied objects are important for further development of existing archeological and historical concepts.

Keywords: neutron imaging, non-destructive methods, cultural heritage, neutron diffraction.

TUNABLE BIO-INTERFACE FOR BIOSENSING APPLICATIONS

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The lecture intends to be an overview on the research activity developed by our group in the sensing field, especially the design of the interface between the physical transducer and the biological recognition elements. The immobilization of the active biological component on the transducer surface represents a critical stage in the biosensors development and it has as a goal the settlement of the bioactive part on the surface of the physical transducer.
The chosen immobilization procedure has to keep the biological component in the native conformation. On the other hand, the physical transducers should have an adequate sensitivity toward the species to be detected.

The lecture will illustrate the practical applications of physical, organic, and inorganic chemistry for surface modification of electrochemical and SAW sensors, focusing on layer-by-layer assembly and thiol-driven self-assembly and sol-gel chemistry, grafting chemistries including click chemistry and practical applications of ‘micro- and nano- bio-interface’ in environmental and biomedical analysis areas.

**Keywords**: enzyme, biosensors, optical, electrochemistry.

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**S5 O1**

**STRUCTURAL INPAINTING TECHNIQUES USING EQUATIONS OF ENGINEERING PHYSICS**

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Digital image interpolation, or inpainting, represents the reconstruction of the missing regions of the image using the information obtained from surrounding areas. The inpainting techniques may have a structural or textural character. Here we consider only the structure-based image interpolation domain, describing the state of the art structural inpainting solutions based on partial differential equation (PDE) – based models of physics engineering, including our own contributions in this area.

The diffusion equations, which describe the random motion of the micro-particles in physics, have been successfully applied in the image restoration and interpolation field in the last 35 years. The nonlinear anisotropic diffusion-based structural inpainting techniques, based on variational and non-variational PDE-based schemes, are disscussed first [1]. Influential reconstruction approaches following variational principles include those using Mumford-Shah functional, Total Variation (TV) Inpainting and its versions, and Euler’s Elastica Inpainting. Some second and fourth-order anisotropic diffusion models for structure-based interpolation developed by us are also described here [2]. Reaction-diffusion equations, which are used to describe pattern-formation phenomena in various biological and physical systems, represent another powerful inpainting tool. The applications of the reaction-diffusion Ginzburg-Landau equation, describing a large variety of physics phenomena, in the inpainting domain, are presented next [3].

Structural interpolation methods using partial differential equations for fluid dynamics are also considered here. Such an important third-order non-variational PDE-based inpainting algorithm that was introduced by Bertalmio et al. is based on the Navier-Stokes equations that describe the motion of the viscous fluids in physics [4]. Another category of nonlinear third-order PDE models for non-texture inpainting are based on curvature-driven diffusion equations, which use the thermal diffusion principle in physics. Curvature-driven Diffusion (CDD) Inpainting scheme provides an effective image reconstruction but has a noise sensitive character [5]. Fourth-order PDE-based structural inpainting solutions are also addressed. Cahn–Hilliard Inpainting [6], a state of the art model using a modified mathematical physics equation describing the process of phase separation is described here.

**Keywords**: image interpolation, anisotropic diffusion models, curvature driven diffusion-based inpainting, equations of fluid dynamics for inpainting.

**Acknowledgements**: This research is supported from PN-III-P4-ID-PCE-2016-0011 of UEFISCDI.
Studies conducted on fiber reinforced plastics (FRP’s) have shown that they have a time dependent behavior [1]. This is caused by the resin, which tends to “flow” in time [2]. This is also confirmed composites with a synthetic fiber (such as carbon or glass), where, composites with a 0° oriented fiber reinforcement tend to behave purely elastic, while having a non-linear visco elastic behavior on all other directions [3].

Recent advancements in FRP’s have had the tendency to lead towards renewable sources, such as plant fibers, out of which, flax fiber is the most proficient [4], with specific mechanical properties close to glass fibers.

However, the complex nature of this fiber, which itself can be considered a composite material [5], gives it, as well, a time dependent behavior [6]. Thus, studies on this subject have shown that flax fiber reinforced plastics (FFRP) behave in a more complex manner than synthetic FRP’s. More specifically, they tend to have a coupling of viscoelastic and viscoplastic behavior.

The present study aims at characterizing and modeling this behavior for a unidirectional flax fiber – epoxy resin unidirectional composite, with a fiber direction of 0°. For this to be achieved, a two series of creep-recovery type tests have been conducted, one with the variation of creep time and the other with the variation of creep stress. To model this behavior, a nonlinear viscoelastic model has been chosen, namely the one presented by Schapery and a viscoplastic model, introduced by Zapas and Crissman.

Experimental results have shown significant scatter, especially the viscoplastic data, which has prompted a sensibility study, conducted by simulating a variation in the mean experimental results, within a ±10% boundry.

Keywords: Bio-composite, Flax fiber, Viscoelasticity, Viscoplasticity.

References
S5 O3
THE NEW FACILITY OF NEUTRON RADIOGRAPHY AND TOMOGRAPHY AT THE RESEARCH REACTOR WWR-K IN ALMATY, KAZAKHSTAN

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One of the basic facilities of the Institute of nuclear physics of the Ministry of energy, Almaty, is the research reactor WWR-K, in which conducts fundamental nuclear physics and materials science research, produces radioisotopes for industry and medicine. Taking into account the importance and wide application capabilities of neutron non-destructive testing methods, a new experimental facility for research using neutron radiography and tomography was built. The new facility for neutron radiography and tomography is located on the channel № 1 of the reactor WWR-K. Neutron beam is formed by a system of collimators placed in a vacuum casing to reduce losses due to neutron scattering in the air. The neutron flux at the sample position, measured by gold foil activation, was equal 1.4*10^8 n/(cm^2*s) with the parameter L/D=100. A specially designed detector system based on scintillation screen and a high-resolution video camera with a mirror is used. At present, the schemes of the drum system for changing the diameter D of the input aperture of the collimator system are being developed, which allow to vary the L/D parameter from 100 to 1400. This paper will present the results of the first test experiments and a description of the main components of the experimental setup.

S5 O4
QUANTITATIVE DETERMINATION OF CEMENTITE IN STEELS USING NEUTRON DIFFRACTION

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Carbides along with retained austenite (RA) are formed during steels heat treatment. Although such dispersed phases have low volume fractions (of the order of one per cent or less), their effects on mechanical properties of steel at low temperatures are very strong.

X-ray diffraction (XRD) is generally considered the most reliable technique for RA evaluation [1]. But there are some limitations for this technique. Firstly, RA content can be evaluated only on the surface of a sample by this technique. Secondly, it can be applied only for texture-free materials. Metal volumes studied by neutron diffraction (ND) exceed those of XRD by several orders that provide promising perspectives in the phase analysis. In particular, very small volume fractions (less than one per cent) of retained austenite, imperceptible with XRD, can be evaluated by means of ND.

Existing procedures [1-2] to determine quantitatively retained austenite in steels are also can be applied for the cementite finding. However, even the procedure based on ND application [2] have serious drawbacks as follows. First, there are no direct ways to verify results accuracy; second, the measurements are highly
affected by a crystallographic texture. Besides, this technique implies that a cementite is the only second phase in steel.

The new technique to determine the cementite in high strength steels using the neutron diffraction method is proposed. This technique based on the proposed by authors method for the retained austenite determination [3]. Measurements of neutron diffraction patterns were carried out at the texture diffractometer SKAT (JINR, Dubna, Russian Federation) in order to eliminate the influence of a texture on the result. Measurements of calibration samples with predefined content of the cementite were fulfilled. On the basis of these measurements the calibration lines were computed. These lines have been used for cementite content determination in medium-carbon steel samples (0.3 to 0.4%) with a yield strength of 1500 MPa subjected to different annealing (400°C to 550°C) after quenching.

**Keywords:** neutron diffraction, cementite, high strenth steels, crystallographic texture

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**References**

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**S5 O5**

**DATING THERMOLUMINESCENCE AND MICROSTRUCTURAL CHARACTERIZATION OF ARCHAEOLOGICAL CERAMIC SAMPLES FROM CORVINS’CASTLE AREA**

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Some ceramics samples from Corvins’Castle area, in different weathering stages, have been analyzed in this paper by different analytical techniques: X-ray diffraction (XRD), Scanning Electron Microscopy - Energy Dispersive Spectrometry (SEM-EDS), porosity and thermal analysis (thermogravimetric analysis (TG) and derivative thermal analysis (DTG) and thermoluminescence (TL) dating.

For identification of the technology employed in the pottery production, the firing temperature could be determined through the presence of some minerals (evidenced by XRD): quartz, calcite, fluorite, illite, feldspar, montmorillonite. Crushed calcite is a good indicator, because it is present in the fabrics which have been tired up to 750°C (under oxidized atmosphere) whereas at a higher temperature it disappears leaving a well-defined rhombohedral shape void. Furthermore, a vitrified fabric suggests that the firing temperature exceeded 850 °C. Also, the clay minerals can be identified by the high-temperature minerals, such as mullite and tridymite, that form at temperatures over approximately 900 °C. By TL the nature of the crystalline network could be detected, ceramics consist of a number of crystalline inclusions (mainly quartz and feldspar) embedded in the ceramic matrix. TL analysis revealed the existence of a single maximum, which suggests that existing defects are of a single type, probably correlated with the pore structure of the material (pore diameter = 0.4 nm). A predominant peak at about 276 °C, when the TL glow was deconvoluted using computerized curve deconvolution analysis.
Also, the peak related to 343 °C is always found in quartz. The date obtained by TL technique was in good agreement with the date assigned by archaeologists (age of 227 years).

**Keywords**: ceramic, thermoluminescence, XRD, SEM-EDS.

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**S5 O6**

**NUMERICAL MODELING OF QUENCH THERMAL PROPAGATION IN A SUPERCONDUCTING HTS COIL**

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In the paper are presented the results of numerical modeling in Comsol Multiphysics of the heat dissipation produced at the occurrence of a quench, in a cylindrical coil made of HTS (High Temperature Superconductor) YBCO material. The coil is of double pancake type with an outer diameter of 220 mm and an inner diameter of 80 mm. The HTS tape, with a thickness of 0.1 mm and a width of 12 mm, is covered with a copper layer of 20 μm. The superconducting coil is made in two versions: with an electrical insulating layer and with no insulating layer between turns. For various reasons (vibrations, fast variation of magnetic field, etc.), the superconductor can suffer locally the quench transition leading to the appearance of a "hot spot" in the winding. This produces local heating of the HTS coil and generates both a considerable thermal jump and a corresponding rise in voltage to the coil terminals. The heat produced propagates both horizontally and vertically at different speeds. The numerical evaluation of the heat propagation speed in the winding allows to obtain an important parameter for the design of the superconducting winding protection systems: the reaction speed. The obtained numerical results also allow for optimization of the superconducting coil cooling process. The cryogenic cooling system is conductive, using a two-stage Gifford-McMahon closed cycle cryocooler: step I at 50K and respectively step II at 4.2K. Numerically, both constructive variants of the coil were evaluated in order to optimize the technology of realizing these superconducting coils and to evaluate the operating parameters of an efficient HTS coil protection system.

**Keywords**: superconductive HTS coil, numerical modeling, quench, thermal propagation.

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**S5 O7**

**CRYOGENIC SYSTEM FOR NEON SOLIDIFICATION AND POSITRON SOURCE COOLING AT ELI-NP**

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In the paper is presented the cryogenic cooling system of a positron source for ELI-NP and solidification of the neon on the source, for the energetic moderation of the emitted positrons. The positron source with an intensity of \( \sim 10^7 \) s\(^{-1}\) consists of several tungsten sheets irradiated with gamma rays. Numerically, in Comsol Multiphysics are evaluated, the thermal transfer in the system as well as the conditions of solidification of the neon on the positron source. The cryogenic cooling system of the source and solidification process of the neon is performed with a closed-loop, Gifford-McMahon, two-stage cryocooler: stage I at 50K and stage II at 4.2K. The cryocooler is isolated with a thermal shield coupled to the cooling stage I to reduce heat transfer by radiation. The whole system is enclosed in a cryostat that allows both the gamma radiation access to the tungsten sheets and thermal insulation from the external environment. The cryogenic system is evaluated numerically to assess the thermal loads on the two stages and the efficiency of the cooling process. Condensation and solidification of the gaseous Ne on the elements of the positron source requires both thermal and mass control. The optimal conditions and optimal value of the parameters required to achieve neon solidification are also evaluated. Thus, the contribution of gas precooling and quantification of the mass of gas introduced into the system is highlighted. A video system monitors in real time the process of depositing / solidifying the neon gas on the positron source. In the paper are presented the obtained results and their correlation with the parameters of the system.

**Keywords:** cryogenic system, positrons, solid neon, numerical modeling.

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**S5 O8**

**MARTENSITIC PHASE TRANSITION IN YTTRIUM-STABILIZED ZRO\(_2\): NANOPOWDERS BY ADSORPTION OF WATER**

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The adsorption-induced structural effects in oxide nanopowder systems are of great interest for the fundamental science and nanopowder technologies applications. Among them are: nanopowder moisture sensors, high-temperature nanoionic capacitors, submicroscopic adsorption mechanical strictors, adsorption heat and electric generators [1], etc. The adsorption-induced phase transformation is the key physical effect due to which the charge state of nanopowder objects can change. The effects of adsorption-induced phase transformations and the effects of interphase electron exchange related to them have not been studied sufficiently. Moreover not so long an existence of such transformation in nanoscale objects has been questioned.

The present study was aimed at revealing the influence of the mechanical stress induced by surface absorbed water molecules on the composition of crystalline phases in the ZrO\(_2\) - 3mol% Y\(_2\)O\(_3\) – nanoparticles. Three basic methods have been used to determine the phase transition: neutron diffraction, Raman microspectroscopic scanning and X-ray diffraction. The fact of phase-structural \[\square\] transformation and the simultaneous presence of two polymorphic structural modifications (\[\square\] - is the phase of the tetragonal syngony and \[\square\] is the phase of monoclinic syngony in nanoscale particles (7.5 nm) under normal physical conditions is established by these methods. Satisfactory consistency was achieved between the results obtained using
different techniques. The scientific basis for use of adsorption-induced effects in oxide nanopowder systems for nanoelectronics, mechanics and power engineering devices has been developed.

**Keywords**: adsorption phase transition in nanopowder systems, size effect of structural stabilization, powder nanotechnologies, zirconium oxide nanoparticles.

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**S5 O9**

**SPATIO-TEMPORAL DISTRIBUTION OF SEISMICITY AND SOURCE PROPERTIES AT IZVORUL MUNTELEUI DAM NORTHEAST ROMANIA**

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The seismic activity in the Eastern Carpathians (EC) is dominated by the intermediate depth events occurred in a small volume in the Vrancea region, located at the EC bending. The significant earthquakes associated with this region generate hazard in southeastern Europe. Towards the northern segment of the EC (NEC) the deformation decreases while seismic activity is increasingly sparse and mostly lie to the west of the marginal fractures of the East European Craton. However, recent developments of the Romanian Seismic Network (RSN) showed an increasing trend of the detected and located events in the NEC by decreasing the magnitude detection threshold. Therefore, the detection and location processes are highly influenced by the number of seismic stations, network geometry and the detection algorithm. At the same time in the NEC is located one of the largest dams built in Romania between 1950 and 1960. Although the dams often produce seismic events as a result of stress variation due to the weight of the water column, Romanian earthquake catalogue (ROMPLUS) reveals only a reduced number of low-magnitude events in the dam area. The present study aims to verify the efficiency of the detection approach used routinely within the National Institute of Earth Physics, the possible triggering effects by the water level fluctuations in the dam and to establish a comprehensive picture of seismic activity around the dam area. To achieve our goals, we ran a multi-channel waveform correlation detector to the seismic data recorded between 2012 and 2018 by a 3-component broadband seismic station and a seismic array located nearby. Our results showed a significant increasing trend of detected and located events. The hypocenters are distributed mostly in the upper crust towards the southwestern part relative to the dam. Nevertheless, we noticed possible contamination with anthropogenic events, since most of the events occurred during the daytime. Statistical and spectral analyses used to separate the sources revealed that only a low number of tectonic events were influenced by the water level variations in the dam.

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**S5 O10**

**MAGNETO-OPTICAL EFFECTS IN BARIUM HEXAFERRITE COLLOIDS**

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Plate-like magnetic particles of barium hexaferrite (BaFe\textsubscript{12}O\textsubscript{19}) were synthesized by hydrothermal method, and the colloids containing BaFe\textsubscript{12}O\textsubscript{19} nanoparticles with a diameter of 60 nm were first prepared (Fig. 1). Magneto-optical effects in BaFe\textsubscript{12}O\textsubscript{19} colloids were studied. Magneto-optical response of an aqueous colloid containing 60 nm plates of barium hexaferrite was found to be by 2 orders higher than the one in cobalt ferrite colloid containing 6-10 nm isometric cobalt ferrite particles. The method for calculation of magneto-optical characteristics was developed. According to the method, the frequency dependence of magneto-optical effects is measured and experimental data are approximated by Debye function. Than characteristic frequency for a given colloid $f_0$ and characteristic size of the particles (or aggregates), responsible for optical anisotropy in a colloid when exposed to a magnetic field, were calculated using this method. In an aqueous BaFe\textsubscript{12}O\textsubscript{19} colloid, containing relatively big (60 nm) plates, a dichroism phenomenon was observed due to a change in light scattering on the particles subjected to magnetic field.

Fig.1 SEM image of barium hexaferrite particles.  
Fig.2. Small-angle X-ray scattering experimental curve of BaFe\textsubscript{12}O\textsubscript{19} nanoparticles (in powder).

Small-angle X-ray scattering experimental curve of BaOFe\textsubscript{12}O\textsubscript{18} nanoparticles is given in figure 2. The measurements were performed on the Rigaku SAXS instrument in function at the MPhTI Dolgoprudny.

**Keywords:** magneto-optical response, barium hexaferrite, hydrothermal synthesis, SAXS.

The reported study was partially supported by the Government of Perm Krai, research project No.C-26/791.

**S5 O11**

**LOW COST NANOSTRUCTURED CUO THIN FILMS DEPOSITED BY SUCCESSIVE IONIC LAYER ADSORPTION AND REACTION (SILAR) METHOD**

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The copper oxide CuO has attracted a lot of attention as a possible absorber materiel for solar cells due to its direct band gap and high absorption coefficient. copper oxide CuO thin films were prepared by the simple and economical successive ionic layer adsorption and reaction method on glass substrates using aqueous solution of hydrated copper chloride (CuCl\textsubscript{2}.2H\textsubscript{2}O) complexed with aqueous ammonia (NH\textsubscript{3}) (25-28%). The structural, morphological, chemical composition and optical properties of these films were investigated. Structural analysis revealed that all the deposited films were polycrystalline crystallize in pur CuO monoclinic structure. The pure phase of CuO was confirmed by X-ray photoelectron spectroscopy (XPS). SEM images show that we have dense homogenous and compact morphological surface of CuO thin films. The energy dispersive X-ray spectrum confirms the presence of Cu and O elements. Optical properties of the CuO thin films were studied by means of UV-Visible spectrometer.

**Keywords:** Copper oxide CuO, SILAR, Thin Films, Solar Cells.
S5 O12

OPTIMIZING THE MECHANICAL STRUCTURE OF THE INNER TRD MODULES FOR LOW MATERIAL BUDGET AND CONSTRUCTION PROCEDURES

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The Transition Radiation Detector (TRD) chambers installed close to the beam pipe at the Compressed Baryonic Matter (CBM) experiment @ FAIR has to operate at particle rates of up to $10^5$ Hz/cm$^2$. Such chambers require supporting structures of low material budget for minimizing the secondary particle production and in the same time, to be strong enough to withstand the mechanical tensions induced by wire plane electrodes without deformation. Mitigating the two requests is rather challenging and we present here ways to accomplish it by detailed static structural analysis of the full chamber design. Additionally, the simplification of the technological procedure for chamber construction, is carefully considered in our analysis.

Keywords: FAIR, mCBM, TRD

S5 O13

FATIGUE BEHAVIOUR AND MECHANICAL PROPERTIES OF AA6061/SiC/20p COMPOSITE AND AA6061-T6 DISSIMILAR JOINT FABRICATED BY FRICTION STIR WELDING

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Friction stir welding (FSW) is a relatively new solid-state welding technique that was developed in 1991 by The Welding Institute of United Kingdom (UK) especially for joining of high-strength aluminum alloys (Thomas et al., 1991). Afterwards, the technique has become a promising joining method for welding of dissimilar materials. In this research, dissimilar joint of AA6061+SiCp composite and 6061-T6 aluminum alloy is produced via FSW using an AISI 4140 steel tool with a shoulder of 20 mm diameter. Defect-free butt welded joint is obtained using a tool rotational speed of 1000 rpm, welding speed of 80 mm/min and a tilt angle of $1^\circ$. Within the study, effects of the FSW process on the mechanical and fatigue properties of the dissimilar FSWed joint are investigated.

Figure: Failure locations of the dissimilar welds after transverse tensile tests

Accordingly, transverse tensile and Vickers hardness tests are conducted to evaluate the tensile properties and hardness of the welds, respectively. Axial loading fatigue tests are also performed by using the dissimilar joint. Furthermore, fracture surfaces of the dissimilar welds are characterized by means of scanning electron microscope (SEM). The obtained results show that minimum hardness values are observed within the
heat affected zone (HAZ) in the base material (BM) at the monolithic alloy side. All tensile test specimens except one fractured on the retreating side (RS) in HAZ close to the BM. Figure demonstrates the fracture locations of the specimens. Failure elongation of the joint also decreases subsequent to the FSW process. The process produces a fatigue strength of 96 MPa that exhibits a joint efficiency of 79.8.

**Keywords**: friction stir welding, metal matrix composites, fatigue, mechanical properties.

**References**

**S5 O14**
COMPLEMENTARY USE X-RAY SCATTERING AND ELECTRON MICROSCOPY FOR STRUCTURAL BIOLOGY

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The main goal of structural biology is deciphering of macromolecular (protein and nucleic acids) structures to understand the mechanisms of their functioning. This is necessary both for solving the fundamental problems of biophysics and understanding the principles of biological systems at the molecular level, as well as the subsequent use of the results for drug discovery and for development of new methods in medicine and pharmacology.

Until now, the main method of obtaining such structures is X-ray scattering. So, X-ray protein diffraction (XRD) is used to obtain atomic resolution structures, and small angle scattering (SAXS) is used to obtain low-resolution structures. Despite its popularity, X-ray scattering methods have certain limitations (high-quality of crystals, the non-physiological conditions, the organization of the protein molecule in the crystal structure, etc.). Nowadays, macromolecular structures obtained by electron microscopy at cryo temperatures (Cryo-EM) is becoming increasingly popular. In contrast to XRD while using microscopy, we can get the protein structure in solution (in the native state) but with worse resolution. Often among the goals of structural biology there is a need to search a low-resolution structure in a solution. This is required to understand the functional state of the protein.

Often when searching for the structures of protein molecules, the use of all this methods is required. We will show that on concrete examples the possibilities that each of the methods and the results obtained by combining information obtained from these methods will be considered.

**Keywords**: electron microscopy, neutron and x-ray scattering, diffraction, structural biology.

**References**
Corrosion is usually defined as being the deterioration of materials (e.g. metals, plastics, wood, concrete) by chemical interaction with their environment [1]. The extracts from the parts of plants (e.g. petals, leaves, peels, seeds, fruits, roots) have been reported as effective corrosion inhibitors in different aggressive environments. Seaweeds are marine macro algae which are found in the shallow waters of sea, estuaries and backwaters [2].

The objective of this work was to investigate the corrosion inhibition effect of seaweed in natural seawater. The small coupons of mild carbon steel were used for corrosion tests. The coupons were polished, degreased, weighed and then suspended in glasses that contain small amount of natural seawater, with and without seaweed. After 14 days the coupons were taken out, washed, dried and weighed accurately. The tests were performed at room temperature. The inhibition effect of seaweed on the corrosion of mild carbon steel in seawater was studied by weight loss measurement. In order to evaluate the corrosion of mild carbon steel, corrosion rate and percentage corrosion inhibition efficiency were calculated.

The obtained results shown that the corrosion rate (calculated by weight loss measurement of mild carbon steel in natural seawater) decreases when the seaweed was used. Also, the value of percentage corrosion inhibition efficiency was more over 65%, when seaweed was used.

The seaweed reduces the corrosion rate and can be considered as an eco-friendly corrosion inhibitor for mild carbon steel in seawater.

**Keywords**: corrosion, natural seawater, seaweed

**Acknowledgements**: The work has been funded by the University Politehnica of Bucharest, through the “Excellence Research Grants” Program, UPB-GEX 2016, project no. 62/2016, supported by a grant of the Romanian Ministry of Research and Innovation, PCCDI-UEFISCDI, project no. PN-III-P1-1.2-PCCDI-2017-0428, within PNCDI III (no.40PCCDI/2018 PC4-FOTOMAH) and supported by a grant of the University Politehnica of Bucharest, GNaC 2018 ARUT, project no. CH37-18-01, Code 32.

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Scaling limitation for sensors have brought in attention the metasurfaces (MTS), interfaces with subwavelength thickness and regular spacing subwaveleght nanostructures, as a particular metamaterial (MTM) case. There is no single 2D material or semiconductor nanostructure that offers superior performance for all applications (e.g. plasmonic sensors or large area metalenses without aberrations) in a given bandwidth or wavelength range. On the other hand, the choices for multiple immunofluorescent stains are complicated by several limitations: Thus, the interchangeability of sensitive surfaces is needed, namely Interchangeable MTS (I-MTS). These I-MTS will be achieved by nanospheres lithography and characterized by Localized Surface Plasmon Resonance enhanced Angle-Resolved Evanescent-Wave Cavity Ring-Down Spectroscopy (LSPR-enhanced AREW-CRDS). The developed I-MTS will be evaluated in order to increase the sensitivity of the staining sensors used in the spectroscopical detection of antibodies (CFH) [1], proteins (GcMAF) [2], inhibitors for cachexia ((N2H5) HSO4) [3] in oncology therapy. The I-MTS staining sensor brings spatial resolution for optical measurements of probes placed in EW field of resonant spectroscopical system. Advantages of this system are: distributed and autonomous, multiple measurements, insertion-based probes, compact signal processing, streamlined, robust optical path.

Keywords: metasurfaces, staining, spectroscopy, sensor

Acknowledgements: 2019 Core Program-Materials, structures and methods with potential for applications in the fields of Bioeconomics and Health

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S5 P3
METASURFACES WITH AVAILABLE CHARACTERISTICS FOR POLARIZATION STATE ANALYZERS, SUPERLENSES OR ELECTRO-OPTICAL MODULATORS

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The metasurfaces (MTS) developed as optical interfaces in the National Institute for Materials Physics are described in the OSIM patent application [1]. Examples of MTS based on metallic coatings on semiconductor with atomic clean surfaces for middle or near-infrared are shown in Fig. 1. They are useful in polarization state analyzers (a serial combination of linear polarizers and quarter-wave retarders), superlenses for near-field or far-field imaging with subwavelength resolution, electro-optical modulators for difficult visibility conditions (twilight, smoke, fog, haze). The new plasmonic materials [2] are now developed on the basis of transparent conductive oxides, transition metal nitrides with optical losses (on free carriers and interband) lower than Au and Ag metals, with high mobility of carriers and nanoscale structure. Current technologies for MTS manufacturing include deposition of metallic or semimetallic coatings, nanoimprint or nanospheres lithographies. Other remarkable examples include wet chemical synthesis, evanescent wave lithography and data compression algorithm (METAsurface Compression) [3], which promise low-cost productivity, precise nanoscale structural control to achieve highly sophisticated structures. The development of these technologies aims at shortening the processing time for large surfaces and lowering the spatial resolution below 10 nm.

Fig.1 Metasurfaces developed as optical interfaces for near and middle-infrared

Keywords: metasurfaces, polarization analyzers, superlenses, optical modulators

Acknowledgements: UEFISCDI, Contract no. 75PCCDI/2018

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1. C. Cotirlan-Simioniuc, A. Rizea, C. Marin, a 2017 00167, OSIM patent request.
3. A. She et al., OPTICS EXPRESS 26(2) 1573 (2018).
Microbial fuel cells (MFCs) is a promising electrochemical device that can directly convert the chemical energy contained in organic matter into electrical energy by the catalytic activity of electroactive bacteria. The surface characteristic of anode materials is one of key factors affecting the bacterial attachment and extracellular electron transfer. Improving the properties of electrode materials could provide a breakthrough solution for the implementation of MFCs as a promising green power sources.

The modification of anode with carbon nanostructures containing hetero-atoms such as nitrogen could provide more active sites for interface electrochemical reactions and better biocompatibility. Carbonization of nitrogen-containing aromatic polymer nanomaterials such as polypyrrole nanostructures is a suitable alternative to prepare nitrogen-containing carbon nanostructures (NCNS), retaining the morphology of the polymer precursors.

In this study, the relationship between the morphology and the nature of nitrogen environment of carbonized polypyrrole, together with their performances as electrodes for MFCs, is investigated. NCNS were obtained from polypyrrole with granular (called PPY-g) and tubules-like (called PPY-t) morphologies. X-ray photoelectron spectroscopy and scanning electron microscopy were used to investigate the morphology and the nature of nitrogen environment in the obtained samples. The results were correlated with their performance as MFC anodes.

Keywords: polypyrrole, nitrogen-containing carbon nanostructures, microbial fuel cell

Acknowledgements: This work was financially supported by The Romanian National Authority for Scientific Research, UEFISCDI, Project No. 40PCCDI/2018.

S5 P5
K-LINE XRF ASSITED BY STANDARDS, MONTE CARLO AND FUNDAMENTAL PARAMETER CALIBRATION METHODS

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The X-ray fluorescence method is widespread and highly applicable as non-destructive method for composition and thickness determination in research and industry. Here we present an enhancement of the XRF method specially developed to quantitatively analyze functional tungsten coatings of plasma facing components exposed to tokamak plasma. One particular application that was solved by K-line XRF is erosion of W coatings thicker than the W L-line equivalent saturation thickness of ~ 5 µm.

The experimental method uses a high energy X-ray source for W K-line excitation and a high energy CdTe X-ray spectrometer. For single layer coatings the most straightforward calibration procedure consists in the determination of calibration curve based on standard samples that converts the signal intensity in calibrated units. The empirical procedure becomes slightly unstable for calibrations measurements of multilayer samples. Thus, Monte Carlo transport simulations and Fundamental Parameter methods were applied in order to assist the empirical protocol, to overcome the need of a high number of quality standards and to improve the measurements accuracy for multilayer samples. The Monte Carlo procedure is a fully statistical approach in which one counts the photons interacting in the detector active area while considering numerous parameters such as incident excitation beam, scattering-absorption effects and sample configuration.

The Fundamental Parameter method is a common approach that is relying on reference samples in order to mitigate the unpredicted distortions caused from the matrix effects. We applied the specific MTF-FP module developed by CrossRoads Scientific that is dedicated for multilayer coatings. To our knowledge this was the first time when the MTF-FP module was applied for W K-line thickness determination.

In this paper we report the thickness profiles of W/Mo reference coatings and the absolute erosion map of W coated C base substrate. The application of the employed calibration procedures is presented in detail.
Keywords: X-ray fluorescence (XRF), Fundamental Parameter, Monte Carlo transport, erosion resistant coatings

S5 P6

TOMOGRAPHY SOFTWARE DEVELOPED IN LABVIEW FOR IN-HOUSE BUILT MICRO-CT FACILITY

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Building a customized X-ray micro computed tomography (micro-CT) facility involved considerable efforts from a combined team of engineers and physicists in order to integrate both hardware and software components. In our laboratory, the micro-CT facility was designed for maximum versatility for advanced applications of research and industry. This involved a constant upgrade and update of the relevant software developed in the LabVIEW environment. In order to build reliable software for an optimized use of the complex facility, multiple adjustable input and monitorization parameters were integrated in a user-friendly interface.

This work presents in-depth the LabVIEW developed software. The digital radiography software is used for real-time sample overview and the tomography software is used for system control and data acquisition. This implies taking multiple images of the sample at different angles in order to obtain its 3D reconstruction. Prior to each micro-CT measurement, the radiography software is used in order to obtain a gray level histogram based on which several optimizations can be performed such as: defining the X-ray source operation regime, choosing the maximum beam energy and current, adjusting the detector gain and integration time and using an appropriate x-ray filter for obtaining an optimal signal to noise ratio. The tomography acquisition software integrates the optimized parameters resulted from the radiography software. Additionally, a real-time source voltage feedback module was integrated in the tomography software in order to pause and re-start the acquisition process if the source intensity drops below a certain threshold.

Several examples of fully 3D scan tomography reconstructions are presented in correlation with the optimizations based on the custom-built software. Illustration of the application of our micro-CT facility and with special purpose LabView developed software in coordinates measurement (metrology) investigations are presented.

Keywords: micro-CT, LabVIEW, digital radiography, tomography, metrology

S5 P7

AQUACULTURE WASTEWATER TREATMENT USING ANTI-BIOTIC RESISTANT BACTERIA

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The using of biochemical processes involving different microbial species in wastewater treatment is an actual domain of research due to its practical applicability.

This research is focused on the assessment of some microbial biofilters treatment efficiency in aquaculture, placed in various growth media (specific medium and synthetic water) by using different optical (UV-Vis spectroscopy) and gravimetric techniques. These media were inoculated with two types of bacteria...
(P. aeruginosa, C. violaceum) which are involved in the biotreatment processes by consuming the nitrate and phosphorus based nutrients. The effect of different oxytetracycline concentrations on the biofilm formation and on the efficiency of the biofilters was also assessed.

The tested biofilters presented higher efficiency by decreasing the concentration of nitrite, nitrate and phosphorus ions, proving practical applicability in wastewater treatment (Table 1). On the other side, the experimental results shown lower efficiency of the P. aeruginosa and C. violaceum bacterial strains in removal of the ammoniacal nitrogen.

### Table 1 – Efficiency of various biofilter – bacteria strain systems in wastewater treatment

<table>
<thead>
<tr>
<th>Biofilters</th>
<th>NO₃⁻ (µg/mL)</th>
<th>NO₂⁻ (µg/mL)</th>
<th>PO₄³⁻ (µg/mL)</th>
<th>NH₄⁺ (mM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial amount: 162.76</td>
<td>Initial amount: 0.647</td>
<td>Initial amount: 4.69</td>
<td>Initial amount: 0.999</td>
<td></td>
</tr>
<tr>
<td>Pa*</td>
<td>C_v*</td>
<td>Pa</td>
<td>C_v</td>
<td>Pa</td>
</tr>
<tr>
<td>F1</td>
<td>90.40</td>
<td>103.60</td>
<td>0.080</td>
<td>0.011</td>
</tr>
<tr>
<td>F2</td>
<td>153.60</td>
<td>104</td>
<td>0.100</td>
<td>0.152</td>
</tr>
<tr>
<td>F3</td>
<td>96.80</td>
<td>97.60</td>
<td>0.104</td>
<td>0.111</td>
</tr>
<tr>
<td>F4</td>
<td>98</td>
<td>97.20</td>
<td>0.094</td>
<td>0.627</td>
</tr>
<tr>
<td>F5</td>
<td>98</td>
<td>97.20</td>
<td>0.031</td>
<td>0.136</td>
</tr>
<tr>
<td>F6</td>
<td>94.80</td>
<td>96.40</td>
<td>0.108</td>
<td>0.106</td>
</tr>
</tbody>
</table>

* Pa – Pseudomonas aeruginosa; C_v – Chromobacterium violaceum

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**S5 P8**

THE EFFECT OF USING FERTILIZERS ON APPLE AND PLUM ORCHARDS

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Metal toxicity in plants is still a global problem for the environment, agriculture and ultimately human health. The aim of this work was to evaluate the elemental profile of various samples from apple and plum orchard – located in Dambovita and Arges Counties - (sampled from soil, bark, leaves and fruits) and to characterize the influence on elemental profiles of different types of fertilizers used commonly in orchards. For this purpose, the effect of fertilizer/pesticide couples was studied by characterization of treated and untreated soil composition (parameters: by elemental composition, organic/inorganic ratio), metal content in fruits related to UE requirements for daily intakes. Heavy metals was used as tracers for fertilizers concentration monitoring, aiming to get information about their overall concentration eventually, critical accumulation into some part of the plant (which shall not exceed the limits regulated by Romanian law and UE directives for fertilizers use in fruit-grower). The most popular used fertilizer in fruit growth Dambovita County is manure, a natural complex material rich in nitrogen and phosphorus assimilable compounds and main microelements. Commonly, the pesticides used by local orchardists consist in different formulations based on copper sulfate containing formulations which are efficient in the annihilation of pests in fruit crops.
The obtained results was useful for better understanding of pesticides and fertilizers circuit in micro-environment crops and for improving methods to analyze and interpret data on crop products.

Keywords: fertilizers, heavy metal, orchards

S5 P9
IN THE SEARCH OF CEMENT MATERIALS FOR STORAGE OF RADIOACTIVE ALUMINIUM BY NEUTRON RADIOGRAPHY AND TOMOGRAPHY

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Nowadays, the question of storage of radioactive wastes is actual. For this purpose special storages are created which require constant monitoring of wear of structures. New cement grades are being searched to prolong the life of such storages. Special attention is paid to corrosion resistance of reinforcing materials of concrete structures under different environment conditions, as well as their micro-pore structure, which is formed at the early stage of cement hardening. The purpose is to find a suitable cement material for storage of radioactive aluminum, which when interacting with the cement paste has not formed cracks and pores.

To determine the structural characteristics of cement materials and concrete, experimental methods of neutron scattering are used, aimed at obtaining detailed data on phase analysis or peculiarities of the crystalline structure, education nanoparticles and grains inside the matrix, aging, cracks and pore evolution. The received structural information allows to understand the nature and origin of mechanical and chemical properties of cement, predicting functional properties, presenting ways of optimization of composite composition of new cement materials.

The paper presents the results of the research by methods of neutron radiography and diffraction kinetics of hardening and solidification of cement of the brand "CEM V" and "CEM V" with the addition of graphite, and the method of neutron tomography investigated hardened cement Materials "CEM V" with the addition of graphite, which is used for storage of radioactive waste. The Main task was to identify the factors influencing the formation of cracks and pores inside concrete samples.

The Experiments on neutron radiography and tomography were carried out on the installation of the NRT, on the neutron diffraction on the diffractometers of the DN-12 at the high-flux impulse reactor IBR-2. Formation of cracks on a place of contact of an aluminium container and cement paste was found out. The dependence of the coefficient of weakening of the neutron beam of cement paste over time is constructed. Anomalies of the neutron beam weakening behavior associated with the beginning of gas and water vapor release during hardening of cement paste were revealed. With the help of neutron tomography define distribution of graphite and cement and hydrogen containing area.

S5 P10
STUDY OF THE PHYSICAL PROPERTIES CHANGES AND THE MEMORY TEST OF THE MAGNETIZED WATER IN EXTREMELY LOW FREQUENCY MAGNETIC FIELD

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Water is an indispensable material present in nature and is used in most of the human activities. Water molecule being a diamagnetic one, it can be affected by the magnetic field presence. Many of research studies have focused on the static magnetic field influence on the water properties and leading to contradictory research results. So far, a small number of research studies have been focused on extremely low frequency magnetic field impact on water properties. The aim of this research study was to evaluate the impact of extremely low frequency (50 Hz) magnetic field on water properties after 300 minutes continuously exposure time for different values of magnetic flux density (1-3-5-7 mT) and to test the “memory” of the magnetized water. For magnetically exposure of water, a laboratory Helmholtz coil system was used. It was generated a uniform magnetic field on the vertical direction. Glass containers with distilled water have been placed in the center of the coils system. For water evaporation prevention during the exposure, closed containers were used. The density, surface tension, viscosity, pH, dissolved oxygen rate and electrical conductivity of the exposed water samples compared with the control one have been measured immediately after exposure. The changes of the water properties, observed after exposure to magnetic field depend on the magnetic flux density. Also, the objective of study was to notice the effect of the passed time since the magnetically treatment on the properties of the magnetized water. So, the properties values were measured at different periods of time passed since the exposure of the water samples. For the analyzed characteristics, a tendency to return to the initial values (for non-exposed water) was observed with the increase of the passed time since the magnetically exposure.

**Keywords:** “memory” of water, extremely low frequency, magnetic field, water properties.

**SS P11**

ENGINEERING OF THE ACHIEVING ON A NEW LABORATORY LINE OF POLYMER FILAMENTS THAT COMPLY WITH 3D / 4D PRINT REQUIREMENTS

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The purpose of the paper is to study the influence of the operating conditions characterizing a laboratory calibration – cooling/rolling line – of own conception and execution, on the diameter, ovality and other defects of the filaments obtained from a customized renewable material.

Figure 1. Ovality, diameter tolerance and 3D printed items achieved with filament shaped from renewable material on the new laboratory line
This study was necessary to determine the line points which need to be improved so the fabricated filaments to be compatible with 3D/4D printing and to not breakdown the printer. The diameter and ovality of the filament were precisely measured by scanning electron microscopy. The obtained results showed that filaments with good ovality, diameter tolerance and corresponding 3D printing behaviour, on the studied line, can be obtained. The laboratory line will be upgraded to increase its performance, mainly for improving the cooling phase and for online measuring of diameter and ovality of obtained filaments.

**Keywords**: 3D printing, filaments, ovality, diameter tolerance

**Acknowledgements**: This work has been funded by the Ministry of Research and Innovation through project no. 40/2018–5/3D-LONG LIFE.

**SS P12**

**DYNAMIC LIGHT SCATTERING FOR SIZING PARTICLES SUSPENDED IN AIR – IS IT POSSIBLE?**

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Small particles, like nanoparticles, undergo a Brownian motion, as the result of the random collisions with the molecules of the fluid they are immersed into. The gravitational and buoyant forces are exerted upon them, as well, causing sedimentation. If the particles are small enough, the resultant of the last mentioned forces is insignificant and the particles remain in suspension.

If a light beam meets a fluid that contains scattering centers (SCs) randomly distributed in suspension, light is scattered. If the incident light is coherent, the scattered waves are coherent as well, therefore they interfere. A detector and a data acquisition system can be used to record the far field interference signal producing a time series that can be later on analyzed to produce the average diameter of the suspended particles or the size distribution and the technique is called Dynamic Light Scattering (DLS).

Typically the fluid is a liquid solvent, the scattering angle is 90° and a photomultiplier is used to produce an electric signal proportional to the scattered light intensity. The extended work presents the results of our investigation on the possibility of using low-cost conventional electronics for recording the time signal of light scattered by particles suspended in air, and software written for this purpose. Moreover, we aimed to use the DLS technique for sizing particles in the air as a carrier fluid. The figure below illustrates the theoretically expected shape of the Lorentzian line, that describes the power spectrum of the DLS time series (computed with the fast Fourier transform algorithm), as a function of the frequency, at a scattering angle of 5°, for particles with the diameters (in nm): 10, 176.7, 343.3, 510, 676.7, 843.3, 1010, 1176.7, 1343.3 and 1510.

Examining the figure we can conclude that DLS is possible on particles suspended in air, but using a small scattering angle, of 5° or lower, with a low-frequency data acquisition rate, of 40 kHz, as the turnover point for the power spectrum line of the 1510 nm particles is around 1000 Hz. This makes the least square...
fitting possible. There does remain the experimental condition of having a reasonably good signal to ratio rate that is mandatory for an acceptable precision of the results, not covered in this work.

**Keywords:** Dynamic Light Scattering, Nanoparticle sizing, Fourier transform

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**S5 P13**

**VERSATILE APPLICATION OF APATITIC MATERIALS FOR ENVIRONMENTAL PROTECTION**

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Removal of various inorganic and organic pollutants represents a very important area of research worldwide. Our group presented the synthesis and characterization of different apatitic materials (using X-ray diffraction, X-ray fluorescence, electron microscopy, thermal analysis, FTIR spectroscopy, specific surface area and porosity analysis, etc.), as well as their application for the removal of both inorganic pollutants (such as heavy metals) and the organic pollutants from aqueous solutions, thus offering an economic, easy to apply and easily to scale-up method for the treatment of polluted water using the proposed adsorbent. The substitution of calcium with other metals (barium, strontium, cobalt, iron, copper, silver, and others) led to differences in absorbance capacity, thus underlying the very different properties of the obtained materials.

![Figure 1. TEM image of hydroxyapatite](image)

**Keywords:** apatitic materials, organic pollutants, inorganic pollutants.

**Acknowledgements:** This work was supported through INCDCP-ICECHIM Bucharest 2019-2022 Core Program PN. 19.23 - Chem-Ergent, Project No.19.23.03.01 and by PFE-CDI Program, Contract No. 31PFE/2018 - TRANS - CHEM.

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**S5 P14**

**CHARACTERIZATION OF HISTORICAL CERAMICS: A CASE STUDY**

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The study presents the archaeometrical characterization of ceramic artifacts with a high historical value. The artifacts were collected from A1_1 Sagu site (Arad county), being date to approx. 1600-1250 BC (Figure 1), belonging to an unfortified Late Bronze Age (LBA) settlement. Due to the impressive amount of ceramic material found and the large area the settlement covered, the mentioned site represents a LBA landmark of in the region.

The artifacts were analyzed using X-ray diffraction, X-ray fluorescence, thermal analysis and FTIR spectroscopy and the analytical results obtained, together with the available hystoric information, allowed not only the establishment of their composition, but also offered valuable insights into the Late Bronze Age habits and technologies.

**Keywords**: ceramic materials; firing temperature, archaeometrical characterization.

**Acknowledgements**: This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0413, within PNCDI III.

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**S5 P15**

**SEISMIC SOURCES FROM WEST AND NORTH-WESTERN PART OF THE ROMANIAN TERRITORY**

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This study approaches the crustal seismicity of the west and north-western part of the Romanian territory to highlight the seismic sources, their geometry, distribution of epicentral and hypocentral distances relative to main populated cities, monitoring of seismic activity in order to assess future seismic hazard in the urban areas. Crustal seismicity, on the Romanian territory is located at the hypocentral depths up to 60 km, depending on the area, for our investigation area up to 40 km.

The Carpathian arch consists of a basement and sedimentary cover knaps, thrusted and overthrusted, formed during compressional period, during the Cretaceous and Pleistocene period. Contact between these units seems to be seismogenetic. Besides subcrustal and crustal seismicity located in Vrancea area, Romania hosts also crustal seismicity in the Apuseni Mountains, Crisana, Satu Mare, Oradea, Arad and Baia Mare.

Observed crustal seismicity has not exceeded Mw = 5.6 in Crisana (from historical data). In rest of the country reported data were generally limited to Mw = 6.
In the north part of the country, in Oradea area is known the Mw = 4.1 earthquake in 1886 and Mw = 4.2 in 1906 at the intersection of two fault systems. One with a NE to SW direction and the other with SE to NW direction.

Other epicentral areas from NW part of Romania are: Sighet Marmatiei-Ukraiina, Baia Mare, Jibou and Valea lui Mihai-Carei.

In the Apuseni Mts. The crustal seismicity not exceed 5.3 (Mw) in the eastern part of Alba Iulia city. Tectonic regime is an extensive stresses regime (normal fault with a component of strike slip) very well correlated with firsts order stresses in region induced by Adria pushing.

**Keywords**: seismic sources, magnitude, faults system, epicentral area

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**ACTIVE FAULTS FROM THE WESTERN PART OF SOUTHERN CARPATHIANS (ROMANIA).**

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This study approaches the crustal seismicity of the active faults from the Southern part of Southern Carpathians (Romania) belonging to the Dacia tectonic unit. To describe the active faults we use the Database of Individual Seismogenic Source Methodology.

The area of interest consist of Hateg-Strei Basin and Danubian Domain with the Median Dacides, Marginal Dacides and External Dacides as main tectonic units. Hateg-Strei Basina is characterized by a ruptural teconic with NW-SE to W-E orientations. Danubian Domain is segmented by a NE-SW to E-W oriented faults and represent Carpathian fault system [Oros et al., 2018]. These are mainly thrusts which delineate WNW verging nappes inside Median and Marginal Dacides (such as Sichevita-Rezeat thrust) or vertical fault such as Oravita-Moldova Noua Fault system, Cerna-Jiu fault system. Ignous rocks are distributed through basement formations being a associated with deep fault system in the Alpine time.

Active faults can be described using different parameters, as:

- Geometrical parameters: length, active length, width and depth of the earthquakes foci.
- Seismological parameters: strike, dip, rake (slip);

Distinguished three main categories of Seismogenic Sources: Individual Seismogenic Sources, Seismogenic areas and Macroseismic sources. Our study is providing geometrical and seismological parameters for the active faults, using only the first and second category of seismogenic sources.

In the studied area, we highlight the main faults form Hateg Basin, Moldova Noua-Oravita Basin, Caransabes-Orsova basin(Teregova) and Orsova-Mehadia-Corneva faults systems.

We present the fault systems, which generate seismic sequences such as: 2002 Moldova Noua, 1991 Mehadia-Baile Herculane, 2014 Teregova, 2011 and 2013 Hateg seismic sequences.

**Keywords**: seismic sources, Danubian Domain, faults system, Hateg-Strei Basin

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THE STUDIES OF THE ROMANIAN ANCIENT CERAMICS USING THE NEUTRON TOMOGRAPHY METHOD

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One of the most important tasks of archeology and other human sciences are comprehensive studies of the cultural heritage items. They give us a chance to allow understanding of the formation of ancestors' lives and civilization development. The special value and uniqueness of such items require the use of advanced non-destructive methods for their studies. One of the non-destructive methods in neutron radiography and tomography. This method is a powerful tool of non-destructive analysis, which plays an important part in industrial and scientific research. The fundamental difference in the nature of neutron interaction with matter compared to X-rays provides additional benefits to neutron methods, including sensitivity to light elements, a notable difference in contrast between neighboring elements and high penetration ability.

On the one hand, fragments of ancient ceramics and pottery items store valuable information about the trade, economic and social development of ancient civilizations and states, and on the other hand, potter items are convenient model objects for the study of degradations and cracking processes occurring in other clay products.

In our work, the ancient ceramics from Romanian archaeological excavations and museums are presented. The studied ceramic objects consist from the clays and often mixed with as-called "tempers", which may be organic materials, sand, ceramic powder, shells or other types of clays. The inner structure, cracks and admixed components spatial distribution of ancient ceramics fragments were the aims of our neutron radiography studies. A difference in the total absorption cross-sections of neutrons for the different elements allows visualizing the distributions of composition or structural heterogeneities in the studied materials, obtaining a three-dimensional model with a spatial resolution of a portion of a millimeter. These studies were prepared at the neutron radiography and tomography facility on the 14th beamline of the IBR-2 high-flux pulsed reactor (Dubna, Russia). The neutron radiography images of investigated objects collected by the detector system based on 6LiF/ZnS scintillator screen with a high-sensitivity camera based on CCD chip.

A 3D analysis of the interior of the ancient ceramics fragments was performed using neutron tomography. Good contrast in the neutron attenuation coefficients between different components allowed us to clarify several structural features of the studied cultural heritage items. The morphological calculations based on the experimental tomography data were used to analyze the spatial arrangement of basic components of the studied ceramics. The characteristics obtained for the internal structure of studied pottery remains are important for improving our concepts of Ancient Roman Empire evolution.

Keywords: neutron tomography, ceramics.
seismicity does not exceed the magnitude of 5.4 (Mw) and it seems to have no relation to the seismic activity of the subduction lithosphere. Seismic activity is characterized by spatial and temporal clustering in the Rămnicu Sarat area through seismic sequences and through seismic swarms in the Vrâncioaia area.

The purpose of this work consists in analyses of ETAS parameters for the sequence recorded on November 22 2014 in Vrancea Area.

The moderate-size earthquake with maximum local magnitude 5.7 which occurred on November 22, 2014 in Vrancea region, at 41 km depth, is the largest crustal event instrumentally recorded at the bending of the Eastern Carpathians.

The Epidemic-Type Aftershock Sequence (ETAS) model is one of the most widely used statistical models to describe the temporal (and later on spatial) clustering of seismicity. [1], [2].

While other models to describe seismicity have been proposed over the years [3], [4].

As its name suggests, ETAS was designed to describe aftershocks, in particular by expressing their rate as a function of time (temporal model) or as a function of time and space (spatiotemporal model). ETAS reflect the fundamental observation that aftershocks tend to cluster near and after a main shock. The model consists of two parts: (1) background events, which occur independently but are often interpreted as being caused by the same underlying process (e.g., tectonic loading due to plate movement) and (2) aftershocks, which are triggered by other earthquakes, either background events or previous aftershocks.

This crustal seismicity is related to the normal fault system associated to Peceneaga - Camena major fault, which separates the Focsani Basin, part of the Moesian Platform, from the North Dobrogea promontory.

**Keywords**: ETAS, seismic sequence, Vrancea area, crustal earthquakes

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**References**


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**S5 P19**

**SPATIAL AND TEMPORAL VARIATION OF SEISMIC b VALUE BENEATH RM. SARAT SEISMOGENIC AREA**

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In this paper, we have studied the seismic activity in relation with geology, and tectonics in order to highlight seismogenic processes recorded in Rm. Sarat crustal area.

Seismic activity is characterized by groups in space and time, in the area of Rămnicu Sarat by seismic sequences and seismic swarms in the Vrâncioaia area. The main shocks of the seismic sequences are often accompanied by clusters of earthquakes or foreshocks.

The seismic sequences recorded in the Rămnicu Sarat area are characterized by the systematic orientation of the strike direction parallel to the orientation of the Carpathian chain. The preferential orientation of the rupture propagation tends to extend along the NE-SV direction, thus perpendicular to the Peceneaga-Camena fault line, which crosses this seismically active area to the north. It should be noted that in all cases, the epicenter of the main shock is located in the southwest end of the after shocks distribution except for the 2005 swarm, suggesting a mechanism in the outbreak with unilateral rupture to NE.
Seismicity is usually described by the empirical relation between the frequencies and magnitudes proposed by Gutenberg–Richter (1954) [1] with coefficients b-value. The space distribution of b-value depends on the stress regime, the tectonic character of the region, the heterogeneities and the temperature (Scholtz et al 2015) [2]. Low b-values have been correlated with areas of asperity, locked part of a fault where the nucleation of earthquakes is likely to happen (Schorlemmer et al., 2004).[3] Large heterogeneities correspond to higher b-values (Mogi, 1962).[4]

Determination of spatial and temporal variations of the b-value is thought to reflect the stress conditions in the crust.

The Vrancea zone is an area of concentrated seismicity at intermediate depths (60-200 km) beneath the bending area of the South-Eastern Carpathians in Romania.

Seismic activity is characterized by spatial and temporal clustering in the Râmnicu Sărat sub-areas through seismic swarms in the Vrâncioaia area.

**Acknowledgments:** This paper was carried out within Nucleu Program MULTIRISC, supported by MCI Project PN19080101

**Keywords:** b value, seismic sequence, Rm. Sarat area, Vrancea area, crustal earthquakes

**References**


**S5 P20**

**FAST-BASED ROUTE TO PRODUCE IMPROVED DEMO DIVERTOR MONOBLOKS**

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A powder metallurgy route based on FAST (field assisted sintering technique) was developed to produce DEMO divertor monoblocks with different materials. The plasma facing part of the W armor is processed from K-doped W foils joined to the suited dimensions by FAST. This 5 mm thick part is then joined to the main W-composite monoblock produced from a mixture of W and nanometric carbides powders. A functionally graded Cu-based thermal barrier material is embedded in the monoblock using the “cake slice” method developed by our group [1]. The joints’ quality in the finite components are investigated by high resolution FE-SEM.

**Keywords:** powder metallurgy, refractory materials, thermal barriers, FAST joining

**Acknowledgement** This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grand agreement No 633053, WP-MAT. The views and opinions expressed herein do not necessarily reflect those of European Commission.

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S5 P21
MICRO-GANTRY - A VERSATILE MOBILE COMPACT GANTRY TOMOGRAPH
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A mobile in-house built modular X-ray system used primarily as a gantry cone-beam tomograph for biology (small animals, plant roots, seeds etc.) and process tomography applications (manufacturing, environmental research).

It features two modules, a gantry frame for performing gantry tomography and an second frame that can accommodate the equipment for performing regular cone-beam micro-tomography (3D-CT) and X ray microbeam-fluorescence (µXRF). The modules can be used one at a time. This multifunctional X-ray system can be used for noninvasive 3-D morphology and composition mapping.

The X-ray sources are of sealed microfocus type with maximum high voltage of 60 kV, maximum power of 50 W and different anode materials (W, Mo or Ag). X ray detection is achieved using a compact high resolution flat pannel (1944 x 1536 pixels, 75 μm pixel size) for tomography and a miniaturized X-ray spectrometer for XRF experiments. A micrometric rotation stage is used for spinning the gantry frame and four micrometric motorized stages aid in sample positioning when using the cone-beam & µXRF module.

Customized software was developed using LabView for axis manipulation, data acquisition and control. 3-D tomographic reconstructions are obtained by a proprietary highly optimized computer code based on a modified Feldkamp algorithm.

Gantry tomography is used for samples than cannot be moved and need to lie on a sample bed rather than stand in a sample holder. It is the case of small animals, germinating seeds or samples that undergo different processes that can be analysed in situ.

For the inspection of miniaturised samples the microtomography analysis is guaranteed for feature recognition down to a few tens of microns. The fluorescence component can provide local qualitative and quantitative information about the sample composition elements. Using the X-Y linear stages, the µXRF system provides high resolution (~20 μm) composition mapping and accurate thickness measurements of multilayer samples.

The presentation is illustrated with applications on both gantry and cone-beam & µXRF modules.

Keywords: mobile compact gantry tomograph, process tomography.

S5 P22
DEVELOPMENT OF SILOXANE COATING WITH OXIDE FILLERS FOR KESTERITIC (CZTS) PHOTOVOLTAIC SYSTEMS
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The photovoltaic system (PV) based on CZTS solar cell demonstrate its efficiency and higher rate. According to the results of the comparative studies, the kesterite structure showed to be ecologically safe and less expensive than other photovoltaic (PV) systems. Research and development in the field of CZTS based PV technologies are extremely relevant now.

Above mentioned results claim for further development of CZTS based PV. One of the most important problems of the CZTS based PV devices creation is obtaining of a high-temperature transparent electrically insulating coating on the metal substrates. It’s was the purpose of this work.
Thin, optically transparent coating substance was created by centrifuging a suspension of polysiloxane varnish with industrial thermal conductive oxide mixture fillers. It was shown the resistance of the resulting coating to short-term high temperatures exposure required for the synthesis of kesterite.

Physicomechanical properties of the surface layers of the coating were investigated by complex of special methods such as surface profilometry, microscopy, Differential Scanning Calorimetry [1].

It was assumed that using of the optically transparent dielectric polysiloxane-based coating should provide an increase in efficiency due to the recovery of the energy of the light flux transmitted through the kesterite layer and reflected from the substrate.

**Keywords**: high-temperature coatings, kesterite photoelectric converters.

**References**


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**S5 P23**

**CHITOSAN AND ALGINATE – PERSPECTIVE POLYMERIC BINDING FOR FUNCTIONAL ENVIRONMENTS OF THE ECOLOGICALLY SAFE BUILDING TECHNOLOGIES**

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In the medium term introduction new environmentally friendly construction technologies with a high share of an active component of energy efficiency is planned [1]. Coming to the forefront new materials and technologies, in particular, technologies of adsorptive conditioning, electro-and heat generation. At the moment in Europe are actively conducted developments of new materials within Horizon program-2020 (project H2020/MSCA/RISE/HUNTER/691010, JINR - Romania Cooperation Programme Project of of 2016-2018), etc. The problem of searching ecologically safe polymeric binding, providing the required mechanical properties and adsorptive capacity of functional building constructions is relevant – adsorptive panels.

Chitosan and alginate polymers have a natural origin, so, they are bio-compatible and are ecologically pure. Thanks to a complex of unique physical and chemical properties, including ecologic safety, bio-compatibility, hydrophily, polarity of molecules, polymeric composites on the basis of chitosan and alginic acids have big prospects for application as a polymeric binding and independent functional element in new technologies of adsorptive conditioning of rooms, in adsorptive power, a bionanoelectronics and a nanopowder sensors. The research of these polymers in aspect of application in perspective construction technologies was the purpose of this work.

With use of a complex of local and integrated research techniques scientific research of their applicability as hydrophilic binding in adsorptive warm and electric generators on a basis the nanostrukurivannykh of porous solid YSZ solutions – systems and CaSiO₃ is conducted. On the example of experimental laboratory models the high functional efficiency of data polymeric binding as a part of warm- and the electro-generating devices is shown.
Keywords: adsorption phase transition in nanopowder systems, size effect of structural stabilization, powder nanotechnologies, zirconium oxide nanoparticles.

The work was supported through the project H2020/MSCA/RISE/HUNTER/691010 and JINR-Romania Cooperation Programme Project of 2019.

References

**S5 P24**

**AN EXPERIMENTAL DEVICE FOR WATER PURIFICATION BY MEANS OF POWDERED MATERIALS**

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Nanostructured materials are a promising selective adsorption solution for water decontamination. An experimental device for immobilized powders efficacy in wastewater cleaning by means of selective adsorbent powders is presented herein [1]. The device is meant to provide both filtration and selective absorption functions while efficiently separating the two functions. Hence the device ensures an efficient pre-filtration of the polluted water (by means of a Millipore Mella-GP Hydrophilic PES membrane filter with 0.22µm average pore size) before it reaches the powder material which is meant to absorb the aimed chemical compounds dissolved in water. Since nanomaterials have very high surface to volume ratio, and often these are obtained in the forms of nanoparticles, a second membrane filter is provided at the output of the central capsule containing the powder adsorbent material (Fig.1). By means of an external glass cylindrical sleeve provided with input/output water connectors, the central capsule containing the adsorbent material can be flooded with water having a controlled temperature, in order to assess the powder adsorbent properties at different temperatures comprised between 1 – 80°C.

Fig.1 The device developed for powder wastewater decontamination efficiency assessment: a. axial cross section view and b. schematic representation of the central capsule containing the powder. Numbers refer to: 1- membrane filters, 2- annular gaskets, 3- cylindrical external glass sleeve provided with 4- liquid connectors.

Because of the two membrane filters and because of the closely packed powder comprised between circular retention membrane and meshes, the testing operations of the device required a relatively high input wastewater pressure (>3 atm), while allowing a relatively low liquid flux (less than a few milliliters/ min) passing through it, but it has ensured retention even of a few nanometers sized nanoparticles.

Keywords: filtration, nanoparticles wastewater purification

Acknowledgments. The presented work has been carried out through the Core- Program, developed with the support of the National Innovation and Research Ministry (MCI), project no. PN19 35 02 03.

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A MULTICHANNEL DATA ACQUISITION SYSTEM FOR ACTIVE SENSORS

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An industrial compliant (with +/-15 V tolerant signal input) multichannel signal acquisition system (DAS) is presented herein. The DAS is aimed for low-frequency multichannel data acquisition, when the input signals are provided by active sensors connected in half-bridge measurement configuration. Active sensors are element circuits that require biasing (by means of a series resistor or by means of a current source) in order to provide a signal dependent on the measured parameter (measurand). In order to best cover the dynamic band of the analog-to-digital converter (ADC) employed for data acquisition, a signal conditioning block is inserted into the signal chain. The proposed DAS (Fig. 1) is composed of a high voltage multiplexer, a signal conditioning subsystem, provided with digital control and an ADC embedded into the microcontroller of an Arduino board.

For the purpose of best framing the aimed values of the measurand and in order to compensate for the influence of the biasing network over measured signal, the signal conditioning subsystem is provided with a digitally controlled offset compensation block, provided with a preset Gain Coefficient (GC) followed by a flexible digitally adjustable signal conditioning block that allows both GC and fine offset adjustment [2]. An output RC first order low pass filter followed by a buffer stage is employed in order to deliver the proper signal for the ADC. The microcontroller provides the required sequence for input signal multiplexing, signal conditioning block parameters setting, data acquisition and transmission. Acquired data is sent to a PC where a LabView program receives, graphically represents and stores the data.

The time required for a channel complete settling, acquisition and specific communication is about 0.1s, therefore 1.6s are necessary for an acquisition sequence for all input channels. The proposed DAS can be employed for multisensor signal acquisition with multiple identical sensors, for example analog temperature sensors employed for a given geometry temperature distribution measurement and monitoring.

**Keywords:** signal acquisition, multisensor system, signal conditioning

**Acknowledgments.** The presented work has been carried out through the Core-Program, developed with the support of the National Innovation and Research Ministry (MCI), project no. PN19 35 01 01.

**References**

CHARACTERIZATION OF SUSPENDED FINE PARTICULATE MATTER IN INDOOR OF REHABILITATED CULTURAL HERITAGE

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The indoor environment in rehabilitated cultural heritage is influenced by several factors, whereas the main influence arises from the environmental conditions (e.g. humidity, temperature, light), gaseous and particulate matter (PM) pollution, and microorganisms, as well. Particulate matter is a potential threat to original structure material of rehabilitated monuments due to soiling and chemical reactions from harmful compounds inside the particles or on the surface between the particle and the deposited surface. The chemical composition of particles is an important factor which affects the preservation of structural materials inside of historical monuments. This research is a first step of an ambitious project, based on a complex acquisition of microclimatic data during a long-term monitoring (i.e. on three complete seasons). The investigations and obtained results are representative for old historical monuments of Romania, rehabilitated without preliminary scientific studies on building materials and climatic changes. Inside of the historical monument, the organic compounds and soot in PM, deteriorated the surface of old ruins, behave a very attractive medium for SO2 capture (this was observed by soiling the structure surface). The ICP-MS analysis was highlighted a rich particles content in iron (6.06-7.25 ng/m3 inside and 75.90-107.80 ng/m3 outside) and manganese (3.10-5.17 ng/m3 inside and 12.80-23.80 ng/m3 outside) and this demonstrated an accelerated oxidation process on the surface of ruins structure. The higher content of metals was detected in suspended particulate matter collected in summer, in comparison of those sampled in winter. Regarding the place, inside and outside of monument, the amount of investigated metals (i.e. Pb, Cd, Cr, Ni, Cu, Mn, Al, Zn, and Fe) was higher outside and this finding may result from the fact that most of metals are accumulated in the finest fraction of PM2.5-10. The measured values of element amount expressed as maximum/minimum/median/mean in analyzed particulate matters were ~ 4-13 times higher for all metals outside comparative with the values obtained for samples collected inside of historical monument.

Keywords: PM; ICP-MS; heritage; environmental conditions.

Acknowledgments: This work was supported by a project of the Romanian National Authority for Scientific Research, UEFISCDI, project 51PCCDI/2018 “New diagnosis and treatment technologies for the preservation and revitalization of archaeological components of the national cultural heritage”.

PHYSICO-CHEMICAL CHARACTERIZATION OF ENEOLITHIC PIGMENTS FROM CHEIA ARCHAEOLOGICAL SITE

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In this paper was studied 8 bivalve shells (with pigments traces) collected from Cheia archaeological site (Eneolithic site, dated probably to the 5th millennium BC, Romania). The present study aims to investigate the morphology and chemical content of samples (shells and pigments). All samples were investigated by Scanning Electron Microscopy coupled with Energy Dispersive Spectrometry (SEM-EDS), Attenuated Total Reflectance - Fourier Transform Infrared (ATR-FTIR) and Raman spectroscopies. The chemical composition of investigated pigments was compared with the shell composition and with other data reported in scientific literature. Principal Component Analysis (PCA) and cluster analysis using IBM SPSS Statistics software to assess the similarities between the investigated samples were performed.

**Keywords**: pigment; bivalve shells; SEM-EDS; FTIR; Raman spectroscopy.

**Acknowledgments**: This work was supported by a project of the Romanian National Authority for Scientific Research (UEFISCDI), project 128/2018 “Personal adornment in the Prehistory of the Northern Danube territory: aesthetic or socio-cultural symbol?”.

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**S5 P28**

**MONITORING OF GAS EMISSIONS IN A SEISMIC AREA**

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Gas emission is a precursor factor in a seismic area. This presentation refers to the monitoring of radon and CO₂ in Vrancea, the area characterized by deep earthquakes at the curvature of the Carpathian mountains. The methods are general but are customized to the geological specificity of the area under investigation. Fault areas have been determined through studies in several national projects. Sensor positioning has been correlated with these results, but it has been necessary to reallocate them in some cases as a result of inconclusive results. The purpose of monitoring gas emissions is to highlight the tectonic stress and to analyze the possibility of realizing a seismic forecasting service based on a multidisciplinary network. This is possible by determining local precursors, choosing the right equipment, and building a real-time monitoring network. Emissions of radon, CO₂ and other gases (e.g. CH₄) are dependent on atmospheric conditions (pressure, temperature, humidity, wind). For this reason each monitored location also has a meteorological station to determine the conditions under which the measurements were made. The first step is to determine the normal evolution of these parameters over a period of at least one year. We are looking for time intervals in which we did not have major earthquakes. After determining the daily, seasonal and annual evolution, deviations from normal and correlation with recorded seismic events can be made. The results of detection, effects evaluation, and data analysis alert the beneficiaries specialized in emergency situations (Inspectorate for Emergency Situations, organizations involved in managing special events).

**Key words**: radon anomalies, multidisciplinary monitoring, precursor phenomena, air ionization monitoring, CO₂ monitoring, cross-correlation.

**Acknowledgements** This work was supported by PN19080101 MULTIRISC NUCLEU program.
ON THE EFFICIENCY OF GYROTROPIC THERMOELEMENTS IN COOLING MODE

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The generalized theory of thermoelectricity allowed developing methods for the discovery of new thermoelement types, and their application in anisotropic media made it possible to devise, investigate and create a number of fundamentally new thermoelement types with unique properties that expanded essentially the opportunities of thermoelectricity. A promising direction in the development of thermoelectric applications is devising new thermoelement types based on gyrotropic media [1-3]. These opportunities of thermoelectricity are little studied, and their implementation will make it possible to expand the element basis of thermoelectricity, to improve the competitiveness of thermoelectric power converters, as well as to create on their basis the thermoelectric products of enhanced performance.

Thermal conductivity equation for a homogeneous gyrotropic medium is given by

\[ \kappa \Delta T + \rho_0 j^2 + 2\alpha_B \left( j_r \frac{\partial T}{\partial r} - j_\theta \frac{\partial T}{\partial \phi} \right) = 0, \]  

(1)

where \( \kappa \) is thermal conductivity coefficient of a gyrotropic medium; \( \rho_0 \) is electrical resistivity; \( j \) is electrical current density vector; \( j_r, j_\theta \) are projections of vector \( j \) in the Cartesian coordinate system; \( \alpha_B = Q_B \) is the asymmetric part of thermoEMF tensor; \( Q_\perp \) is the Nernst-Ettingshausen coefficient.

With regard to the axial symmetry of the system, we write Eq.(1) in the polar coordinate system

\[ \kappa \Delta T + \rho_0 j^2 + 2Q_\perp B \left( j_r \frac{\partial T}{\partial r} - j_\theta \frac{\partial T}{\partial \phi} \right) = 0, \]  

(2)

where \( j_r, j_\theta \) are the radial and azimuthal components of current density vector \( j \), \( r_1 \leq r \leq r_2 \) is thermoelement radius.

Computer simulation of temperature fields for gyrotropic thermoelements of the rectangular, spiral and optimal shapes was performed. BiSb, Ag2Te and InSb thermoelectric materials for gyrotropic thermoelements were considered. The calculation of temperature distributions in gyrotropic thermoelements was done by finite element method. Computer simulation was used to determine temperature distributions in gyrotropic thermoelements of a number of shapes for Ag2Te material in a magnetic field with induction \( B = 1 \) T. The temperature dependences of \( \Delta T_{\text{max}} \) for gyrotropic thermoelements of various shapes were obtained. It was shown that the use of Ag2Te is more reasonable in the temperature range of 150 – 300 K, when \( (\Delta T)_{\text{max}} \approx 36 \) K, and in the range of 80 – 120 K it is better to use BiSb – \( (\Delta T)_{\text{max}} \approx 17 \) K.

**Keywords:** gyrotropic thermoelement, magnetic field, thermoelectric material.

**References**

MEASUREMENT AND EVALUATION OF RADON IN SALT MINES IN ROMANIA

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For to domain development of speleotherapy in Romania, the paper presents the results of an indoor radon concentration levels analysis in some salt mines in Romania. The knowledge of atmospheric radon concentration levels in underground, (salt mines and caves) environments is essential for therapeutic purposes of different respiratory and rheumatic diseases. Have been chosen three salts mine test areas placed in the Northern part of Romania: Ocna Turda, Cacica and Ocna Dej in stable areas between 32–240 m depth. The measurements were conducted using the portable radon system PYLON AB 5, designed for atmospheric radon measurement. The analysis was performed by means of integrated measurements of radon and its short-lived daughter products for a period of a few years, using the radon monitor endowed with Lucas 300A alpha cell and the passive CPRD meter counter. The measuring of the natural background ionizing radiation in salt mines was made using the Berthold Umo LB 123 portable integrated impulse debit meter equipped with a gamma probe counter-timer and an integration time of 1 h/measure. The measurement and calibration procedures were conducted in conformity with the procedures for work of the accredited and notified laboratory SALMROM, in accordance with referential SR EN ISO/CEI 17025: 2005. The analyzed environmental conditions and recorded low levels of indoor mean radon concentrations (9.7 ± 0.8 and 64.9 ± 4.2 Bq/m$^3$) demonstrated the best suitability of the investigated three salt mines in Romania for speleotherapeutic applications and balneary treatment.

Key words: Radon concentration, Radiometric measurements, Speleotherapy, Salt mines.

PERFORMANCE, LIMITATIONS AND COMPARISON OF THE RESULTS FOR AN IN-SITU SPECTRO-TRACER WITH THE LABORATORY GAMMA RAY SPECTROMETRY

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The selection of an appropriate detector for field measurements, in case of natural radioactivity, is an important task taking into account constraints given by data reliability, time and cost effectiveness. This paper provides the necessary data when choosing a portable spectrometer Gamma Surveyor II based on BGO crystal (6.3 in$^3$). The proven efficiency of the crystal, the weaker energy resolution but still good and comparable results with HPGe results obtained for $^{238}$U, $^{232}$Th, $^{40}$K, often makes it a good choice. Thus, in this paper some functional parameters, as energy calibration, energy resolution and background of the system were analyzed. Field data, concentrations of radionuclides $^{238}$U, $^{232}$Th, $^{40}$K (ppm) in surface soil on the Bucharest area are compared with laboratory measurements using HPGe detector. Some soil samples were taken from the same locations where measurements with the Gamma Surveyor II were done. The results for $^{238}$U, $^{232}$Th and $^{40}$K were plotted against HPGe results to show the consistency of the measurements, depicted in Fig. 1. The obtained data are well correlated.
In conclusion, there are many advantages of using this system, such as:
- less time-consuming regarding acquisition and time analysis, the reporting of the data being instantaneous, at the elapsed time; 
- does not require liquid nitrogen, as for the in-situ HPGe detectors; 
- the BGO crystal contributes to a good response to the presence of radionuclides in the soil; 
- cost-effective way to obtain concentrations of natural radionuclides in soil.

Among the weaknesses of the system would by the fact that although it has a built-in library of 19 radionuclides (natural and artificial) that are recognized in the spectrum, it does contain an algorithm for their concentrations calculation. From this point of view this represents a loss, because in the samples measured on the HPGe detectors, $^{137}$Cs has been measured with activities between few Bq/kg up to more than 100 Bq/kg.

**Keywords**: Soil survey; Geophysical techniques; Gamma ray spectrometry.

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**S5 P32**

**N-WATCHDOG – FORECASTING AND DIAGNOSING VIRTUAL NUCLEAR EMERGENCIES**

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N-WATCHDOG is a cooperative R&D endeavor undertaken by Horia Hulubei National Institute of Physics and Nuclear Engineering IFIN-HH, Bucharest; SC SIVECO Romania SA; and the University Politehnica of Bucharest, within The Research, Development and Innovation National Plan II, Program Partnerships in Priority-Domains, Collaborative Projects of Applied Research, under the monitoring and financing by The Executive Unit for Financing the Higher-Education, Research, Development and Innovation System. The project aimed at creating a coherent, multi-disciplinary, stakeholder-oriented and practical software platform for monitoring vulnerabilities induced in people, natural environment, infrastructure and assets by nuclear facilities and events, with a pronounced preoccupation for precautionary, anticipatory assessment and early warning. A core function of the system is to iteratively forecast, as frequently as the user decides (including around the clock), over time windows spanning from 8 to 72 hours, the virtual radiological impact of hypothetical atmospheric radioactive releases from nuclear facilities anywhere in the World, as the assumed releases are driven cross-country by the true meteorology of the regions (winds, atmospheric stability, precipitations).
The product took the solution sought from a Proof of Concept to an Experimental Model which, while seen as the final deliverable of the Project itself, is also feeding promising prospects of scope expanding into the CBRNE realm and, possibly, marketability beyond.

Keywords: Nuclear Safety, Health and Environmental Threats, Risk Assessment, Emergency Management.

Acknowledgements. This work was financed by The Executive Unit for Financing the Higher-Education, Research, Development and Innovation System (UEFISCDI), The Research, Development and Innovation National Plan II, Project no. 298/2014

S5 P33

WEB APPLICATION FOR SUPPORTING THE FIRST RESPONDERS IN TRANSPORTATION INCIDENT INVOLVING DANGEROUS MATERIALS

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Dangerous goods or hazardous materials are daily transported by road and rail. These transports, in the event of incidents or accidents, may be a potential hazard to the population and the environment. When such incidents occur, the first responders must take a series of safety precautions.

The web application was created using “Emergency Response Guidebook – 2016” and has, as backend, a database who contains the following information:

- UN ID number of the substance;
- Complete name of the substance;
- Substance class (explosives, gases, flammable liquids or solids, etc.);
- Isolation distances for small and large spills;
- Protection distances for small and large spills, for both day and night periods.

The application is fully customizable by the user, in terms of: type of the substance, location, time of the day (day or night), type of spill and wind characteristics (speed and direction), characteristics who can be estimated by user or automatically taken from a free weather service.

The results, isolation and protection distances, are displayed to the user on a map, based on the previously inserted parameters.
Keywords: web application, hazardous materials, first responders, emergency response.
Acknowledgements: This work was supported by the Romanian Ministry of Education and Research through Grant SOL 7/2017 / RR – CBRNE.

S5 P34
WATER AND HYDROGEN TRANSPORT MODELING THROUGH THE MEMBRANE-ELECTRODE ASSEMBLY OF A PEM FUEL CELL

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Membrane Electrode Assembly (MEA) formed by a proton exchange membrane (PEM), two catalyst layers (CLs) and two gas diffusion layers (GDLs) represent the heart of the PEM fuel cell system, being the place where the electrochemical reactions are developed in order to generate electrical power. Due to a complex water production and transportation process through the porous media of MEA, the water management represents one of the most critical issues for the low temperature PEM fuel cell systems, working at 30 – 80°C. Production of water at cathode after reaction of oxygen ions with protons and electrons will result in a gradient of the water concentration across the membrane and a consequent diffusion of water from the cathode to anode, as the water back-diffusion mechanism. So, the net water flux across the membrane at any cell operating conditions represents a combination of diffusion and electro-osmotic drag. In the present paper, a one-dimensional mass transport PEMFC model for estimation of net water flux across the Nafion type membrane was implemented with the Comsol Multiphysics software, based on the Finite Element Method (FEM). Hydrogen crossover phenomenon, which may cause a degradation of the reaction sites inside MEA, was also included in the model. The numerical model offered a reasonable prediction of the fuel cell electrical performance in the form of current-voltage characteristic, validated through experimental measurements. Fuel cell performance was investigated by modifying the temperature and pressure inside the cell, along with the relative humidity (RH) for reactant gases.

Keywords: water activity, ionomer phase, relative humidity, molar fraction.

S5 P35
PHOTOCATALYTIC PROPERTIES OF NANOCOMPOSITES BASED ON SILVER AND ZINC OXIDE

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The new composite nanomaterials based on silver and zinc oxide (Ag-ZnO) were obtained in red cabbage extracts. The silver nanoparticles (nanobio silver) were first obtained in aqueous extract, on the basis of the Ag(I) reduction with phytochemicals from red cabbage. The nanocomposites were obtained in the same extract, by the decoration/deposition of blue ZnO nanopowder with different amounts of Ag nanoparticles. The structure and properties of Ag-ZnO nanocomposites were determined by XRD, SEM, TEM, FTIR and UV-vis spectroscopy. The TEM investigation demonstrated that ZnO are agglomerated in larger aggregates, which are deposited onto or decorated with Ag nanoparticles, depending on ZnO/Ag ratio. The band gap
energy values, calculated on the basis of Tauc equation, are in the range of 3.44 – 3.65 eV, superior to that of ZnO functionalized with anthocyanins [1].

The photocatalytic activity of nanocomposites was determined in the bleaching of an azo dye solution (Congo red, an anionic dye). For low concentrations of silver, a slight growth of photocatalytic activity with the silver content was noticed and values of photocatalytic activity in the 84.52 - 88.39% range were determined after 120 min of photocatalytic reaction. For the highest Ag content (Ag/Zn = 1/7), the lowest value for photocatalytic activity (67.46%) was determined. A similar dependence on the silver content was demonstrated by other authors for nanocomposites based on silver and ZnO [2].

The high photocatalytic activity for low silver content, up to 1/12, and an expected antimicrobial activity due to the synergic effect of ZnO, Ag and anthocyanins, make these materials very suitable for use in the wastewater treatment [3].

Keywords: Ag-ZnO nanocomposites, optical properties, photocatalysis.

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References

S5 P36

OPTIMIZED X-RAY SYSTEM FOR SELECTIVE WELL PLATES IRRADIATION

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Radiotherapy is one of the main strategies for cancer treatment and recent advancement in pre-clinical radiotherapy research have stimulated the development of precise irradiators for both small animals and cell cultures. The main purpose of present study was to develop an efficient and accessible method to perform high precision irradiations on cell cultures in terms of delivered dose, energy, exposure time, X-ray beam geometry, and irradiation selectivity. Our X-ray system provides the possibility to selectively deliver different doses in specific wells for the same plate without influencing the cells from the nearest wells. The plate is loaded with several cell cultures and is manipulated only once, after which dedicated Labview software is used to controls the X-ray operating parameters and the motor stages that position each well in front of the X-ray beam. The X-ray beam profile is delimited by round aperture pinholes and their corresponding scattering pattern is registered using EBT3 films. Additionally, the X-ray spectral shape dependence on energy and irradiation geometry was investigated by Monte Carlo simulation. The delivered doses for different working parameter of the X-ray source (current and voltage) were calibrated with a high performance secondary standard Unidos dosimeter connected to a plan parallel camera for low X-ray energies. A preliminary experiment on the survival rate of A375 cell in relation to the delivered dose was performed using the above-mentioned irradiation system. Next step is to accommodate to the irradiation head an XRF sensor in order to carry out an image guided irradiation protocol for nanoparticle loaded cell cultures.
ENERGY RECOVERY FROM NOISE AND VIBRATIONS

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Energy recovery from alternative sources is a preoccupation of our century in the conditions where conventional energy sources are exhaustible and does not provide the needs of existing consumers. Therefore, new directions of applied research in the field of energy are necessary. Its use in cogeneration or trigeneration systems is also a point to be considered.

The capture and conversion of vibration and noise into energy is also studied at national and international level. In this study we will develop methods of capturing and converting energy from noise and vibrations from the ambient environment. The novelty element consists in creating an optimized method of converting vibrations and noise from the environment into energy, for a dedicated area (Cluj-Napoca), with the delivery of a data base of the energy potential from sources of vibration and noise and a efficiency model by increasing this potential. Scientific description: Assessing the current state of technology of recovering energy from parasitic noise and vibrations, based on a literature review of the literature. 1. Studies on vibration and noise potential for Cluj in several areas of interest chosen on the basis of expected data: stadium, airport, train station, center, very populated districts, mall, etc ...) Choose the areas of interest with the largest population and traffic and estimate the energy output. 2. Measurements and preliminary results of vibrations and environmental noise 3. Statistical database on the energy potential that can be obtained from vibrations and noise based on measured measurements 4. Method of characterization of vibrations and noise in the area of the municipality Cluj-Napoca.
19th
International Balkan
Workshop on
Applied Physics

ABSTRACTS

S6 – Topics in Physics Education Research

- Physics curriculum design
- Active learning techniques
- Classroom teaching, demonstrations and laboratory experiments
S6 P1
QUANTUM ENTROPY AND REVERSIBILITY IN COOPERATIVE INTERACTION OF ATOM SYSTEM WITH BI-MODAL CAVITY FIELD IN RAMAN CONVERSION

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The restoration of the initial state of the two atoms and quantified bi-modal field in the Raman interaction with Pump and Stokes (anti-Stokes) cavity modes is analytical and numerical study. It is proposed the representation of bimodal field and a system of two atoms in scattering interaction.

The exact non-stationary solution of the system of two atoms in interaction with the bimodal field is found, considering that at initial time the atoms enter in the cavity and the wave functions of atoms and cavity field are disentangled. During the flying time, the system of two atoms exchanges the energy to the bi-modal field of cavity according to Raman scattering process. It is demonstrated that after this complicated nutation process during the absorption and emission of the photons from Stokes and pump modes the restoration of disentangled states between the system of atoms and field is possible.

In this communication, it is analytical demonstrate that the restoration of field and atom initial states is possible. Another attractive effect is connected with stationary trapping effect in the bimodal field, during which the exchange of the energy with the field during the absorption and emission processes is stopped.

Keywords: bi-modal field, Stokes and anti-Stokes cavity modes, trapping effect.

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References

S6 P2
AN INTERACTIVE EXPERIMENT FOR TESTING BELL-CHSH INEQUALITY

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Education in quantum technologies is paramount for the success of the second quantum revolution. In order to familiarize the students with basic concepts of quantum information, we set up the Applied Quantum Information Laboratory. The Lab, the first of its kind in Romania, is designed around the entanglement demonstrator quED from quTools [1]. In the Lab we can perform several landmark quantum experiments. Here we present an interactive experiment and a dedicated, in-house developed code, designed to test the violation of Bell-CHSH inequality [2] for different quantum states.

Entanglement is a quintessential quantum property. Entangled states have quantum correlations stronger than any classical correlations. Consequently, entanglement is an important resource for quantum technologies (teleportation, sensing, communication etc). A sufficient (but not necessary) condition for a quantum state to be entangled is to violate Bell-CHSH inequality. A classical system always satisfies Bell-CHSH inequality.
$S \leq 2$, where the Bell parameter $S$ can be calculated from the state of the system. However, for a quantum system this inequality is violated: there are quantum states with $2 < S \leq 2\sqrt{2}$.

The quED system (see figure) has several components: (i) a 405nm pump laser; (ii) two orthogonally-mounted BBO crystals for type-I SPDC; (iii) a half-wave plate for pumping the crystals at $45^\circ$; (iv) a detection and control module. For the detection and analysis of the photon pairs each arm contains a polarizer mounted on a rotational stage, a filter, an optical fiber coupler and an APD detector. Single and coincidence count rates are displayed on the touch screen of the control module.

To determine the Bell parameter $S$ we measure coincidence rates $\{N_1, ..., N_{16}\}$ for 16 different settings (angles) of the two polarizers. These values are recorded by the quED interface and the $S$ value and the standard deviation are automatically displayed. We developed a C++ code to vary the values $\{N_1, ..., N_{16}\}$ within $\pm 10\%$ of the experimental values and to compute $S$ for these states.

If we remove the half-wave plate before the BBO crystal, generated photons are no longer entangled and they satisfy Bell-CHSH inequality, $S \leq 2$.

In the Lab we can also demonstrate four other experiments: single-photon interference, quantum eraser, wave-particle duality, quantum random number generation.

**Keywords**: quantum information, entanglement demonstrator, Bell inequality, interactive code.

**Acknowledgements.** The authors acknowledge support from a grant of the Romanian Ministry of Research and Innovation, PCCDI-UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0338/79PCCDI/2018, within PNCDI III.


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**S6 P3**

### INTERDISCIPLINARY ACTIVITIES FOR STUDENTS

**Narciza TOPOR**

1 High School “Decebal” Constanta,

“Why do we learn math? Why do we learn physics? Why do we need to learn all this things?”

Carrying out educational projects and even optional disciplines can answer to this kind of questions that come from students.

Developing competences through knowledge and life skills is one of the major targets of education. In Physics one of the competences regards protection of one’s self, others and the environment. To reach an optimum level of this competence one needs to understand natural phenomena and anticipate their effects on everything that happens on Earth. In developing life competence in a formal and non-formal way, besides compulsory disciplines, optional disciplines have an important role as well as extracurricular projects. On school level, we proposed as an optional discipline Seismology and Elements of Astronomy. During compulsory disciplines, I propose to my students research activities.

During Seismology classes, my students watch documentaries, experiment and practice survival skills for earthquakes. Students are also involved in scientific activities through partnerships, such as ROEDUSEIS.

Cosmic phenomenon affect our daily life and this is why I consider that students have to know about this and not be taken by surprise. The Elements of Astronomy course offers students the opportunity to fill out what are stars, planets, what are the rules that govern the Universe and how this affects our life on Earth.

Materials and information gathered by teachers during communication sessions are very important. Participating to European Geosciences Union, knowledge from Geosciences Information for Teachers: PLATE TECTONICS AND EARTH’S STRUCTURE YESTERDAY, TODAY, TOMORROW was very helpful for interdisciplinary activities.

**Keywords**: Physics, Astronomy, Seismology, Students
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