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TOPIC 1

Thin Films and Nanostructures for Modern Electronics

PL-1 Effects of ionizing radiations on the performances of A2-B6 thin films photovoltaic cells for 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 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, the photovoltaic cells based on CdS/CdTe thin films, produced by thermal vacuum sublimation, were irradiated with protons and alpha particles, (both components of cosmic rays), at room temperature. The irradiation energy for both protons and alpha particles was 3 MeV and the fluencies were 1014 protons/cm2 and 1013 alpha particles/cm2, respectively. 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. The parameters characterizing a photovoltaic cell, short-circuit current, open circuit photo-voltage and fill factor were calculated before and after protons or alpha particles irradiation and the obtained values are comparated. A discussion about the possible origin of those defects is given. In this sense, it was found that proton irradiation in the above mentioned conditions results mainly in the introduction of defects at the CdS/CdTe interface.

PL-2 Photosensitive Ge-TiO2 films with tuneable detection wavelengths from VIS to NIR

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Quantum dots (QDs) present strong confinement, being tailorable in terms of size, crystallinity and shape. The research based on them, in particular on Ge QDs represents a major driving force for the scientific community as they are promising for applications in photodetectors, solar cells, and non-volatile memories. One route to obtain films based on them, having targeted photoconductive properties to be used in different applications is to manufacture films formed of Ge QDs embedded into dielectric matrices such as TiO2. The use of Ge QDs has two important advantage, first being that in Ge nanocrystals the quantum confinement effect is more pronounced and second, the thermal budget of the formation process of QDs is reduced in comparison with other nanocrystals, for example Si QDs. An additional advantage of TiO2 films with embedded Ge QDs is given by TiO2 which has excellent optical properties which make it suitable for a wide palette of applications in photocatalysis and photovoltaics. In this work, we employ the magnetron sputtering method for Ge-TiO2 films deposition combined with subsequent annealing under controlled conditions for films nanostructuring with the aim to manufacture Ge-TiO2 films with tailored structure and consequently with targeted electrical and photoconductive properties. This can be achieved by changing the Ge content and annealing temperature. We obtain nanostructured films formed of Ge QDs with cubic structure and TiO2 nanocrystals with anatase structure, all of them having sizes in the range of 10 – 15 nm. In the films, the Ge QDs are surrounded by the mixed oxide of Ti and Ge, i.e. (TiGe)O2 having rutile structure. In this structure Ti and Ge atoms are randomly distributed in the same lattice. More than that, these films are photosensitive from visible to near-infrared interval, the spectral dependence of the photocurrent showing a fine structure which can be tuned by changing the Ge content and annealing temperature. These films with tuneable photoconductive properties are appropriate for further employing in photodetection applications.

PL-3 Epitaxy of Ferroelectric Complex Oxides on Semiconductors for Field-Effect Devices

Lucie Mazet[1], Romain Bachelet[1], Guillaume Saint-Girons[1], Lamis Louahadj[1], David Albertini[2], Brice Gautier[2], Jean Jordan-Sweet[3], Martin M. Frank[3], Vijay Narayanan[3], Martin Hytch[4] , S. Schamm-Chardon[4], C. Dubourdieu[1]
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Ferroelectric oxides integrated on a semiconductor substrate are of particular interest for various applications such as nanoelectronic devices, electro-optic components or as piezoelectric materials for sensors and actuators. In this talk, I will briefly review the challenges associated with the monolithic integration of crystalline complex oxides on a semiconductor and more particularly with the integration of ferroelectrics. Molecular Beam Epitaxy (MBE) provides unique advantages to precisely construct, almost atom by atom, the oxide/semiconductor interface, which plays a major role, especially when transport is involved in the semiconductor. I will then present an experimental work on the epitaxy of $BaTiO_3$ thin films on silicon and $Si_{1-x}Ge_x$ substrates. Films are grown by MBE, in the thickness range of 1.2-20 nm. Different growth conditions such as temperature and oxygen pressure are explored to optimize the $BaTiO_3$ film quality and to minimize the SiO_2 interfacial layer regrowth between the semiconductor and the $SrTiO_3$ buffer layer. The crystalline structure is studied by conventional and synchrotron x-ray diffraction. It is also investigated at the nanoscale using advanced transmission electron microscopy techniques. Strain maps determined with high precision (0.05%), 5 nm spatial resolution and with a large field of view (1 µm) using dark field electron holography will be shown for selected samples. The crystalline domain orientations (c- versus a-domains) will be discussed with respect to the growth conditions and thickness. The ferroelectric properties are investigated by piezoresponse force microscopy (PFM). Ferroelectric films are obtained in optimized conditions that will be discussed. I will conclude with perspectives on the integration of such heterostructures in quantum metal field-effect transistors for low power logic applications.

I-1 Integration of ferroelectric $BaTiO_3$ thin films and artificial multiferroic heterostructures with silicon

Mateusz Scigaj[1], Nico Dix[1], Ignasi Fina[1], Romain Bachelet[1], Vassil Skumryev[1], Gervasi Herranz[1], Josep Fontcuberta[1], Florencio Sánchez[1]
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Multiferroic materials are appealing for its application in microelectronic devices, but coexistence of ferroelectricity and ferromagnetism in a single material is generally restricted to low temperatures. Artificial multiferroics, combining ferroelectric and ferromagnetic phases are an alternative. High quality multiferroic ferromagnetic/ferroeletric heterostructures can be fabricated on oxide single crystals, but its integration with silicon is elusive. We show here that high quality epitaxial CoFe2O4/BaTiO3 bilayers can be grown on buffered Si(001). The use of a complex LaNiO3/CeO2/YSZ buffer layer was found key to obtain c-axis orientation of BaTiO3. Consequently, CoFe2O4/BaTiO3/LaNiO3/CeO2/YSZ heterostructures were deposited on Si(001) in a single process by pulsed laser deposition assisted with high energy electron diffraction (RHEED). Atomic force microscopy, X-ray diffractometry, and RHEED confirm high structural quality of the CoFe2O4/BaTiO3 heterostructures. CoFe2O4/BaTiO3 bilayers display good multiferroic properties, with high values of magnetization (> 200 emu/cm3) and polarization (>C/cm2) at room temperature. Remarkably, the polarization of CoFe2O4/BaTiO3 bilayers is enhanced compared with bare BaTiO3 films and there are no fatigue up to more than 3x109 cycles. Finally we show the influence of the CoFe2O4 on the ferroelectric polarization and current leakage of the BaTiO3 films.µ15

I-2 ZnO Nanorods

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The past few years have seen extensive research in enhancing the electrical and optical properties of ZnO for the design of new optoelectronic and electronic devices. This interest is motivated by the prospect of forming various types of nanostructures such as nanowires, nanotubes, and nanorods. ZnO nanorods are of great interest for various nanodevices because of their large surface area. In order to improve the practical applications, it is necessary to improve the shape, morphology and size of ZnO nanorods. A wide range of these adjustable parameters provide a versatile control over the optical properties of the ZnO nanorods for broadening their applications in nanodevices. In this study, the effect of shape of ZnO nanorods on optical properties was investigated.

I-3 Where do the Electrons go in STM? Real-space imaging of electron dynamics on the Si(111)7x7 surface

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The dynamics of hot-electrons is central to understanding and hence improving or harnessing the properties of nanometer scale silicon transistors, solar cells and the optical and electrical transport properties of graphene. However, due to the short-lived nature of hot-electrons (typically ~ 100 fs) and associated nm length-scales it is challenging to directly measure their properties. Here we image with atomic resolution the outcome of precise hot-electron injection into the Si(111)-7x7 surface. We show that the injected hot-electrons are responsible for the manipulation (desorption or diffusion) of adsorbate molecules some distance (~ 10 nm) from the injection site. The length-scale of this nonlocal effect is dependent on both the energy of the injected hot-electrons and the temperature of the silicon substrate. The underlying hot-electron dynamics are well described by a two-dimensional diffusive model with a single decay channel.

I-4 The effect of the substrate temperature and the acceleration potential drop on the structural and physical properties of SiC thin films deposed by TVA method

Victor Ciupina[1]
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Crystalline Si-C thin films were prepared at substrate temperature between 200°C and 600°C using Thermionic Vacuum Arc (TVA) method. To increase the acceleration potential drop a negative bias voltage up to -1000V was applied on the substrate. The 200nm thickness carbon thin films was deposed on glass and Si substrate and then 200-500 nm thickness Si-C layer on carbon thin films was deposed. Transmission Electron Microscopy (TEM), High Resolution Transmission Electron Microscopy (HRTEM), X-Ray Photoelectron Spectroscopy (XPS), and electrical conductivity measurement technique characterized the structure and physical characteristics of as-prepared SiC coating. At a constant acceleration potential drop, the electrical conductivity of the Si-C films deposed on C, increase with increasing of substrate temperature. On the other part, significant increases in the acceleration potential drop at constant substrate temperature lead to a variation of the crystallinity and electrical conductivity of the SiC coatings XPS analysis was performed using a Quantera SXM equipment, with monochromatic AlKα radiation at 1486.6eV. Electrical conductivity of the Si-C coating on carbon at different temperatures was measured comparing the potential drop on the sample with the potential drop on a series standard resistance in constant mode.

I-5 High Accuracy AFM with Advanced Scanner Structure

Kevin Ryang[1]

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Although atomic force microscope (AFM) is a very useful instrument in characterizing nanoscale features, it lacks accuracy and repeatability in measuring absolute dimensions. The primary reasons are the poor behavior of piezoelectric tube scanner and the tip wearing that constantly changes the tip geometry. Together with complex setting of operating parameters, AFM could not be made as widely adopted as other microscopy such as optical microscope or scanning electron microscope (SEM). In order to improve the core performance of AFM, we have developed a flat scan system, where the x-y scanner moves the sample in the horizontal plane and the z scanner moves only the probe in the vertical axis. The accuracy of the x-y scan was improved with feed-forward algorithm, Hann function, and dual servo system. The speed of the z scanner was increased by minimizing the mass of moving part of the scanner to which the probe is attached. The resulting z servo bandwidth was high enough to enable the non-contact mode in ambient atmosphere and made it stable enough to become practical for routine operation. The non-contact mode preserves the sharp tip and, therefore, provides highly accurate and repeatable measurements of the sample geometry through tip de-convolution.

I-7 Revealing The Ultrafast Process Behind The Photoreduction Of Graphene Oxide

Regis YN Gengler[1,2], Daniel S Badali[1], Dongfang Zhang[1], Kostas Dimos[3], Kostas Spyrou[3], Dimitrios Gournis[3], Dwayne RJ Miller[1]

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Effective techniques to reduce graphene oxide are in demand owing to the multitude of potential applications of this two-dimensional material. A very promising green method to do so is by exposure to ultraviolet irradiation. Unfortunately, the dynamics behind this reduction remain unclear. Here we perform a series of transient absorption experiments in an effort to develop and understand this process on a fundamental level. An ultrafast photoinduced chain reaction is observed to be responsible for the graphene oxide reduction. The reaction is initiated using a femtosecond ultraviolet pulse that photoionizes the solvent, liberating solvated electrons, which trigger the reduction. The present study reaches the fundamental time scale of the ultraviolet photoreduction in solution, which is revealed to be in the picosecond regime.

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O-1 Effect of Deposition Conditions and Doping on Structural and Optical Properties of ZnTe Thin Films

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The zinc telluride (ZnTe) is one of the important compounds of the II–VI group due to it low cost and high absorption coefficient for application to photovoltaic cells and various optoelectronic devices. The ZnTe thin films were prepared by close space sublimation method (CSS). Cleaned glass slides and covered with SnO2 were used as a substrates. The structure and optical properties of undoped ZnTe thin films have been studied as a function of substrate temperatures in an attempt to optimize the growth conditions. The films deposited at higher substrate temperatures were found to have larger grains and nearly stoichiometric composition. Also, ZnTe films successfully doped with Ag using ion exchange process and thermally treated have been investigated. For undoped and doped ZnTe thin films, the structure is the cubic phase with a (111)-preferred orientation as shown by X-ray diffraction (XRD) measurement. XRD patterns indicated that the crystallite size had increased after silver immersion in as-deposited ZnTe thin films. Scanning electron microscopy (SEM) and EDX analysis was used to observe the change of as-deposited and doped sample's grains sizes and confirm the presence of Ag in the ZnTe thin films after doping. The optical studies showed the decreasing in energy band gap after Ag-doping. Transmission also decreased after doping. The observed changes in the physical properties in relation to the concentration of Ag for the films of different thicknesses will be reported and discussed.

O-2 Transparent amorphous oxide semiconductors: Advanced characterization by spectroscopic ellipsometry and x-ray reflectivity

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In addition of the electrical properties (resistivity, charge carrier mobilities), the optical properties are important parameters of a transparent conductive oxide (TCO) and of a transparent amorphous oxide (AOS). The transparency spectral range, the refractive index dispersion, as well as the absorption coefficient dispersion (or extinction coefficient) define the optical properties, and can be used for example to estimate the amount of light that reaches the core p-n junction of a photovoltaic cell. Inx−wGawZn1−xO1+0.5x−1, known as IGZO or GIZO, have been proposed as a suitable thin film transistor's channel semiconductor. Such amorphous oxide semiconductors (AOS) can be used on already developed silicon based platforms or on novel proposed fully transparent devices, while IZO can replace as TCO the most expensive Sn:In2O3 (ITO). Due to the different structure in which ZnO (hexagonal wurzite), In2O3 (cubic bixibite) and Ga2O3 (monoclinic) crystallize, the intermixture of these compounds has for a large concentration range an amorphous-like structure, whereas the electric properties can be tailored by modifying the stoichiometry. This amorphous nature is a big advantage versus pure ZnO which has a strong tendency to form polycrystalline phase, which diminishes the electrical and bending functionality. The optical properties of the amorphous IZO and IGZO films having various In and Ga concentrations were determined by analysis of spectroscopic ellipsometry data. The refractive index of non-absorbing materials ($k=\alpha=0$) in the corresponding transparency spectrum is linearly dependent on the mass density, determined by X-Ray Reflectivity. However, this dependence between the refractive index and the mass density breaks down in the case of a weak absorbing compound. At certain cations concentration, a semiconductor-metal transition occurred, as proved by the free carrier light absorption and by the specific band-gap blue shift.

O-3 On the spectral response of photovoltaic cells based on CdTe

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Photovoltaic cells based on cadmium telluride (CdTe) were prepared by thermal vacuum evaporation (TVE) technique onto optical glass substrates covered with ITO or ITO/IGZO as transparent conductive oxides (TCO's). Indium gallium zinc oxide (IGZO) thin films were deposited in situ onto indium tin oxide layers (ITO), by magnetron sputtering. Optical investigations were made for both, the transparent conductive oxide layers and photovoltaic cells component films, using a Perkin Elmer spectrometer. The optical transmittance spectra were drawn at room temperature in the 190 – 1100 nm and the obtained values were higher than 60% for all transparent oxide layers. From absorption spectra of cadmium sulfide (CdS) and CdTe the optical gap values were determined and were similar with those from literature. The morphological analyses of the prepared photovoltaic cell's surface were performed by scanning electron microscopy (SEM) and the structural features for cadmium sulfide and cadmium telluride thin films were determined by X-ray measurements. A well-defined crystalline structure was observed for both CdS and CdTe layers. The external quantum efficiency (EQE) values were determined for the prepared PV cells, at room temperature. The obtained experimental data proved that IGZO thin film can be used as TCO's replacing ITO; moreover, a photoelectrical behavior was revealed improving the photovoltaic performances of the prepared samples.

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O-4 On the physical properties of different metallic oxides obtain by direct thermal oxidation

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Different metallic thin films (Zn, Zn:Al, In:Sn, Ni, Ti) were deposited onto optical glass substrates by magnetron sputtering, in two configurations: perpendicular (denoted horizontal) and parallel (denoted vertical) to the plasma flow. Transparent oxide thin films (ZnO, AZO, ITO, NiO and TiO2) were obtained by direct thermal oxidation, gradually, from room temperature (RT) to 550°C. The whole processes took place in open atmosphere. The structural, morphological, electrical and optical investigations were made for oxide thin films and, for metallic layers, respectively (when appropriate). The structural features revealed a well-defined crystalline structure for all prepared oxide thin films and an optical transmittance higher than 60% for both, vertical and horizontal deposition arrangements. The morphological analyses were performed by atomic force microscopy (AFM), in contact mode and scanning electron microscopy (SEM). It was observed that the deposition configuration influenced the thickness and the roughness of the prepared samples no matter of the nature of the deposited film. Electrical behavior was analyzed by van der Pauw measurements in 300 K – 50 K. The obtained results proved that direct thermal oxidation can be an alternative in order to obtain transparent oxide thin films that can be used as buffer or dielectric layers for different electronic and optoelectronic applications.

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O-5 Investigation of optical properties of nickel oxide thin films deposited on different substrates and understanding their influence over properties of nickel oxide.

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Nickel oxide is investigated for several potential applications, namely, ultraviolet detectors, electro chromic devices, displays, diodes for light emitting, transparent conductive electrode and opto-electronic devices. These applications requires deep analysis in understanding its optical properties, such as transmittance, absorption coefficient, dielectric constant, real and imaginary parts of refractive index, optical conductivity, extinction coefficient, direct and forbidden band gap. Optical properties of material are investigated by depositing thin film of material on glass substrate. Hence, optical properties determined or deduced from measurements add effect of glass substrate, which modifies the information obtained. In view of this, we investigate optical properties of nickel oxide on different substrates to study differences in optical properties of same film deposited on Insulators (glass, quartz, sapphire) and wide band gap insulators (potassium bromide and calcium fluoride windows).

O-6 Studies on optical properties of antimony doped SnO_2 films

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Antimony doped tin oxide thin films were grown by spray method on microscope glass substrates. The antimony doping was varied from 0 to 4 at. %. The structural properties of the films were investigated by X-ray diffraction method. It was determined that the films formed at polycrystalline structure in tetragonal phase and structure was not changed by doping ratio. The optical transmittances of thin films were measured with UV-Vis-NIR spectrometer in the

300−1500 nm wavelength range. The transmittances of the films were decreased in an apparent way with doping and wavelength near the IR region. A simple analysis according to Swanepoel's method [1] was applied to derive the real and imaginary parts of the complex index of refraction plus film thickness. The dispersion of refractive index was investigated in terms of the single-oscillator Wemple and DiDomenico model [2] and the important oscillating parameters such as the dispersion energy E_d, the oscillation energy E_o, the high frequency dielectric constant ε_∞ were determined. The analysis of the refractive index has been carried out to calculate the lattice dielectric constant ε_L and the ratio of carrier concentration to the effective mass N/m^* according to procedure [3]. The absorption coefficient and, therefore, the extinction coefficient have been determined from transmission spectra. The real and imaginary parts of the electronic dielectric constant and optical conductivity were analyzed. The optical band gap, E_g values of the films were obtained from the spectral dependence of the absorption coefficient, using the Tauc relation [4].

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O-7 Tuning the structure and electrical behaviour of GeSi nanostructured films by annealing temperature

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In this work we report on the growth of GeSi nanostructured films and on the structure investigations and electrical properties. The films are deposited by magnetron sputtering and annealed in N2 at 700, 800 and 900 oC for GeSi nanocrystals formation. The films structure was studied by using XRD and TEM methods, and the electrical properties by measuring current-voltage and current-temperature curves. In the annealed films we evidence two different structures. The films annealed at 700 oC are formed of small GeSi nanocrystals separated each other by very thin amorphous space, while with the increase of the annealing temperature, the size of nanocrystals strongly increases and the boundaries between them become completely crystallized. The electrical behaviour of the films is in accordance with their structure, so that the conduction mechanism (in the current-voltage characteristic) in 700 oC annealed films is the tunnelling of carriers between nanocrystals assisted by high electric field, while the 800 and 900 oC annealed films show a polycrystalline behaviour.

O-8 Nanomechanical characterization of amorphous and nanocrystalline FeCuNbSiB thin films

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Over the past decades, FeCuNbSiB alloys have shown a fundamental scientific interest and a promising potential for industrial applications [1].

The purpose of this paper is to show how the films' thickness, substrate's nature and nanocrystallization process influence the mechanical properties of $Fe_{73.5}Cu_1Nb_3Si_{15.5}B_7$ thin films. The samples, having thickness in the range of 1.4 μm to 2.0 μm, were deposited by HiPIMS on different substrates (glass, aluminum, silicon, and sapphire). The analyses were performed on as-deposited films, as well as on films isothermally treated under high vacuum, for 1 h, at temperatures between 300°C and 475°C.

The surface chemical nature, the thickness and the structural, topological and mechanical properties of the films were analyzed by X-ray photoelectron spectroscopy, interferometry, X-ray diffraction, atomic force microscopy and nanoindentation techniques, respectively. The Oliver-Pharr method was used in order to determine the hardness, H, and reduced Young's modulus, E_r, of the films, while for the effective Young's modulus, E, the mechanical properties of the substrate were taken into account [2].

In as-deposited state, the films are amorphous with uniform surfaces and RMS roughness values less than 1% of their thickness. In nanocrystalline state, the average grain size of the b.c.c. α-Fe(Si) grains is about 12 nm for the samples thermally treated at 463^{o}C and about 15 nm for those thermally treated at 475^{o}C.

According to the contact stiffness dependence on the normalized indentation depth, the film-substrate systems exhibit different types of characteristics: hard-soft (film-aluminum and film-glass), soft-hard (film-sapphire) and nearly elastically homogenous (film-silicon).

Increasing the thickness of the amorphous films, E value remains approximately constant, while H value increases up to 1 GPa. In the case of nanocrystalline films, for the same thickness, increasing the annealing temperature up to 475^{o}C, E value decreases by about 13%, while hardness value increases by about 13% with respect to the as-deposited state.

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O-9 Influence of n- ZnO channel layer characteristics on switching properties of the transparent thin film transistor

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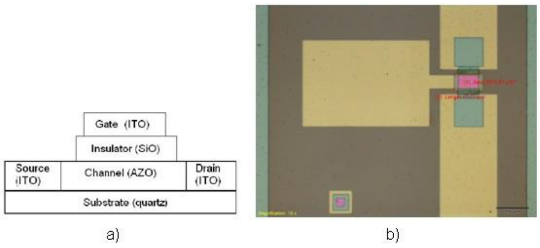
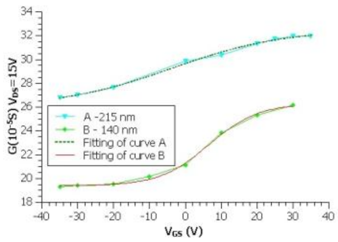
Thin film transparent transistors (TTFT) based on metal-oxide thin films as building blocks of transparent electronics are widely investigated tacking into account films properties and characteristics in order to be used as active devices in high performance flat panel display and sensors. In this paper we investigated and analyzed an all TCO films based TTFT with n-ZnO channel (l=150 µm, w=70 µm) in coplanar top gate configuration, structure is presented Fig.1 a,b. n-ZnO channel layers of the thickness in range 90-215 nm were deposited by RF assisted Pulsed Laser Deposition (RF-PLD) using a AZO ceramic source (ZnO with 1 % Al). The deposited n-ZnO films presented a polycrystalline structure, (222) oriented and below to 2 nm roughness and 85 % optical transmission in the visible spectral range. Electrical characterizations, IDS(VDS) for various values of voltage applied on the gate, were performed using a Keithley 4200 in dark and white light illumination conditions.



a) Schematic cross-sectional view of TTFT; b) Optical image of the n-ZnO coplanar top gate processed TTFT



c) Conductance versus gate source voltage extracted from I-V characteristics and fitting functions

From the , IDS(V_{DS})/V_G corresponding to the structures that have channel thicknesses 93 nm , 140 nm, 215 nm were extracted conductance and depletion layer thickness versus gate source voltage, presented in Fig 1c. The conductance versus gate source voltage characteristics were modeled by using the following function:$G(V_{GS})=a+(b-a)/(1+\exp[(V_{GS}-V_0)/c])$ where a, b, c are fitting parameters. The thickness corresponding to device switching for -20 V gate source voltage is 35 nm as results from the extracted values of the depletion region thickness. By using the conductance versus gate source voltage characteristic we can estimate device behavior in the given range of drain-source voltages.

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O-10 Nanometric Titanium Oxide Films: Composition And Properties

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Currently nontraditional methods are very often applied to form surface layers that have special properties that differ of those the base material has. The progressive direction of modern technology is corrosion protection of metal surfaces. Despite the fact that titanium is a metal resistant from the point of view to corrosion in the most harsh environments, it intensively corrosives in H_2SO_4 water solutions. The paper [1] proposes electro-spark alloying (ESA) method for the formation of Pd depositions to enhance the corrosion resistance of titanium surface. The results show that the corrosion resistance in H_2SO_4solutions of the processed surfaces increases by 1÷2 orders. The present paper proposes a method of formation nanometric oxide films on the surface of titanium and its alloys by applying electrical discharges in impulse (EDI). Processed surface layer consists mainly of titanium oxides and nitrates in the amorphous state, which leads to the passivation of the surface and, as a result, to the increase of surface electrical resistance by 107 times and to the increase of corrosion resistance up to 100 times in H_2SO_4 solutions.

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P-1 DC conduction mechanism of some new lower rim substituted calixarenes derivatives in thin films

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In this work study of temperature-dependent electric conductivity of some recently synthesized organic compounds, lower rim substituted calixarenes derivatives, is reported. Thin-film samples (d=0.10-0.60 μm) deposited from chloroform solutions (an immersion technique) onto glass substrates were used. Organic films with reproducible electron transport properties have been obtained by submitting freshly deposited films to a heat treatment within temperature range of 295−483 K. The studied organic compounds are polycrystalline (as shown by XRD analysis) and display typical semiconductor behavior. The activation energy of the electric conduction ranges between 1.35 and 2.36 eV. Study of optical absorption revealed direct band gaps ranged between ∼2.50 and 3.60 eV. Some correlations between semiconducting parameters and molecular structure of the organic compounds have been discussed. In the higher temperature range (T>420 K), the electron transport in examined compounds can be interpreted in terms of the band gap representation model, while in the lower temperature range, the Mott’s variable-range hopping conduction model seems to be appropriate. Some of the investigated compounds hold also promise for thermistor applications.

P-2 Optical and electrical properties of (Ba1−xCax)(ZryTi1−y)O3 polycrystalline thin films growth by pulsed laser deposition

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Piezoelectric and ferroelectric materials are keys to modern technologies due to his high dielectric constant and strong piezoelectric response. The well known Piezoelectric material are the lead zirconium titanate (PZT) but the main drawback of PZT is the high toxicity of lead and for that reason new materials are being developed. Recent studies [1-3] demonstrated the possibility to obtain lead-free (Ba1−xCax)(ZryTi1−y)O3 (BCZT) ferroelectric materials with very high dielectric permittivity and piezoelectric coefficients, opening the way to competitive devices free of toxic elements. In this work, BCTZ thin films, with different compositions,.were deposited using pulsed laser deposition method (PLD) with a ArF excimer laser, on platinum coated silicon substrate in a reactive environment (oxygen). The targets have been prepared by conventional ceramic processing and sintering at temperatures of about 1500 oC. The properties of the BCTZ thin films such as optical and electrical properties, thickness, roughness and dielectric constant were investigated by X -ray diffraction, Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and Spectroscopic Ellipsometry (SE) techniques. The films deposited on Pt/Si substrates are policrystalline and show (110) and (111) orientation. Atomic force microscopy evidenced a uniform surface microstructure with small roughness. Using spectro-ellipsometry (SE) technique, the optical behavior and band gap characteristics were determined. A high refractive index and low extinction coefficient for a large spectrum of wavelength (n>2 and k<10-4 for near UV-VIS-near IR) was found. The thickness of samples and their rough layer obtained from SE was compared with SEM and AFM results and were found in good agreement. Dielectric spectroscopy measurements carried out at room temperature and different frequency values. Excellent dielectric properties (relative permittivity of about 2000 and tangent loss ~ 3% at frequency of 10 KHz) have been measured.

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P-3 The Effect of Oxygen Flow Rate on the Electrical Properties of CuO Films Coated By DC Magnetron Sputtering Technique

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The structural, optical and electrical properties of cupric oxide (CuO) films coated by DC magnetron sputtering method under different oxygen flow rate (0%, 35%, 70%) were examined. The electrical transport mechanism of the films was also investigated in a temperature range of 110−400 K. Electrical conductivity of the films mainly affected by oxygen flow rate since density of states (DOS) was critically dependent on the oxygen flow rate. Considering oxygen flow rate, a direct link between the DOS and electrical properties of the films was established.

P-4 Advanced characterization of amorphous oxide semiconductor thin films by X-ray reflectivity and thermally stimulated current spectroscopy

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There is a growing interest for the use of amorphous In-Ga-Zn oxide (a-IGZO) as channel semiconductor in transparent field effect transistors (TFET). Numerous reports on devices containing a-IGZO as active layer can be found, but scarce information regarding their in-depth physical properties which govern their functionality is presented. The electrical instability of a-IGZO-based TFETs when are exposed to white light is now well-known. The TFETs performance deterioration as a consequence of aging effect with increasing work time has been proposed. The presence of the trap levels can be the source of these drawbacks. In this work a-IGZO thin films are analyzed by thermally stimulated current spectroscopy (TSC) in order to depict the nature and position in energy of the trap levels. As it was showed in previous articles, the working parameters of a-IGZO-based TFETs together with the electrical stability are significantly improved after soft thermal treatment of the devices. Although IGZO remain amorphous after such typical annealing procedures, variations of electrical conductivity were recorded. The structural changes that occur after annealing in the IGZO cannot be emphasized by X-ray diffraction. In order to examine the influence of the thermal treatment over the in-depth uniformity, interface roughness and density of the IGZO films, X-ray reflectivity measurements have been employed.

P-5 Effect of buffer and interlayer on the adhesion and magnetic properties of anisotropic Nd-Fe-B single layer and multilayer films

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Nd-Fe-B films with crystallographic c-axis of $Nd_2Fe_{14}B$ phase perpendicular to the substrate plane have attracted much attention due to some potential applications, such as fabrication of the thin magnets, microelectromechanical system, millisize motors or actuators, and microstructured magnetic sensors [1-2]. A suitable buffer layer is crucial both in the growth of $Nd_2Fe_{14}B$ grains with c-axes perpendicular to the film plane and for adhesion to the substrate for thick layers. Many metallic elements can be used as buffer layer for Nd-Fe-B films in order to obtain $Nd_2Fe_{14}B$ grains with the c-axes perpendicular to the film plane. Among them, Ta and Mo [3] are known to act in sense of promoting the growth of c-axis texture of the $Nd_2Fe_{14}B$ phase, and to protect the Nd-Fe-B films from oxidation from the substrate.The X/NdFeB/Mo and X/[NdFeB/Mo]x3/Mo films were deposited in vacuum by magnetron sputtering onto Si substrates, where buffer layers used are X= (Mo, and Ni/Mo).The Nd-Fe-B films were deposited on a substrate/buffer ensemble heated at ≤ 470°C and then have been annealed for 20 minutes (optimum annealing time) at 500°C. It was found that the c-axis orientation depends on the nature and thickness of buffer layer and interlayer, and temperature of heated substrates of Nd-Fe-B film in single layer and multilayer variants. Good c-axis orientation and adhesion on substrate was obtained by using a composite Ni (10 nm)/Mo(40 nm) buffer. Supplementary, the layering of Nd-Fe-B film with a Mo film used as interlayer further improves the anisotropic hard magnetic characteristics of Nd-Fe-B films. In comparison with Mo/NdFeB(540)/Mo single layer film, the multilayer Mo/[NdFeB (180)/Mo(5)]x3/Mo film exhibits an increase in coercivity from 800 kA/m to 1220 kA/m and in the remanent ratio from 0.92 to 0.99. For the qualitative assessment of adhesion to the substrate of the Nd-Fe-B films the scratch test was used. If a Ni film with an optimal thickness of about 10 nm is used as buffer layer, besides Mo film of 40 nm, the adhesion to substrate is improved and this is very promising for the use of Nd-Fe-B thick films in MEMS applications.

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P-6 Effect of annealing treatment applied to TCO samples on the structural and optoelectronic properties

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Oxide layers (ITO, AZO(2%) and SnO2) with thicknesses of 30 nm and 50 nm were deposited onto glass substrate by rf magnetron sputtering technique, and next subjected to heating at a temperature of 350°C for 1h performed in open atmosphere. The characteristics of the oxide depositions as well as the obtained layers were investigated. XRD, XPS and SEM analysis indicates that the obtained films possess a polycrystalline structure and the crystallites have a preferred orientation. Atomic force microscopy measurements show a roughness on the order of nanometers (i.e. 0.7 nm to 5 nm) for the ITO, SnO2 and AZO layers. An increase in surface roughness was observed after subjecting the samples to annealing treatment. Structural parameters depend on the oxidation conditions. Electrical behaviour of TCO films was investigated during annealing treatment. It was observed that after the first heat treatment, temperature dependences of electrical conductivity becomes reversible. We conducted spectrophotometric investigations of these layers in the 0.2-1.8 μm wavelength range. A high transmission in visible and near infrared range as well as a value of 3.70 eV and 3.75 eV for the energy band gap (calculated from the absorption spectra) were particularly noted for these layers. The present investigations of oxide layers are also useful in applications of transparent conductive oxides.

P-7 Thin films of AZO-derivative compounds for non-linear optical applications deposited by laser techniques

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Matrix-assisted pulsed laser evaporation, at low fluences (0.2–0.7 J/cm2), using a Nd:YAG pulsed laser device (λ = 266 nm, τ = 7 ns, ν = 10 Hz) was employed for the growth of azo-derivative compounds thin films due to their optical properties (e.g. two-photon absorption, second harmonic generation, optical limiting and all-optical poling). The structure, morphology and optical properties of the films were investigated by spectroscopic-ellipsometry, Fourier transform infrared spectroscopy, scanning electron microscopy, and atomic force microscopy techniques. Second harmonic generation (SHG) capabilities were evidenced when irradiating the films by a Ti:sapphire pulsed laser (λ = 780 nm, τ = 60 fs, ν = 80 MHz, Pmax = 700 mW). The as deposited films were used as donors for printing micrometric pixels, by laser-induced forward transfer (Nd:YAG, λ = 355 nm, τ = 50 ps, ν = 10 Hz) and the pixel's morphology, structure, and optical behavior are presented and discussed.

P-8 XPS Analysis Of AuGeNi/Cleaved GaAs(110) Interface

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Chemical composition of Au-Ge-Ni along the entire volume of the thin layer acting as ohmic contacts on n-GaAs was investigated by XPS technique combined with in-situ Ar ion sputtering for every new cleaved surface. The purpose of the experiment was to study the obtaining of ohmic contacts in a new in situ device realised by metallic deposition on cleaved surfaces. A 200 nm metallic layer was deposited on n-GaAs cleaved surface in high vacuum and annealed at a 430° Celsius temperature for 5 minutes. A total of 18 sessions of XPS measurements and Ar etching sessions were performed until de metal/semiconductor interface has been revealed. The atomic concentrations of the chemical elements found were calculated and their chemical behavior investigated. Au4f, Ga3d, Ga2p, As3d, As2p, Ni2p3/2, Ge3d, O1s and C1s spectral lines were recorded and processed. The Au, Ge and Ni have a homogenous distribution while Ga and As tend to diffuse to the surface [1]. Oxygen is present in the first layers of the surface while carbon completely disappears after the second etching step. The existence of a AuGa alloy was detected and XPS spectra show only metal Ni and Ge within the layer and at the interface. As far as we now, in literature there are no studies about the depth profile chemical composition of

AuGeNi layer and the AuGeNi/GaAs interface by X-Ray Photoelectron Spectroscopy (XPS). Therefore, our research effort was to provide an extensive analysis for AuGeNi contacts on GaAs by using XPS combined with Ar+ sputtering to obtain depth profile information for the metallic layer and for the AuGeNi/GaAs interface. The main and original goal of our work is to determine the chemical composition and interdiffusion processes in AuGeNi film and GaAs at the interface.

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P-9 The effect of annealing temperature on structural, optical and electrical properties of MnS thin films prepared by SILAR

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MnS thin films were prepared on glass substrates by using Successive Ionic Layer Adsorption and Reaction (SILAR) method at room temperature. The annealing temperature effect on the structural, morphological, optical and electrical properties of the films was investigated. The X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) studies showed that all the films exhibited polycrystalline nature and were covered well on glass substrates. The crystalline and surface properties of the films were improved with increasing annealing temperature. The band gap values were changed from 3.19 to 3.05 eV depending on the annealing temperature. The refractive index (n), optical static and high frequency dielectric constants (εo, ε∞) values were calculated as a function of the annealing temperature. The electrical properties of the films were investigated and it was found that resistivity decreased with increasing annealing temperature.

P-10 An XPS study of the GaN layers grown on silicon by HVPE method

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Gallium nitride is a wide band gap (3.4 eV) semiconducting material with a high breakdown voltage and, as such, it is ideal for high frequency, high power and high temperature applications [1]. GaN thin films have been prepared by hydride vapor phase epitaxy (HVPE) in a horizontal quartz reactor. In a first stage, the AlN buffer layer was deposited at 1100oC on the silicon substrate. In a second stage, AlN and AlGaN intermediate layers were deposited at lower temperatures, followed by the GaN layer. Buffer layers were used to reduce lattice mismatch and substrate surface wetting characteristics incompatibility at the interface between the GaN thin film and the substrate. As transport gas, hydrogen purified with a palladium filter was used. Ammonia, hydrogen chloride, aluminum and gallium with 5N purity were used in the current experiments. The elemental composition in the surface of the GaN films was found by X-ray Photoelectron Spectroscopy (XPS). The XPS spectra revealed the signals of Ga 2p, N ls, Al 2p and O 1s peaks. The binding energies of Ga 2p and N ls electrons were approximately equal to those of GaN in the literature. The N:Ga molar ratio depends on the growth mechanism and deposition conditions. The effect of substrate temperature of buffer layers on the XPS spectra of GaN thin films will be discussed in the full-length manuscript.

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P-11 Development of Nb/Pb photocathodes prepared by pulsed laser ablation deposition for application in superconducting RF guns

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We propose a Nb/Pb photocathode whose configuration consists of a Pb bulk covered by a coating of Nb deposited using the pulsed laser ablation technique. The cathode was obtained masking the central part of a Pb disk by a circular shield of 1 cm in diameter while all the rest of disk was completely cover by a thick film of Nb. This clever configuration is useful in R&D of photocathodes for superconductive guns because the Nb coating of the cathode preserves the quality factor of the superconducting cavity made of Nb while the central part assures the photoemission from a robustness Pb bulk with better performances with respect to Nb. This device was characterised by an array of diagnostic techniques including scanning electron microscopy to deduce the morphology and by X-ray diffraction to obtain structure information on both Nb film and Pb bulk. The weak and strong points of this new concept of photocathode will be presented and discussed.

P-12 Plasma polymerization of aniline and dichlorobutyne for smart card applications

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The need for high performance electronics has led the scientific community to the recent development of organic devices. Printed electronics using organic conductive polymers present a series of advantages compared to classical electronics, like reduced costs, availability, versatility and simple processing. Among their disadvantages, low performance is a major bottle neck to be overcome. In this study, we report the deposition of polyaniline and polydichlorobutyne from suitable monomers onto plastic substrate by plasma polymerization. The aim is identifying the range of negative differential resistance (NDR) behavior in I-V characteristics and their correlation with the conduction mechanisms and space charge distribution. The deposited thin films were characterized by UV-VIS, FT-IR-Raman spectroscopy and AFM/STM/SEM topography. The polyaniline-polydichlorobutyne system show NDR ranged in 0.5 – 1 V, values that are closely related to requirements in designing of smart card devices based on tunnel diodes.

P-13 Compositional Analysis Of Amorphous, Conductive And Transparent Indium Zinc Oxide Thin Films

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The use of amorphous, conductive and transparent oxides (a-TCOs) is key for the development of transparent electronics, solar cells top electrodes and displays. By controlling their stoichiometry, a-TCOs can be used in thin film transistors (TFT channels, semiconductive behavior or as transparent electrodes, conductive behavior). Recently, room temperature deposited indium zinc oxide (IZO) and indium gallium zinc oxide (IGZO) were shown to exhibit a very good transparency in the visible range, low resistivity, and high mobility. The optical and electrical properties of IZO and IGZO thin films strongly depend on the In/(In+Zn) or In/(In+Ga+Zn) values. Therefore, the measurement of these ratios is critical for future developments and applications. Here we report on the relationship composition - properties of IZO and IGZO thin films synthesized using a Combinatorial Pulsed Laser Deposition technique. Monitoring of the thin films elemental composition was performed by Laser-Induced Breakdown Spectroscopy (LIBS), a technique that could be used for in-situ and real-time analysis and process control in case of a-TCOs fabrication. The analytical approach is based on plasma modeling, the recorded spectra being compared to the spectral radiance computed for plasmas in local thermal equilibrium. The relative fraction of indium and zinc measured via LIBS varied from about 60 to 90 and 40 to 10 at %, respectively and was very similar to values measured by EDAX, X-ray fluorescence, and Rutherford backscattering spectrometry. The optical properties (thickness profile and refractive index determination) of the combinatorial thin films, along its longitudinal direction were inferred from spectroscopic ellipsometry (SE). Complementary investigations have been performed by fitting the measured X-ray reflectivity (XRR) curves with simulated ones using a dedicated model to obtain the thickness and density of the deposited films. The room temperature electrical properties were investigated using typical four-point probe geometry and Hall measurements. These investigations helped us understand the interdependence between composition and properties in IZO and IGZO thin films.

P-14 Ar Ion Irradiation Effects On The Structure And Properties Of Polycrystalline SiC Thin Films

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Thin SiC films were grown on (100) Si substrates using the pulsed laser deposition (PLD) technique. Films were deposited under an atmosphere of CH4 at a substrate temperature of 1000 deg. C. Results of X-ray reflectivity investigations showed that films were dense, with mass density values from 3.15 to 3.20 g/cm3, very close to the tabulated value of single crystal SiC. X-ray photoelectron spectroscopy investigations revealed a low oxygen content in bulk, around 1-2 %, while grazing incidence X-ray diffraction showed that films were nanocrystalline. Nanoindentation results found hardness values around 40-45 GPa, the films being very hard. The deposited films were irradiated by 800 keV Ar ion at a dose of 1014 at/cm2. After irradiation, grazing X-ray diffraction investigations showed that the lattice parameter slightly increased, while nanoindentation results indicated a significant decrease of the hardness and Young modulus with respect to the values measured on as-deposited films. Raman investigations also showed that the ion irradiation induced changes in the films corresponding to the amorphisation of SiC film and the appearance of C-C bonds.

P-15 Characteristics Of Transitional Metal Nitrides Thin Films Grown By Pulsed Laser Deposition

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Thin ZrN and TiN films were grown by the pulsed laser deposition (PLD) technique on Si substrates at moderate temperatures, from 300 to 700 °C. By controlling the deposition conditions films with different grain sizes and chemical compositions were obtained. The deposited films exhibited good physical, chemical and mechanical properties (density, hardness, Young modulus) for application in nuclear industry and space exploration as hard and protective coatings under extreme irradiation and temperature conditions. X-ray reflectivity (XRR) measurements revealed mass densities of deposited thin films close to the bulk values while X-ray diffractograms showed that the films were <111> textured. Mechanical properties evaluated by nanoindentation were excellent, with hardness values in the 30-40 GPa range. The optical reflectance of the films was measured from the visible to the mid-infrared region to extract the dielectric function and the optical conductivity. The deposited films were irradiated with 800 keV Ar ions. After irradiation the modification of the crystalline structure and mechanical properties were measured to assess the effect of radiation induced defects in such thin films.

P-16

ZnO-SnO_2 Mixed Oxides For Gas Sensing Applications

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ZnO and SnO_2 are wide bandgap (Eg = 3.3 eV, respectively 3.6 eV) n-type semiconductors, with various applications as transparent conducting electrodes and materials in sensor technology. In this work we analyzed the gas sensing properties of ZnO-SnO_2 mixed oxides. The investigated samples were obtained by mixing Zn and Sn oxides in different concentrations, obtaining a powder which was uniaxially pressed and heat treated at 1100°, for 3 hours. The crystalline structure was investigated using XRD technique, while the surface characteristics were investigated with SEM. Quantitative analysis of the samples was found using the Rietveld full-pattern fitting method. The samples were tested as humidity sensors, with good sensitivity in the range 80-100 % relative humidity. The gas sesing properties were studied for three gases (acetone, ethanol and LPG) at temperatures varying from 20° up to 350°. A maximum sensitivity of 27 % was found at 175°C for LPG.

TOPIC 2

Fundamentals of Plasma and Laser-Material Interactions and Processing

PL-1 Silver nanoparticles from LASER ablation in liquids for surface-enhanced Raman scattering

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In the past years, laser ablation of a solid target in a liquid environment has been widely used in preparation of nanomaterials and fabrication of nanostructures, and a large variety of nanomaterials such as metals, metallic alloys, semiconductors, polymers, and etc, have been synthesized using laser ablation in liquids (LAL). Surface-enhanced Raman scattering (SERS) has showed promise in overcoming the low-sensitivity problems inherent in Raman spectroscopy for application of detecting and indentifying molecules. Colloidal suspensions of noble metal NPs are the most common SERS substrates, which enable us to provide enhancement factors of about 1010–1011 for dye molecules respect to the normal Raman signal of nonadsorbed molecules. Ag NPs is one of the most promising nanomaterials for SERS substrates. In this study, we have synthesized Ag NPs by laser ablation in liquids. The Ag target with 99.99% purity is fixed on the bottom of a quartz chamber and immersed in pure de-ionized water (18.2 MΩ). Then a second harmonic produced by a Qswitched Nd:YAG laser device, with wavelength of 532 nm, pulse width of 10 ns, laser pulse power of 50 mJ and repetition frequency of 5 Hz, is induced and focused onto the surface of the Ag target under the water layer thickness with 5mm. In this case, we evaluate the performance of the Ag NPs as SERS substrates by using R6G as the probe molecules. Spectra are excited by an argon-ion laser with incident wavelength of 514.5 nm. The synthesized Ag NPs showed the super SERS sensitivity, e.g., they can detect the SERS spectra of rhodamine 6G at concentration as low as 5×10-16 M, and have a EM EF on the order of 1012, which is much larger than that of the theory prediction (about on the order of 106–107), and reaching the single molecule detection requirement. These investigations thus showed that silver nanostructures with highly active surface can make the utmost of Ag nanostructures function as super-SERS-active substrates and multiple antibiotics.

Yang G. W. (2007). Laser ablation in liquids: applications in synthesis of nanocrystals. Progress in Materials Science, 52, 648-698.

PL-2 Two-Temperature Warm Dense Matter

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Laser materials processing has many scientific, medical and industrial applications. Ultrashort lasers are widely used in laser materials processing [1]. A better understanding of the quantitative details of the early time of the ultrashort laser solid interactions is important. The results provide the much needed details which can be used for detailed modeling and optimizing the processes in many applications. When a high intensity ultrashort laser pulse is absorbed by a solid target, a two temperature warm dense matter with electron temperature of several electron volts, ion temperature near room temperature and density remains as solid is formed initially in less than a picosecond. During the subsequent several picoseconds the electron temperature reduces and ion temperature rises and the heated target eventually disassembles into an expanding plasma. The ultrashort laser produced warm dense matter which lies in between the condense matter and plasma states is related to two forefront research areas in materials science under extreme conditions, namely, the warm dense matter science [2] and the high energy density physics[3]. In this talk, I will present results of our study on the time evolution of AC conductivity of two temperature warm dense gold [4]. In the experiment, freestanding 30nm-thick gold foils are excited by 400nm, 45fs (FWHM) laser pulses to energy densities up to ~4MJ/kg. Temporal evolution in AC conductivity of the resulting state is determined from simultaneous measurements of reflection and transmission of a chirped pulse probe at 800nm. This yields two important benchmarks for comparison with theory. The conductivity value at the end of the femtosecond laser pulse is a measure of its dependence on electron temperature as the ions remain cold. Subsequent changes then provide a measure of conductivity as a function of both electron and ion temperatures as thermal equilibration between electron and ion progresses. These data are compared with results from ab-initio quantum simulations [5] to extract information about electron heat capacity and electron phonon coupling coefficient of warm dense gold.

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PL-3 Nano-structuring of polymers by laser radiation

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Laser surface nano-structuring simultaneously at large areas can be done either by using colloidal nano-particle lens arrays deposited on the material surface or by using interference lithography. In the former case the dielectric nano-spheres serve as the near-field lenses when irradiated by the laser pulse. We show that here the individual colloidal particle cannot be considered as an independent lens; on the contrary, the mode coupling effects are significant. Nano-structured surfaces can be employed for numerous applications in photonics and biomedicine. The employment of high-power femtosecond lasers allows obtaining high-quality surface structures from ablation nano-craters and nano-bumps. In this communication, we report on the advantages of using bi-chromatic femtosecond laser pulses having both the fundamental-frequency (FF) and the second-harmonic (SH) spectral components. Experimentally, we show that conversion of a part of the beam energy into the second harmonic decreases the modification threshold and improves the localization of the structures. Theoretical consideration supports the experimental findings. Laser irradiation results in formation of either ablation craters or bumps. The features of the mechanisms of creation of such structures at nano-scales are discussed. Attention is paid primarily to laser swelling – the least studied but very promising effect, which is used first of all for the surface nano-structuring of polymers and glasses. Nano-structured materials can also be produced even by laser exposure without tight focusing if irradiation leads to the development of instability resulting in the formation of nano-clusters or nano-inhomogeneities in an initially homogeneous medium. As examples, we consider the photo-induced formation of metallic and semiconducting nano-clusters within dielectric matrices and the laser-induced bubbling.

PL-4 Low-temperature plasma processing for biomedical applications

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In this talk, recent experimental results on plasma surface functionalization of nano-structured materials for biomedical applications are presented. The main objectives are; (1) to fabricate nano-structured materials by various plasma processing, (2) to modify their surfaces by plasma chemical modification, and (3) to immobilize the desired materials onto the surface of nano-structured materials for biomedical application. In order to achieve the objectives described above, graphite-encapsulated magnetic nanoparticles, vertically aligned carbon nanotube dot-arrays (for a biochip sensor) and ZnO nanoparticles (as fluorescent materials) were used to investigate the low temperature plasma processing. With the graphite-encapsulated magnetic nanoparticles, we studied the plasma processing by using the two-step plasma treatment, Ar plasma pre-treatment followed by NH3 plasma post- treatment, to introduce the functional groups onto the surface of the nanoparticles. With conventional chemical procedures, the amino group population of magnetic nanoparticles having a typical diameter of 20 nm was evaluated to be about 8 x 104 molecules per nanoparticle. Immobilization of the antibody of influenza virus onto the surface of aminated magnetic nanoparticles has been carried out for aiming at developing the feasibility of the collection and condensation of virus. We observed a significant enhancement of collection rate of the influenza virus using the antibody-immobilized magnetic nanoparticles. The present result suggests the feasibility of the magnetic condensation method for rapid detection of influenza virus. This surface modification processing was also utilized in the case of the ZnO nanoparticles

as a fluorescent material for bioimaging application. As the second topic, the selective ultrafine surface modification of functional groups onto the polymeric substrate or vertically aligned CNT dot-array with a dot size of 5 μm and 50 μm spacing was investigated using the atmospheric pressure plasma jet with a nano/micro-sized capillary. The micro-sized surface modification of amino or carboxyl groups introduced onto the substrate were confirmed by the fluorescence labelling technique.

I-1 3D direct laser writing by multi-photon polymerization: physical limitations and possibilities for improvement of spatial resolution

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Direct laser writing (DLW) is a powerful technique that employs multi-photon photopolymerization for making arbitrarily-shaped three-dimensional solid structures with submicron detail for applications in biomedicine, photonics, optoelectronics, plasmonics, micro electro-mechanical and microfluidic systems, etc. [1] The structures are written by the focused beam of the ultrashort-pulse laser in the transparent resin. The polymerization is photoinitiated only in the focal spot of the beam due to the multi-photon absorption. After irradiation, non-polymerized resin is dissolved and washed away. The formation of sub-diffraction-sized features (e.g., single lines and voxels) is possible due to nonlinear response of the resin to the laser radiation. The common model for that relies on polymerization threshold, which is the minimal energy density that must be absorbed for local transformation of the initial resin into the insoluble polymer. Here, we discuss different physical mechanisms that could stand behind the phenomenological polymerization threshold. One of them is concerned with the radical quencher, which prohibits the growth of polymer macromolecules. Thus, the polymerization may occur only in the part of the irradiated volume where the quencher is totally consumed. Another mechanism [2] relies on the gel transition. For the cross-linking polymerization, the gel is the macromolecular network connected by the covalent bonds. Such network cannot be dissolved during the development stage, whereas the distinct macromolecules can be washed out. In order to avoid dissolution during the development, a polymerized volume must contain the gel fraction. The transition between distinct macromolecules and the polymer gel is the percolation-like connectivity phase transition, which has a sharp onset. We discuss the limitations imposed by the non-local phenomena, such as the diffusion of the quencher and size effects of the connectivity phase transition on the spatial resolution of DLW. We also discuss how to use some of those phenomena to improve the spatial resolution when writing both single nanofeatures and complex structures containing multiple nanofeatures at sub-diffraction distances [3].

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O-1 Behavior of historical printing inks on paper in HF cold-plasma discharges

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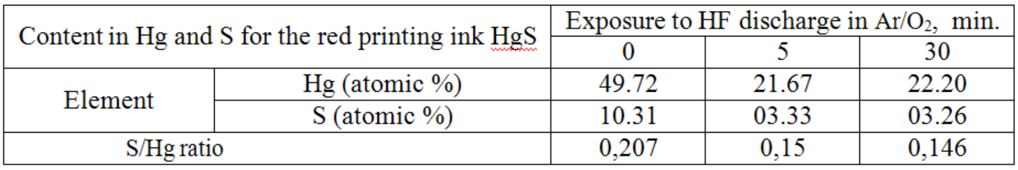
In case of cellulose-based materials, namely paper, HF cold-plasma treatment allows the activation of the surface and is also suited both for cleaning and decontamination purposes. A capacitively coupled HF cold-plasma unit designed for biologic decontamination, cleaning and polymer protective coating has been used for studying the behavior of 19th century printing inks on paper. The behavior of printing inks based on black carbon and red-colored cinnabar (αHgS) as pigments was studied in two working gases: inert (N2) and oxidative (Ar/O2). Changes in the pigments crystal structure was studied using scanning electron microscopy, energy dispersive spectroscopy, X-ray powder diffraction.



Content in Hg and S for the red printing ink HgS		Exposure to HF discharge in Ar/O_2, min.		
		0	5	30
Element	Hg (atomic %)	49.72	21.67	22.20
	S (atomic %)	10.31	03.33	03.26
S/Hg ratio		0,207	0,15	0,146

Chemical composition of the cinnabar-based ink layer in the oxidative (Ar/O2) plasma discharge

In Ar/O2 discharge the EDX data (Table 1) reflects the onset of a change in cinnabar-based inks, which can be associated with plasma exposure.

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O-2 The dynamics of the upper atmosphere and sporadic e layer of the ionosphere

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This article relates to research the cosmic space near the Earth to determine the effects of the action of various factors on the plasma in the ionosphere. It was found that sporadic E layer can serve as an indicator of the dynamics of the upper atmosphere. Statistical analysis of vertical sounding of the ionosphere with electromagnetic waves highlighted some important features of the temporal variation of the probability of formation of sporadic E layer. Are presented the research results link between dynamic processes in the E region of ionosphere and other experimentally observed effects - f0F2 critical frequency variations, the probability of F-spread phenomenon, the formation of multi-layered inhomogeneities and others. It is analyzed the influence of the sporadic E layer on the conditions of electromagnetic wave propagation of the navigation systems and telecommunications.

O-3 Langmuir probe investigations of a LASER produced plasma

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Pulsed laser ablation evolved in several directions such as medicine engineering or technological applications. As a result of this development the number of applications for laser ablation is impressive. Laser ablation is used in nano-structuring and patterning of polymers and silicon , in removal of biological tissue, cleaning of delicate artwork, elemental mass analysis, fabrication of waveguides by lase deposition, pulsed laser deposition for functional optical films, laser propulsion thruster for space transportation. Although the number of laser ablation’s applications is high, the study of the basic mechanism involved in the process of the material removal or in the plasma formation and evolution are proving to be quite difficult. For a better understanding of these complex processes, over the years, optical and electrical investigations and numerical simulations were performed.

In this paper we present an electrical study of a laser produced plasma on a Nickel target. The experiments have been performed in a stainless steel vacuum chamber pumped down to 10-5 Torr residual pressures. The radiation from a 3rd harmonic of a Nd-YAG nanosecond laser (355 nm, 5ns, variable fluences) was focused by a f = 25 cm lens onto the target placed in the vacuumed chamber. The estimated spot diameter at the impact point was 0.3mm. The Nickel target rotated during the experiments and was grounded from the vacuum chamber.

Two important phenomena were observed: a splitting in the transversal plane of the expanding plume which was attributed to a symmetry breaking process induced by the dissipative and the dispersive effects through changes in the ionization/recombination rates and a third plasma structure was observed for measurement angles close to the maximum expansion direction.

P-1 LASER-induced metallic solid nanostructured films: design and applications

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Nanostructured materials attained interest for many applications due to their size effects on the physical and chemical properties [1]. Actual technologies can fabricate these materials in various compositions, forms, and structures. Besides, a combination of different methods for investigation and validation provides more possibilities to design these nanostructured materials for targeted applications [2]. In this work we present a computer controlled design of some metallic submicro- and nanostructured substrates by direct laser writing (DLW) at the room temperature using metallic doped matrix. Optical microscopy investigations indicate a uniform size distribution of the particles inside of the structured patterns. The exception is the outside of the patterns, where the particles are very few and considerably bigger, probably due to the light spot scattering effect. Spectroscopic investigations reveal specific plasmonic responses and attenuation of the optical density connected with the process parameters. A spectral image processing algorithm, that simulates the functionality of these substrates in visible light, is used to show the effects of these materials when are applied on the color checker test image [3]. The algorithm converts the spectral image into CAT 02 color appearance model and then into RGB color space. Also, the algorithm reconstructs the spectrums of the substrates from the reflectance of the spectral image. This latter feature of the algorithm validates the capability of the substrates to act as optical spectral filters.

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P-2 Experimental plasma enhanced biodiesel reactor

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Current biodiesel production methods involve dissolving a catalyst, such as sodium hydroxide, in alcohol, then agitating the alcohol mixture with vegetable oil in large vats for two hours [1]. The liquid then sits for up to 24 hours while a slow chemical reaction occurs, creating biodiesel and glycerin, a byproduct that needs to be separated. This glycerin can be used to make soaps, but first the catalyst in it must be neutralized and removed using hydrochloric acid, a tedious and costly process. A microreactor based on the effects of high frequency cold plasma eliminates the mixing, the standing time and the need for a dissolved catalyst [2]. We designed, built and tested an efficient, fast and portable system that in the near future will enable farmers to produce a cleaner-burning diesel fuel substitute on their farms using seed crops they grow on their own land. In case of the biodiesel production in our cold plasma reactor, the high energetic electrons replace the conventional chemical catalyst during the transesterification reaction [3]. The non-thermal plasma being a highly reactive environment, a shorter reaction time is expected compared to the conventional transesterification process, which requires more than 60 minutes to be completed. Another advantage of the plasma reactor technology for biodiesel production is the easy separation or purification process due to no soap and glycerol formations during the plasma reaction.

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P-3 Effect of excimer laser beam spot size on carbon laser-produced plasma dynamics

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The effect of excimer laser spot size on carbon laser produced plasma dynamics is investigated. From ICCD fast imaging, at higher fluences, an unusual plume shape was observed, the laser crater effects leading to an arrow like plume geometry. The origin of such behavior was explained through the laser created crater profile measurements and space-resolved optical emission spectroscopy. The energy distribution in excimer laser focalization spot plays a significant role on laser plasma dynamics. For particular beam focalization an arrow type expansion process was observed, resulting from two colliding plasmas.

P-4 Investigations of hard TiC films grown by Pulsed Laser Deposition

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TiC films (400-500 nm thickness) were synthesized on Si substrates heated to 500°C by pulsed laser deposition using a KrF excimer laser source. The experiments were conducted in methane or nitrogen atmosphere at pressures of 10-4 to 10-5 mbar. The films surface morpholo-gy was investigated by scanning electron microscopy. Films thickness, profiles and surface features were extracted from confocal microscopy image processing. All films had very smooth surfaces and were very dense, as also indicated by the simulations results of X-ray re-flectivity curves. The films structure was investigated by grazing incidence and symmetrical X-ray diffraction. The use of a high laser fluence (~6 J/cm2) during deposition resulted in the synthesis of films with small crystallite sizes, which influenced the mechanical properties of the films. Hardness and elasticity of the films have been studied by nanoindentation. The variable pa-rameter was set to be the indentation depth, at no more than 25% of the film thickness. Lower indentation depths resulted in inconclusive results. The hardest coatings were obtained in ni-trogen atmosphere (Hit~35 GPa). Samples synthesized in methane ambient had hardness val-ues of ~ 30 GPa. The samples were quite rigid, with Young's modulus of ~300 GPa for films deposited in nitrogen and ~250 GPa for samples produced in methane atmosphere.

P-5 HiPIMS process optimization by external pulsed magnetic field

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In conventional high power impulse magnetron sputtering (HiPIMS) a large fraction of the sputtered material is ionized by the high density plasma formed near the target, in the magnetic field trap. Due to their positive charge, these ions are attracted by the target (negatively biased during the pulse) affecting their transport to the substrate, resulting in low target material deposition rates. This drawback can be overcome by applying a magnetic field of relative weak strength (up to 100 Gauss) in the region of the target which serves weakening the confinement of plasma electrons and allowing plasma to escape towards the substrate whilst enabling sufficient metal ionization. An external pulsed magnetic field was created with a current carrying coil surrounding the target in order to guide the deposition material through the substrate. The magnetic field generated by the coil is opposite to the magnetic field of the central pole of the balanced magnetron. The external magnetic field may be pulsed synchronously or it may be shifted in time with respect to the discharge. Radial distributions of ion current density, floating potential and optical emission intensity were measured for different magnetic field pulses and delays. Electrical measurements were performed using 8 concentric rings as probes. The electrical signals collected from each probe were simultaneously measured with a National Instruments data acquisition system (DAS) with 64 channels (8 acquisition boards NI PXI 6133 of 8 channels each), at a maximum acquisition frequency of 2 MHz. The deposition rate and the space-and-time ion distribution at the substrate position were significantly changed when the external pulsed magnetic field was applied. Moreover, uniform ion density distribution and deposition rate can be achieved by the appropriate choice of the strength and shape of the pulsed magnetic field and by adjusting the delay between coil current pulses and discharge pulses.

P-6 Laser produced plasma dynamics : a non-differentiable approach

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Ablation plasma has proven to be a very favorable environment for the development of instabilities and transitions from ordered to disordered (low and high dimensional chaotic) states, at the same time being a strong nonlinear dynamic system with many freedom degrees. Accordingly, at all possible space-time scales, the ablation plasma implies chaotic behaviors and self-similarity. For large temporal scales, the deterministic trajectories can be replaced by a collection of potential trajectories while the concept of definite positions by that of probability density.

Since non-differentiability appears to be a specific feature of ablation plasmas, a theoretical model based on Non-Standard Scale Relativity Theory with an arbitrary constant fractal dimension (value different from 2) can be developed. Therefore, the movement of the expelled particles on non-differentiable curves implies that all occurring interactions throughout the expansion of the laser-produced plasma will depend not only on space-time coordinates, but also on space-time scales, as the experimental results suggest. Therefore, it will be no longer necessary to use the classical "arsenal" of quantities. Moreover, the ejected particles may be reduced to and identified with their own trajectories so that by means of geodesics in a non-differentiable space-time, the ablation plasma will behave as a special "fluid" lacking interaction. In such conjecture, when studying the plume particle dynamics, one can use the non-differentiable hydrodynamic equations with isentropic viscosity stress tensor type, in dissipative approximation of motion.

TOPIC 3

Materials for Energy and Environment

PL-1 Materials for supercapacitors with high energy density

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Supercapacitors are advanced energy storage devices with characteristics between these of dielectric capacitors and those of conventional batteries. Supercapacitors can improve hybrid electric vehicles and electric vehicles performances. In some specific application, supercapacitors replace completely batteries. Safety, cycle and storage life, low temperature performance and cost are major concerns for successful application and commercialization of supercapacitors. Currently, our researcher groups are working on above supercapacitor materials and technologies in order to provide insight into how these electrochemical systems can be made more efficient. Many different types of supercapacitors are described in the literature. This work is dedicated to investigation of hybrid supercapacitors with Li intercalation compounds. Lithium technologies provide superior improvement of energy and power capability for hybrid supercapacitors. In our work, many efforts have been done for hybrid supercapacitors design and optimization of their performance, effective scale-up and also for the prognostics and diagnostics of their cycle life and storage life issues. Moreover, detailed mathematical modeling of electrode processes has been developed for fundamental understanding phenomena, which allow improving supercapacitor performance. In summary, we have developed different lab scale high-performance supercapacitors. The specific energy of such hybrid systems is at least twice higher than common supercapacitors based on activated carbon in both electrodes.

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PL-2 Low cost and high efficient, second generation thin film solar cells

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Photovoltaic power is forecast as a leader among other alternative energy sources for the future. Thin-film solar cells offer the advantages of low cost, light weight, and mechanical flexibility compared to bulk silicon devices used so far. For reduced cost, ITO, containing the expensive and scarce element Indium and serves as the transparent electrode, is replaced by ZnO. To further increase the efficiency of the devices, partial coverage of the interface between the upper electrode and the active layer with an array of mono-dispersed nanoparticles (e.g., Au, Ag) is used that provides an efficient trapping of the solar light inside the active layer via its plasmonic resonance, thereby offering increased light absorption without compromising charge collection. Different kinds of active layers are used to implement the thin film geometry such as: heterojunction films composed of polymer:fullerene, amorphous Si:H films, CIS /CIGS, etc. The metallic back electrode of the device, usually Al, Mo (for CIS/CIGS) may be also functionalized in a similar way as the front electrode with metal nanoclusters, for light backscattering into the active medium. ZnO-covered glass and the back electrode layers are prepared by pulsed laser deposition (PLD). The metallic nanoparticles are deposited either by a dual-PLD or in a post-deposition process. Organic and amorphous Si:H layers are prepared by spin coating and PLD, respectively. CIS/CIGS active layers are deposited by e-beam evaporation. After optimizing the efficiency of the device, further cost reduction may be achieved by employing sol-gel techniques for the compound ZnO electrode deposition.

Once the design and relevant parameters of such a single, model plasmon-enhanced solar cell is optimized, and in view of building monolithic solar cell arrays in the future, laser micro-scribing for each deposited layer will be applied to electrically interconnect the individual cells. This may further reduce the fabrication costs.

Financial support by the Greek General Secretariat for Research and Technology under the ERANet RUS program, STProjects-212, «FilmSolar» is acknowledged.

I-1 Preparation of $CuInSe_2$ thin films by the metal organic deposition process using organic metal salt

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$CuInSe_2$ (CIS) and Cu(In･Ga)Se_2 (CIGS) attracts much attention as a promising compound of the optical absorber for the solar cells, because it has a large absorption coefficient of the order of 10^5 cm^{-1}, which is approximately two orders of magnitude larger than that of crystal or amorphous silicon. CIGS-based thin film solar cells have attracted attention as a next-generation solar cell, having demonstrated high conversion efficiency and long-term reliability. These thin film solar cell have achieved conversion efficiencies exceeding 20% and are already being manufactured for sale in Japan, Germany, and the United States, with the conversion efficiency of solar cell modules exceeding 15%. Recently, a supply shortage in the market for metallurgical-grade silicon has been identified, and it is hoped that such solar cells will become low-cost thin-film replacements for the Si solar cells that comprise approximately 90% of current market share. The metal organic deposition (MOD) process using organic metal salt method is one of the growth of thin film by wet process and enables deposition on substrates that have an uneven surface or complex form. Furthermore, this method is a simple apparatus for the deposition of thin film, and the equipment used has a lower cost compared with sputtering and vacuum evaporation which are dry process used for a mass production line. Therefore, it can be expected for producing low cost of CIGS based thin film solar cells. Recently, we prepared CIS thin films by MOD process using organic metal salt to prepare large area solar cells applicable for the mass-production with low-cost. CIS thin films were grown by selenizing with Se ambient vapor in the Cu-In precursor thin films that were prepared by thermal decomposition of metal-naphthenates. Diethylselenide (DESe) was reported as a useful selenization source for the preparation of good crystallinity CIS thin films. Therefore, we expect preparation of CIS thin films with large area, mass-production and low-cost using this method. In this presentation, we introduce about the characterization and preparation of CIGS thin films by MOD process using organic metal salt.

I-2 Structural characterization of functional oxide materials

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Nowadays amorphous systems have again their renaissance. The knowledge of the short and medium range order is essential for understanding and interpretation of the physical-chemical and optical properties. We have studied two types of covalent glasses, i.e. alkali borosilicate and boromolybdate systems, being interesting both from basic and applied research. Alkali borosilicate based glasses are of significant current interest as suitable materials for isolating host media for radioactive waste material storage (i.e. UO3 or PuO2) [1-3]. We have undertaken a systematic study in this field, including preparation of new sodium borosilicate based glass series and their characterization by different methods. Here we present neutron- and X-ray diffraction study starting from the ternary Si-B-Na-oxide glasses, through the multicomponent Si-B-Na-Ba-Zr-oxide glasses up to the uranium loaded glasses [4,5]. The role of the components forming the network structure and making suitable the glass for incorporation of radioactive uranium-oxide will be discussed. Rare-earth molybdate phases exhibit a great variety of important physical properties including high ion- and electron conductivity of fast oxide ion conductors, non-linear optical response and luminescent properties. In contrast to crystalline molybdates, the preparation and structural information on amorphous molybdate systems is far not well known. Here we present our neutron- and X-ray diffraction study on Mo-Nd-B-oxide system prepared and studied by spectroscopic methods [6]. In order to get structural information, both the traditional Fourier transformation technique and the reverse Monte Carlo (RMC) simulation of the experimental data have been applied. RMC is a widely applied, successful method to generate reliable 3-dimensional atomic configurations and to calculate the partial atomic pair correlation functions, the coordination number- and the three particle angle distributions. The characteristics of the network forming structural units and the details of the atomic correlations are considered and discussed in the terms of glassy composition.

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I-3 Electron transfer and dye regeneration from new Co(II) complexes as electrolytes for dye-sensitezed solar cells

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We report the resuts of a combined experimental and theoretical study regarding a new series of mixed ligand Co(II) complexes, [Co(AA)(BB)2]X2, where AA and BB are derivatives of 1,10-phenanthroline and 2,2'-bipyridil, X=Cl-, TFSI- (TFSI= bis(trifluoromethanesulfonyl)imide), as redox electrolytes for dye-sensitized solar cells (DSSC). Compared to the I3-/I- system, the cobalt(III/II) polypyridyl complex redox shuttles have low visible light absorption, and the ease of tuning their redox potentials is a very significant aspect for accomplishing a photovoltage enhancement. In particular, our goal is to increase the open circuit voltage and the overall photovoltaic conversion efficiency of the device. The synthetic strategy of such heteroleptic compounds is a challenge due to the tendency of the Co(II) ion to form tris chelates compounds or to disproportionate and included in the first step the synthesis of [Co(AA)Cl2] and [Co(BB)2Cl2] complexes followed by the addition of the second aromatic diamine and TFSI anion. The compounds were characterized by spectral (IR and UV-VIS spectroscopy) and structural (X-ray diffraction) analysis. Density functional theory (DFT) calculations provided optimized geometries and IR spectra. Optical absorption spectra of all complexes were simulated using the time dependent (TD) DFT method, both in vacuum and in acetonitrile solvent. The simulated spectra compare well with the experimental data, allowing for a reliable assignment of the various transitions. We also performed calculations to understand the dye regeneration mechanism of three purely organic dyes, L0, D35, and Y123, in conjunction with three different cobalt(II) complexes: [Co(terpy)2]2+, [Co(bpy-pz)2]2+, and [Co(phen)2(bpy)]2+, respectively. Investigation of the electron transfer from the cobalt electrolyte to the oxidized dye was performed by calculating reorganization energies for high-spin and low-spin pathways, the latter being characterized by a lower energy barrier.

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O-1 Comparative study of window layer materials effects on the CdTe and CIGS thin films based solar cells

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The objective of the present work is the study of the effect of SnO_2 and ITO window layers on the performances of thin film solar cells based on CdTe and CIGS semiconducting materials. We focused on the essential characteristics of the solar cell, namely: The open circuit voltage Vco, the short circuit current Jcc, the form factor FF, the efficiency η and the spectral response of the cell. Our results were simulated with the calculation code SCAPS in one dimension that uses DC and AC electrical characteristics of thin film heterojunctions. We found that the cell based on CdTe gives the best performances with a SnO_2 window. Contrary, the cell based on CIGS gives the best performances with an ITO window.

Keywords: Solar cell, Thin films, Window layer, TCO, CdTe, CIGS, SnO_2, ITO, SCAPS.

O-2 Photovoltaic Devices Based On Binary Compounds With Nanostructured TiO2 Layers

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TiO2 thin films were prepared on glass substrates by radio frequency (RF) magnetron sputtering in a plasma environment of a mixture of Ar and O2 gases. Two sets of TiO_2 thin films were studied. The first set of undoped TiO_2 films was vacuum-annealed at 420°C for 30 min in the deposition chamber at a pressure of $4.0 \cdot 10^{-5}$ mbar and in hydrogen atmosphere at a pressure of $2.0 \cdot 10^{-3}$ mbar. A second set of TiO_2 films was doped with Nb and annealed under the same condition as the first set. All the films have been characterized by optical absorption spectroscopy and X-ray diffraction (XRD). The XRD study revealed that the annealed Nb-doped TiO_2 films exhibited a superior crystallinity with respect to the pristine titania ones. All band gap values obtained for TiO_2 thin films are in good agreement with the reported values from the scientific literature, 3.60 – 3.75 eV for the direct band gap and 3.05–3.20 eV for the indirect band gap. TiO_2/CdTe and TiO_2/CdSe photovoltaic devices were subsequently fabricated by CdTe and CdSe layers deposition on the Nb-doped TiO_2/glass substrates by close space sublimation method. We found that the photovoltaic parameters of the devices are influenced by the value of substrate temperature during CdSe and CdTe film growth. The highest efficiency values of about 2 % were obtained, while the fill factor was low for both TiO_2/CdTe and TiO_2/CdSe photovoltaic devices.

Hyojung Bae, Seung Hwan Park et. al.The Effect of Rapid Temperature Annealing with N2 and H2 on Photoelectrochemical Properties of TiO2. J. Electrochem. Soc. 2013 volume 160, issue 11, H800-H802.

O-3 Effect of surface modification Of PET by plasma on collagen and/or silver nanoparticles immobilization for biocompatibility and antibacterial activities improvement

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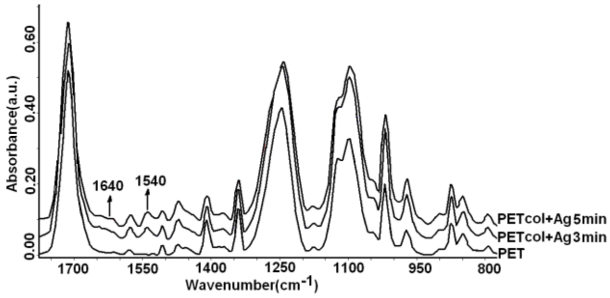
The use of silver as an anti-bacterial agent can be traced back to ancient times by the extraordinary wound- healing abilities of silver when incorporated into bandages,

or by silver salt of sulfadiazine proved to be highly efficient in reducing burn-wound sepsis [1], which is also currently the treatment for burn-wound therapy as it is active against gram-negative and gram positive bacteria, fungi, protozoa, and certain viruses. The creation of an anti-colonization and biocompatible polyethyleneterephthalate (PET) surface, by means of plasma followed by wet chemical modification to incorporate silver ions, is the focus of this publication. Two kind of chemical modifications were studied: one by using a sodium citrate/silver nitrate solution and the second one by using a collagen/sodium citrate/silver nitrate solution. In order for the chemical solution modifications to have the highest yield of collagen and/or silver possible in a reproducible fashion, the parameters of plasma treatments (time, power) were tailored.



FTIR measurements

Various surface characterization methods revealed the effects of the combined treatments on the polymer surface: x-ray photoelectron spectroscopy (XPS) analysis, contact angle measurements, atomic force microscopy measurements (AFM), Fourier transform infrared spectroscopy attenuated total reflection (FTIR-ATR) measurements and small angle x-ray scattering method. The combined surface modifications inhibited bacterial adhesion for both positive and negative gram-bacteria on the treated polymer and conclusions concerning the best combined parameters of plasma treatments were revealed. The results of this work suggest that the proposed surface modifications that incorporate silver ions would be extremely effective at reducing bacterial colonization to polymers. Acknowlegments The work has been funded by the Sectoral Operational Programme Human Resources Development 2007-2013 of the Ministry of European Funds through the Financial Agreement POSDRU/159/1.5/S/132395.

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P-1

Lithium electrochemical intercalation in Saponite

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The development of consumer electronics and limited stocks of natural resources demand constant quality improvement of parameters of lithium power sources. These factors determine the research advance of new substances and parameters of commonly used electrode materials. New materials have to provide high values of capacity, discharge voltage, current densities of charge/discharge processes and to be inexpensive and environmentally benign if possible. Considering the above mentioned demands Saponite became an attractive material for lithium power sources as it possesses a layered structure. The subject of this study is thermodynamic and kinetic parameters of process of Lithium electrochemical intercalation in Saponite. Raw natural saponite and saponite covered with polypyrrole were used with this purpose. The X-ray diffractograms of the solids were registered on DRON-3 diffractometer using CoKα radiation (λ=0.1790nm). Lithium cells contained lithium anode, saponite based cathode and 1M solution of LiClO4 in propylene carbonate. Electrochemical impedance investigations of saponite powders were carried out with PGSTAT-30 impedance spectrometer at open circuit voltage. The scan frequency range was 105-10-2 Hz and amplitude of the input signal was 5mV. Results of our investigation show well that both raw and modified saponite demonstrate different behavior as electrode materials of lithium power sources.

P-2 Synthesis of carbon xerogels-graphene composites under centrifugation

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Carbon xerogels containing rapheme are commonly synthesized via sol-gel polymerization of resorcinol with formaldehyde in the presence of rapheme oxide (GO) and acidic or basic catalysts. This study reports a variation on the classical method for carbon xerogel-graphene synthesis, where the xerogel cross-linking process is performed in a centrifugal field, resulting in monolithic cylindrical configurations. We synthesize resorcinol-formaldehyde-GO (RFGO) xerogels by sol-gel polycondensation of resorcinol with formaldehyde in the presence of GO as the acidic catalyst in centrifugal fields of various magnitudes (125G/75G/37.5G) – the final pyrolysis stage of the method reduces GO into rapheme. For comparison, we synthesize resorcinol-formaldehyde-graphene (RFG) xerogels without centrifugation, so we can investigate the effects of the process on the electrochemical and physicochemical properties (i.e. density, mechanical strength, porous structure and specific surface area) of RFG. This method allows for the control of RFG xerogel properties for applications of interest: electrodes for supercapacitors and for batteries, gas diffusion layers in fuel cells.

Keywords: carbon aerogel, rapheme oxide, centrifugation

P-3 Carbon xerogels as gas diffusion layer in PEM fuel cells

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We design a novel gas diffusion layer (GDL)/catalyst/membrane assembly using carbon xerogels as an alternative to the carbon paper which traditionally sustains the MEA assembly in proton exchange membrane Fuel Cells (PEMFCs). Xerogel synthesis requires the catalytic polycondensation of resorcinol and formaldehyde in the presence of an acidic catalyst, followed by aging treatment and pyrolysis at high temperatures. Platinum-ink, serving as FC catalyst, is directly sprayed on the xerogel plate and incorporated in the FC assembly by hot-pressing against a Nafion membrane. The integrated PEM FC presents a maximum current density between 600 and 800 mA for the given catalyst loading ─ 0.6 mg/cm^2.

Keywords: PEM fuel cell, carbon xerogel, MEA assembly

P-4 Graphene based materials as low cost hydrogen fuel cell catalyst

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Despite various technology upgrades to achieve a low cost and reliable proton exchange membrane fuel cell, there is still a pressing need for increasing the catalytic stability and durability. Among others advances, new carbon-based materials are

considered to be applied within Membrane – Electrode Assembly. Due to the high surface area, high conductivity, unique graphitized basal plane structure and potential low manufacturing cost, graphene nanosheets have been investigated as a support for low temperature fuel cell catalysts. The basic idea in these exploratory activities is the use of graphene as support material for platinum catalysts as fuel cell electrodes, with the expected effect o improving catalytic activity and decrease the platinum loading, with direct consequence of cost decrease. Within this paper, the partial results of an ongoing project, which is intended to implement graphene-based electrodes for the PEM fuel cells manufacturing line from NCHFC Ramnicu Valcea are shown and discussed. The first stage of the project was focused onto synthesis methodology and characterization of fuel cell graphene-based electrodes. Electrochemical proprieties and surface morphology of the electrodes were characterized using cyclic voltammetry, ac-impedance spectroscopy, electrochemical polarization technique, X-ray diffraction, and microscopic techniques. The main conclusion which arise from this stage of exploratory activity was that new graphene-based catalyst is a stable catalyst, by far, more affordable, than commercial standard system from production cost point of view, and moreover the synthesis technology is straightforward.

P-5

Ni- based catalysts for urea electrochemical decomposition

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Urea is a non-toxic, non-flammable hydrogen carrier which can be easily transported and stored. Electro-oxidation of urea in the presence of a Ni catalyst is considered an effective approach for hydrogen production via urea decomposition. In this work, three different catalysts based on Ni metallic particles were synthesized, characterized and used as catalyst for urea electro-decomposition. The physico-chemical properties of electro-catalysts were investigated by Scanning Electron Microscopy, Fourier transform infrared spectroscopy, Cronoamperometry and Cyclic Voltammetry. Electrochemical measurements showed that the Ni is an alternative catalyst material for applications in waste water remediation, hydrogen production and fuel cells.

Keywords: Ni- catalysts, urea decomposition, hydrogen production

P-6

PVA membrane for urea fuel cells

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Urea Fuel Cells employ a non-toxic, non-flammable and transport-friendly fuel that can be easily recovered from waste water. The present study investigates the properties of an anion exchange polyvinyl alcohol polymer as membrane for urea fuel cells. The physico-chemical properties of the polyvinyl alcohol polymer membrane are investigated using FT-IR spectroscopy, thermo-gravimetric analysis, dynamic scanning calorimetry and electrochemical impedance spectroscopy. An anion exchange membrane-electrode assembly was tested in urea/air fuel cell system, with Ni catalyst load of 20mg/cm^2 at anode and Pt catalyst load of 1mg/cm^2 at cathode, reaching a maximum current density of 10-50 mA/cm^2 at a voltage of 0.4-0.5V, for different urea concentrations, ranging from 1 to 7 M.

Keywords: urea fuel cells (UFCs), PVA membrane

P-7 Cylindrical carbon xerogels as all-carbon electrodes in supercapacitor assemblies

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Carbon xerogels are traditionally synthesized via the catalytic polycondensation of resorcinol and formaldehyde in the presence of an acidic catalyst, followed by aging treatment and pyrolysis at high temperatures. A variation of the classical method isolates the xerogel cross-linking process in a centrifugal field, resulting in monolithic cylindrical configurations; such monoliths are then employed as all-carbon double electrodes in supercapacitor assemblies, where they are infused with a gel electrolyte acting as both ionic provider and separator. We test both inorganic (acidic) and organic ionic liquids as electrolytes, and the xerogel porosity (as a function of the synthesis parameters) is correlated to the electrical properties of the assembly. Finally, the performance of the xerogel supercapacitor is compared to all-carbon capacitors built with more traditional materials, e.g. activated carbon.

Keywords: Carbon xerogel, centrifugation method, supercapacitor electrodes

P-8 PEMFC- in cylindrical geometry with carbon xerogel as gas diffusion layer

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The consumption of fossil fuels and the need for clean energy has lead to the fast development of renewable energies and especially of fuel cells. The classical configuration, 2D membrane electrode assembly (MEA) has permitted the development of fuel cells stacks, with increased voltage and current density up to 1000 mA/cm^2 respective and specific weight of ~4 g/W. To improve performances and reduce the specific weight and cost, there is a need for new approaches in fuel cells design. In this respect, the study deals with a new geometry of PEMFC developed on cylindrical carbon xerogel synthesized using a proprietary technology. Cylindrical PEMFC could be considered an improved alternative to the classical configuration. At the standard Pt loading for anode and cathode (0.3 mgPt/cm^2, respectively 0.6 mg Pt/cm^2) and Nafion membrane the PEMFC reach similar performances at lower specific weight around of 1-2 g/W.

Keywords: PEMFC, xerogel, catalyst, centrifugal

P-9 The influence of iron dopant on TiO_2 structure of sol-gel nanopowdwers with photocatalytic properties

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Chemical methods, such as sol-gel process, allow various possibilities of synthesis of oxide materials with different structures, compositions and morphologies and provide especially an attractive route for TiO_2 nanomaterials recognized for their photocatalytic

properties. TiO_2 is well-known as an excelent photocatalyst that permits the degradation and finally the mineralization of xenobiotic compounds from water. Enormous studies have been focused to the research of TiO_2 material, which led to many promising applications in different fields, ranging from optics to gas sensors via solar energy. These applications can be roughly divided into „energy“ and „environmental“ categories, many of which depending not only on the properties of the TiO_2 material itself but also on the modifications of the TiO_2 material host and of its interactions with the environment. Generally, doping of TiO_2 with transition metal cations was reported as a good tool to improve the photocatalytic properties and for enhancement of visible light response. In the present work, un-doped and 0.5, 1, 2 and 5 wt% Fe-doped sol-gel TiO_2 nanopowders have been prepared and structurally characterized. The study clears up the correlation between the structure, magnetic properties and photocatalytic activity underlying the role of Fe dopant on morpho-structural changes of TiO_2 nanopowders. The influence of iron on TiO_2 crystallization was studied in detail based on an own calculus program. Lattice parameters, crystallite sizes and internal strains, as a measure of the structural disorder, were determined. XPS and magnetic measurements completed the structural data study. The photocatalytic activity of the prepared nanopowders has been tested in the degradation of nitrobenzene from water. The sample with 0.5 wt% Fe dopant concentration thermally treated at 400°C presented the best photocatalytic activity.

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P-10 Comparative structural study of sol-gel cobalt and nickel doped TiO_2 nanopowdwers with photocatalytic properties

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In the last time the photochemistry of nano semiconductor particles has been one of the fastest growing research areas in the physical chemistry field. The semiconductor assisted photocatalysis is considered an economic and environmental friendly water treatment technology in order to efficiently remove the organic pollutants from wastewaters. In search for a photocatalyst with optimal features, titania remains a benchmark against which any alternative photocatalyst must be compared. Although titania presents well recognized advantages as high photocatalytic activity, chemical stability, long-term stability, nontoxicity, and relatively low price, it also has the drawback of a limited photocatalytic activity to irradiation wavelengths in the ultraviolet (UV) region. In order to extend the TiO_2 spectrum response to the visible light region, many attempts have been made, such as doping with transition metals. The doping can be produced in different ways, one of the most employed being the sol-gel method. The aim of the work was to study the effects of Co and Ni dopants on TiO_2 structure of sol-gel prepared nanopowders. Un-doped TiO_2 and 0.5, 1 and 2 wt% Co and/or Ni-doped TiO_2 nanopowders have been prepared. A detalied XRD analysis, based on an own calculus program, has established the lattice constants, the average size of the crystallites, and the average lattice strains, which can give some information about the structural disorder. The structural changes due to the thermal treatment and the dopants concentration were established. The concentration of 1 wt% Co and Ni dopant thermally treated at 400°C ensures the best photocatalytic activity in the advanced degradation of nitrobenzene from water.

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P-11 Quantum chemical modeling of adsorption of molecular oxygen and its compounds on the spinel $NiCo_2O_4$ surface

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Reduction of oxygen on the surface of a heterogeneous catalyst can occur in the presence of molecular adsorption, which exist on the surface during the collision of protons with adsorbed molecules and the formation on surface structures such O_2H-, H_2O_2, H_2O-OH-. The limit reasons of time-life of molecular adsorption are a rapid transition of O_2 in the gas phase and dissociation into atoms [1, 2]. The process of oxygen electroreduction in acidic medium can pass through two main mechanisms: 2- and 4-electron. In order to identify the electronic factors which influence on an activity of the catalyst, based on the direct spinel $NiCo_2O_4$, were performed ab initio quantum-chemical calculations of the electronic structure of stoichiometric molecular cluster $NiCo_2O_{10}N_{12}$, oxygen adsorption complex $NiCo_2O_{10}N_{12}$-O_2 and adsorption complexes of oxygen compound. Quantum-chemical calculations were done by MO LCAO - method in the extended Gaussian basis functions with full optimization of geometrical parameters [3]. According to the calculation results, O_2 molecule adsorbed on the Co-cation associated in the curved fragment form on the neutral cluster $NiCo_2O_{10}N_{12}$. A weak coordination bond 2.37 Å length and the binding energy of 0.3 eV were formed between molecules and clusters. In the case of the adsorption on the electronegative cluster, molecule of O_2 reacts with cobalt cations with formation of two, approximately equal length of Co-O, adsorption bonds. It was shown that due process $2ZO_2 + 2e + 2H+$ on the cluster surface can be formed structure HO-OH, where Z - center adsorption. The calculated binding energy between the cluster and the HO-OH is set to 1.10 eV. In the case of HO-OH desorption from the surface, the process of oxygen reduction will end by formation of peroxides. If the desorption is absence, recovery process of O_2 will be continue until the formation of water according to the scheme: 1) $ZO_2H_2 + 2\ e^- + H^+ \rightarrow ZH_2O_2H^-$, 2) $ZN_2O_2H^- \rightarrow ZOH^- + H_2O$ (desorption). It is important to note that the adsorbed water molecules can form strong one-center adsorption Co-O bonds with the cluster cations with reducing efficiency of the catalyst.

P-12 Alkaline fuel cells cased on carbon xerogels and Raney type Ni catalysts

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Skeletal nickel alloys, notably Raney type alloys, constitute promising catalyst materials for low temperature alkaline fuel cells. The aim of this work is to investigate skeletal nickel catalysts used for hydrogen oxidation reactions (HOR).We employ thermionic vacuum arc deposition to obtain Ni - Al thin films. The method implies the use of two independent, constant electron beams emitted by externally heated cathodes inside a vacuum chamber. The resulting Ni - Al alloys were leached at 850°C, followed by a conventional activation process with concentrated sodium hydroxide solution (20 wt% in water). The characterization of the Ni - Al thin films is performed by SEM; skeletal nickel nanostructures oxidation potentials are evaluated by cyclic voltammetry and tested in an alkaline fuel cell to define open circuit potentials and maximum current densities.

Keywords: AFC, electric arc deposition, skeletal nickel catalyst

P-13 Magnetic nanocrystalline ribbons for energy harvesting devices

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An energy harvesting device based on nanocrystalline ribbons, able to convert mechanical vibrations to electricity is presented [1]. A multilayer cantilever beam based on the magnetic nanocrystalline ribbons was implemented to build an energy harvesting device with superior characteristics (voltage and power) comparing with piezoelectric or pure magnetostrictive devices. The value of the induced voltage depends on the acceleration and frequency spectrum of the vibrations, geometry of the multilayer amorphous ribbons beam, number of turns for the surrounding coil, but especially on the magnetic and elastic properties of the nanocrystalline ribbons. Different types of nanocrystalline ($Fe_{52}Co_{28}B_{13}Nb_4Si_2Cu_1$, $Fe_{73.5}Si_{13.5}B_8$ $Nb_3Cu_1Ta_1$, $Fe_{73.5}Si_{13.5}B_9Nb_3Cu_1$) ribbons obtained by melt spinning have been used and their magnetic and magneto-mechanic properties were optimized by using different annealing and annealing in magnetic field. The influences of the fabrication parameters and annealing on the magnetic properties have been monitored by magnetic measurements (hysteresis and permeability). By increasing the relative magnetic permeability trough annealing, we almost doubled the output voltage of the energy harvester device. The power density achieved for our harvester using nanocrystalline ribbons is 45mW/cm^3 at 1g (resonant frequency 60 Hz) and seems to be among the highest reported in literature.

A wireless sensors monitoring system was built using a combination of ultra low power MSP430F2274 microcontroller and CC2500 2.4-GHz wireless transceiver. We used Texas Instruments SimpliciTI™ wireless communication protocol to set up a simple network in which network sensor nodes, powered by the harvesting device, communicate sampled data from embedded sensors (temperature, voltage, acceleration, etc.) to a network access point.

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[1] Application patent No. a 2013 00158 - State Office for Invention and Trademarks Romania (2013).

P-14 New solutions for collecting wind end solar energy

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One of the main objectives of mondial energy politics have as a purpose the reduction of energy consumption,the increase of energy supply security , the protection of the environment and the development of viable energy technologies, it is represented by the development of renewable energy collecting systems. At present new solutions and technologies for collecting wind energy are being needed, which alongside the solar energy collecting systems, will be applied to ensure the necessity of energy for relatively isolated urban areas. The collecting of wind energy in the urban environment is a real problem due to the wind variation determined by pertubations which exist in these areas especially in the presence of buildings. Starting from these problems the objective of this work is based on presenting some actual sistems for collecting wind end solar energy which can serve small communities or can be connected at the National Energy System. These systems adapted for urban areas can be placed in any other location because their architecture can be framed in the traditional urban architecture.

Keywords: wind energy, hibrid wind-solar systems

P-15 Assessment the possibility of reducing the impact on shoreline using actual sistems of collecting waves and marine currents energy

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Renewable energy sources of the planet, as those provided by the planetary ocean waters can be collected and transformed in useful energy. The use of these especially in the coastal areas and shore which represents 15% of the land, with a 40% concentration of the population of the earth, it will ensure the necessity of energy. Collecting technology of those energies have known an accelerated progress in the last period of time. With all of these no optimal cost-efficiency reports haven't been obtained. Although these systems represent the starting point for the new technologies which will allow the collection and stocking of energy which the planetary ocean has. In this respect the present work represents an assessment of how current technologies to collect energy of waves and marine currents can be used to reduce the impact on shoreline.This aspects will serve as a beginning of reports for the new systems and technologies which collect wave and marine currents energy, regarding the environmental protection and in special the shore ones.

Keywords: waves energy, impact, shoreline protection

P-16 Thin film of Yttrium doped bismuth ferrite obtained by pulsed laser deposition

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The perovskitic materials such as bismuth ferrite (BiFeO3, BFO) were intensive studied in last period of time due their small band gap value. BFO is a ceramic material with perovskite structure high remnant ferroelectric polarization (95 μC/cm2) and Curie temperature (Tc~1103 K), that simultaneously exhibit both ferroelectric and ferromagnetic properties The band gap value (Eg~2.8 eV) corresponding to maximum absorptivity at visible wavelengths [1], is much smaller than most of the ferroelectric materials. If a doping is used (with Yttrium for example) an additional sub-band will be created within the charge gap of the material. Doping bismuth ferrite with Y atoms the values of band gap can be changed from Eg=1.90 to Eg=2.57 for 5% and 10% Y doped BFO. Also the band gap value can be changed by different annealed temperature, from Eg=2 eV to 2.57 eV [2] for 5% Y doped BiFeO3. In this work, Y dopped BFO thin films were deposited using pulsed laser deposition method (PLD) with a ArF excimer laser on Nb doped SrTiO3 substrates. The purpose of this study was to obtain thin films of Y:BFO with different values of band gap which make this material a candidate for photovoltaic applications. A parametric study on the influence of substrate temperature and distance between target and substrates, on the properties of the Y:BFO thin layer was carried out. Crystallinity properties and topography of surface of Y:BFO thin films were studied using X-ray diffraction and atomic force microscopy (AFM). Optical properties have been investigated using spectroscopic ellipsometry (SE) witch is non-destructive and precise technique. Thicknesses of the films and of their rough layer are extracted from Cauchy-Urbach model. The dispersion of the refractive index and extinction coefficients in the 300 − 1700 nm range were calculated using a Lorentz oscillator model witch is fully Kramer consistent. The values of band gap were determined from Tauc plot.

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P-17 Photocatalytic property of titanium dioxide thin films deposited by radio frequency magnetron sputtering in argon and water vapour plasma

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Titanium dioxide is one of the most studied photocatalytic semiconductors due to its chemical stability, non toxicity, theoretical relevance, and low cost. The photocatalytic activity of TiO_2 surfaces is related to hole and electron photogenearation and their subsequent redox reactions with surface adsorbates. Various techniques as impurity doping, charge separation, and control of structure and surface morphology have been used to enhance the TiO_2 photocatalytic activity [1]. The present work is investigating the photocatalytic activity of TiO_2 thin films deposited by radiofrequency magnetron sputtering of a pure TiO_2 target in Ar and Ar/H_2O plasmas. In a previous work [2] we have shown that using relative high values of Ar pressure (1.3 Pa) determines deposition of amorphous TiO_2 thin film with excellent photocatalytic activity. Also, it has been proved that adding H_2O vapour in the deposition chamber determines a noticeable increase in the electric conductivity of the deposited films [3].In the present work we use Ar/H_2O gas (ratio 10/1) at a pressure of 4 Pa to deposit amorphous oxyhydrogenated TiO_2 thin films with improved photocatalytic activity. The film structure, surface morphology and photocurrent decay in nitrogen and oxygen were studied in order to elucidate the mechanism of the improved photocatalitic activity of the deposited films.

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P-18 Photocatalytic properties of Nb doped TiO_2 thin films

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The present communication reports the structural, morphologycal, optical, hydrophilic and photocatalytic properties of the undoped and Nb doped TiO_2 thin films deposited by using sol-gel (spin coating) technique on glass substrates. The samples are amorphous as shown by X-Ray Diffraction analysis. The AFM studies revealed very smooth surfaces for all the studied films, with root mean square roughness that increases with the increase of the Nb content, but not exceeding 5 nm. Hydrophilic investigation showed that, by increasing the Nb amount in pristine titania films, results in superhydrophilic surfaces, even in the absence of the UV irradiation. The optical band gap shifts towards higher energies, by increasing the Nb content in the films. The photocatalytic properties were investigated via oleic acid decomposition under UV irradiation.

P-19 The influence of the Mo content on some physical properties of the titania thin films

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Titanium dioxide is well known for its remarkable hydrophilic and photocatalytic characteristics under UV irradiation. Increasing surface area and doping can enhance these properties, and can make this material to be absorbent in the visible domain.

In this paper, we have studied Mo-doped TiO_2 thin films deposited by spray pyrolysis on different substrates (glass and Si). This method allows to obtain rough pronounced surfaces. The structural studies showed the formation of anatase, or anatase/rutil mixed phases, depending on the used substrates. Mo enters in the TiO_2 matrix as Mo^{5+}, determining a slight red shift of the absorption edge. From FT-IR analysis performed before and after irradiation, providing information on the relationship between hydrophilicity and the amount of the adsorbed hydroxyl groups, we certify once again that the anatase phase (present in proportion of 100% in the films deposited on glass) is superior concerning the hydrophilic properties. Mo enhances wettability for the films deposited on silicon, compared to the undoped one, even if determines a rise in the rutile weight percentage, as a combined effect with the substrate nature. The photocatalytic measurements confirms that titania films with higher hydrophilic performances are also good photocatalysts, confirming in fact that investigating the hydrophilic properties of these films constitutes a much simpler way to obtain information on their photocatalytic activity.

P-20 Depositing Pt on Cr doped TiO_2 thin films surface to improve the hydrophilic properties

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We have prepared TiO_2 thin films doped with increased amounts of chromium by RF reactive sputtering. We have examined the influence of Cr doping on the films structure, morphology, optical band gap and hydrophilicity. All the deposited films were polycrystalline with the presence of anatase and rutile phases. With the increase of Cr content, the weight percentage of the rutile phase increases. The AFM studies revealed very smooth surfaces for all the studied films, with roughness values increasing from 0.97 nm for the undoped sample, to 2.19 nm for the sample with the highest Cr content. Cr determines a significant red shift of TiO_2 absorption edge, which is important in self cleaning. Unfortunately, the Cr doped films did not show promising hydrophilic properties. To improve them we have applied a novel surface modification method, reported in literature for powders, namely, surface metallization. We have observed that, by depositing Pt islands on the film with the highest Cr content, its hydrophilic properties improve for a certain metal coverage area. The explanation was made based on FT-IR analysis for the irradiated and non-irradiated films which gives information on the relationship between hydrophilicity and the amount of the adsorbed hydroxyl groups.

P-21 Tuning the properties of Graphene quantum dots towards application as organic sensitizers

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The study aims to emphasize the auspicious potential of an essentially luminescent graphitic material for future implementation as active layer in organic photovoltaic devices [1]. A few nanometers size aqueous solution-processable GQD with different surface functionalities were synthesized through a bottom-up approach , specifically microwave assisted hydrothermal method using D-(+)-Glucose, D-(+)-Glucosamine hydrochloride and 2-Amino-2-(hydroxymethyl)-1,3-propanediol as the main carbon source. Crystallinity of colloidal nanoparticles was evidenced by HR-TEM analysis and the average particle size was established around 4 nm. XPS t[ns]) features of photoluminescence and to enhance quantum yield (ΦF) to over 7%. Further, cyclic voltammetry was performed using 0.1 M TBAP electrolyte prepared in ACN purged with nitrogen,in order to determine HOMO and LUMO values. Finally, GQD nanostructures were attached on titanium oxide surface in a typical solar cell assembly and dark current analysis was used to determine the ligands present on the surface and their chemical state relative concentration. By carefully choosing the appropriate surface functionalities enabled us to control optical properties like optical bandgap energy (Eg), static (PL) and lifetime (I(V) characteristics along with open-circuit potential (Voc) and short-circuit photocurrent density (Jsc [mA/cm^2]) were recorded. During electrical characterizations the cell active area of 0.36 cm^2 was illuminated with a broad band ozone-free Xe source through a standard AM1.5G filter, at a power density of 1 Sun (100 mW/cm^2). Acknowledgements: This work was supported by the strategic grant POSDRU/159/1.5/S/137750.

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P-22 Humidity sensors applied characteristics of tungsten spinel and hexaferrite materials

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Ceramic materials and especially ferrites show a particular importance because of potential applications in various fields such as electronics, sensors and actuators [1-5]. In this study are investigated the humidity sensors applied characteristics of Cu-Zn spinel ferrite and Ba hexaferrite with various tungsten substitutions. Although ferrites are magnetic materials, their electrical properties indicate them to be useful for humidity or gas sensors. From this perspective, our analysis highlights their usefulness, according to their conductivity, for both resistive and capacitive sensors. The comparative sensitivity, response and recovery times characteristics of humidity sensors based on tungsten spinel and hexaferrite materials are analyzed.

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P-23 Advances in laser-scribed planar supercapacitors

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Past studies have documented various implementations of direct laser writing on graphite oxide (GO) thin films, accounting for the latest developments in printing and lithographic techniques for patterning microscale supercapacitors. Further improvements in the technology of laser-scribed supercapacitors need to focus on scalability and form factor. The present work expands on the theme of electrode geometry by investigating pseudo-fractal patterns that capitalize on scaling parameters to account for vastly increased internal lengths over finite surfaces. Fractals are generated by simple iterative algorithms that can result in space-filling curves, whose length-to-surface ratio increases with the number of iterations, pertaining to a fractal dimension that converges at two at the upper bound - for a unit Euclidean dimension of the fractal curve. We examine the implications of design (stacking and orientation) and the effects of resolution (dictated by the laser operating parameters) on the geometrical properties of the imprinted electrodes, the electrochemical properties of the supercapacitor and the scaling potential of the device. We suggest a number of architectural implementations of the above (photolithographic) principles to produce 2D (planar) supercapacitors, employing either self-standing GO films or GO deposited on flexible substrates, e.g. PET, PET-ITO.

Supercapacitors, graphite oxide, fractal geometry

P-24 Investigations of Ar ions irradiation effects in ZrC thin films grown by pulsed laser deposition

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Thin ZrC films (<500 nm) were grown on (100) Si substrates at a substrate temperature of 500 oC by the pulsed laser deposition (PLD) technique using a KrF excimer laser under CH4 or N2 atmosphere. Grazing incidence X-ray diffraction showed that films were crystalline, with crystallites sizes in the range of 15-30 nm and exhibited rather large values of micro-stresses. Modelling of the X-ray reflectivity curves recorded from the deposited films indicated that the films were very dense and smooth. X-ray photoelectron spectroscopy showed that films contained small amounts of oxygen, incorporated into an oxy-carbide type of compound. The films were used to study the effect of 800 keV Ar ion irradiation on their structure and properties. After irradiation with a dose of 1014 at/cm2, the lattice parameter and crystallites average size did not significantly change. However, after irradiation with a 1015 at/cm2 dose, a clear increase in the lattice parameter accompanied by a significant decrease in nanohardness and Young modulus were observed.

P-25 Photocatalytic ZnO for air purification applications

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The photocatalyst materials have various functions, such as self-cleaning, antifogging, antibacterial actions, deodorization or decomposition as removal of pollutant. These effects of photocatalyst's functions are the responsible for the development of a broaden range of so called smart materials used constructions. TiO2 and ZnO are most widely used semiconductor photocatalysts due to their high photosensitivity, photochemical stability, large band gap, strong oxidizing power and non-toxic nature. In particular, anatase TiO_2 has been reported as the most extensively used semiconductor photocatalyst for industrial applications and pollution clean-up since 1970s. Recent reports highlight ZnO to show an even better activity than TiO2 in the photodegradation of some dyes in aqueous solutions, since it can absorb more light quanta. The successful exploitation of such catalysts requires the development of techniques for controlling their size, morphology, structural and surface characteristics, as well as efforts to enhance their photochemical response to visible/solar Pillumination. Up to date, there are quite few reports in the literature presenting state of art approaches of use of ZnO material onto textile substrates for several applications as antibacterial, deodorizing and UV protection, and none regarding any systematic approach of direct growth and optimization with respect the textile support. More than that, up to our knowledge, there is no available study in the literature about ZnO coated textiles used as photocatalytic active support for gaseous compounds decomposition. The present presentation will present recent advances on photocatalytic ZnO onto textile supports for air purification applications.

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P-26 New Fe-based highly active catalysts containing an imidazolium salt and a Schiff base for the removal of pollutants

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Numerous studies have reported a great variety of pharmaceuticals and personal care products (PPCPs) in concentrations of ng/L to µg/L in sewage treatment effluents, rivers, surface and ground waters, and drinking water. Even at low concentrations, these pollutants may still have chronic effects if continuously released into the environment. This is the case of carbamazepine (CBZ), an antiepileptic pharmaceutical. Due to its ubiquitous presence in the aquatic environment, carbamazepine has been reported as an anthropogenic marker of urban pollution [1]. Because of the large volumes of micropollutants released into the environment, as well as their bio-persistence and bio-accumulation, their removal by conventional methods is difficult and costly. Therefore, these compounds should be removed from water supplies before being discharged into general aquatic environments. The scope of our study was to prepare Fe-based highly active catalysts for water treatment processes. To prepare such catalysts, stable ligands are essential. Taking this into consideration, we proposed ligands that contained both an imidazolium salt and a Schiff base moiety, which have been previously reported to be suitable candidates for synthesis of multifunctional catalysts [2]. The sensitized catalysts were characterized by X-ray diffraction, vibrating sample magnetometry, scanning electron microscopy, and energy dispersive X-ray spectroscopy. Important variables such as effect of hydrogen peroxide concentration, UV light, the amount of catalyst and contact time for the catalytic wet hydrogen peroxide oxidation of CBZ were examined. In addition, the oxidation products were analysed using high performance liquid chromatography (HPLC/MS). The results indicate that after only 15 minutes at room temperature, 200 µmol/L H2O2 and 1g/L catalyst, under UV light, without the significant leaching of Fe ions, the CBZ removal was completely removed at pH=6.6. By using these catalysts, is possible to extend the range of pH values for which Fenton-type oxidation can occur and no iron hydroxide sludge is formed. Acknowledgement: The present work was supported by the CNCS–UEFISCDI through the national grant PN-II-ID-PCE-2012-4-0477.

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TOPIC 4

Magnetic Materials and Spintronics

PL-1

Bulk Fermi surface and electronic properties of the Rashba spin-split semiconductors BiTeX (X=Cl, Br, I)

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The V-VI-VII semiconductors BiTeX (X=Cl, Br, I), with strong spin-orbit coupling and without inversion symmetry, have attracted considerable attention as candidates for spintronic materials. Similar to the effect of time-reversal symmetry at the surface of topological insulators, spin-orbit interaction can also lift the spin degeneracy of electrons, this time in the bulk of these non-centrosymmetric semiconductors, giving rise to a large bulk Rashba spin-splitting of their electronic bands. The existence of surface states has also been established, and BiTeCl was even found to be an ambient pressure topological insulator. We combined Shubnikov-de Haas (SdH) oscillations and optical spectroscopy experiments in order to characterize the electronic properties and Fermi surface of the Rashba spin-split semiconductors BiTeX. I will show that the quantum oscillations observed in our data clearly originate from the bulk Fermi surface in all systems. Using the SdH frequencies and the onset of the interband transitions observed in our optical data, we are able to provide very accurate estimates for the magnitude of the Rashba spin-split of the bulk conduction bands. Our results will be discussed and compared with those from photoemission experiments and from band structure calculations.

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I-1

Magnetocaloric effect in perovskite-type complex oxides

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We report the magnetic and the magnetocaloric properties of some perovskite-type complex oxides which have potential to be used in magnetic refrigeration applications. The main aspects of the magnetocaloric effect are analysed in detail in a few series of perovskite manganites and cobaltites like: $La_{0.55}Ca_{0.45}MnO_3$, $Pr_{0.7}Ba_{0.3}MnO_3$, and respectively $Pr_{1-x}Sr_xCoO_3$, $Pr_{0.7}(Ca:Sr)_{0.3}MnO_3$,. These compounds show paramagnetic to ferromagnetic phase transition. We have found that the magnetocaloric properties are strongly related with the critical exponents, which are used to describe the transition. To estimate the magnetocaloric effect we calculated the magnetic entropy change $\triangle S_M$, using isothermal magnetization measurement data. The critical behavior of these compounds, around the paramagnetic-ferromagnetic phase transition, was studied by both using the modified Arrot plot method and the field dependence on magnetic entropy change. The results of these studies indicated either long-range (mean-field model) or short-range magnetic order (3D Heisenberg model) in the transition region. The large magnetocaloric effect on a broad temperature range, recommend these compounds as possible magnetic refrigerants. In comparison with rare earth metals and their alloys, the perovskite-type complex oxides exhibit higher chemical stability and higher electrical resistivity, which lead to reduced eddy-current heating, and in addition, they have lower costs.

1. I.G. Deac, A. Vladescu, J. Magn. Magn. Mater. 365(2014) 1-7.

I-2 Magnetic properties of 3d transition metals in selected rare-earths based intermetallics

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The magnetic properties of 3d transition metals, (M), - rare-earth, (R), intermetallics are rather complex. Function of the magnetic contribution of M and R elements, several types of magnetic behaviour were evidenced. The magnetic properties of Fe, Co, Ni and Mn in binary and pseudobinary RM_2, RM_3, RM_5, RFe_{13} are reported. Magnetic measurements in external field up to 12 T and temperature range 4-700 K were performed. Additionally band structure calculations were also done. The calculated moments per formula unit described well the experimentally determined magnetizations. The band structure calculations and magnetic measurements suggested that there is an interplay between induced R 5d band polarizations and M3d magnetic moments. The R 5d band polarizations influence the M3d magnetic moments, which in turn contribute additionally to their polarization. The transition metal contribution to R 5d band polarization is related both to the number of M-neighbor atoms, and R elements and their moments. Finally, the possible technical applications of these materials are discussed.

I-3 Co ferrite based magnetostrictive materials for sensors

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Co ferrite based materials possessing large values of magnetostriction have been considered as promising candidates for torque sensor applications in automotive industry. The desirable characteristics of such materials are large strain derivative, reasonable saturation magnetization, minimum magnetomechanical hysteresis, low magnetic anisotropy, low Curie temperature, good mechanical properties and low cost. Most of the earlier studies on the magnetostrictive properties of cobalt based ferrites have been carried out on single crystals and the results were explained on the basis of respective magnetic anisotropy contributions of the cations present to the magnetostriction. Recent investigations on the polycrystalline cobalt ferrites with different substitutions have shown to be very interesting with improved magnetostrictive properties. Therefore, it is aimed at presenting the state of the art on substituted cobalt ferites in this paper while reviewing the observations of major research groups engaged in carrying out these specialized studies. Further, it is also proposed to suggest future formulations for improved magnetostrictive properties in finding out more suitable materials for torque sensors

I-3 Structural aspects of magnetic fluids stabilization: neutron scattering investigations

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Magnetic fluids (ferrofluids) are fine liquid dispersions of magnetic nanoparticles (characteristic size ~10 nm) covered with surfactants for preventing their coagulation in different conditions. The understanding of mechanisms of ferrofluids stability is an important factor in the synthesis of highly stable magnetic colloids with defined properties. Diagnostic of aggregation and determination of the aggregation regimes and their control in biocompatible magnetic fluids are necessary for their development in biomedical applications. Small-angle neutron scattering (SANS) is powerful method for structure diagnostic of various objects within length scale 1-100 nm. In this work the successful application of small-angle neutron scattering is presented by example of structure diagnostic of ferrofluids. The structure analysis of various types of magnetic fluids for biomedical applications is presented in the given report. Also the microstructure of non-polar ferrofluids with excess of surfactant and inter-particles interaction are investigated by SANS. Additionally the interaction characteristics between surfactant/polymer molecules used in stabilization of magnetic fluids are investigated, which is very important for understanding the synthesis procedure of highly stable magnetic fluids with controllable properties

O-1 Room temperature giant magnetoresistance in $La_{0.67}Ba_{0.33}Ti_{0.02}Mn_{0.98}O_3$ epilayers

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Perovskite manganites, $R_{1-x}A_x(Mn^{3+}{}_{1-x}Mn^{4+}{}_x)O_3$ (R – trivalent rare earth, A - a divalent alkaline) have attracted considerable attention due to their magnetocaloric and/or magnetoelectric properties. With this respect, they are potential candidates to be used in various applications such as: electronics, spintronics, magnetic refrigeration, field sensors, magnetic information storage or faster reading devices. Downscaling perovskites is prerequisite for integrated them in nowadays miniaturized devices. Another important aspect regards the best functionality at room temperature. In this work we tested the magnetic and magnetoelectric properties of $La_{0.67}Ba_{0.33}Ti_{0.02}Mn_{0.98}O_3$ thin films obtained by pulsed laser deposition on $SrTiO_3$ substrates. The thin films grew epitaxially as proven by X-ray diffraction and transmission electron microscopy. The analysis of XPS spectra gives a stoichiometry close to the one of the ceramic target. From M(T), a Curie temperature very closed to room temperature was determined. The magnetic entropy change and relative cooling power will be also presented. A giant magnetoresistance effect (150% at 300 K under 5 T) was found in the highly epitaxial $La_{0.67}Ba_{0.33}Ti_{0.02}Mn_{0.98}O_3$ layers.

O-2 Domain walls in the helimagnet $Ba_2CuGe_2O_7$

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$Ba_2CuGe_2O_7$ is a layered spiral antiferromagnet (helimagnet) thanks to a Dzyaloshinskii-Moriya (DM) anisotropy. Early experiments [1] revealed a Dzyaloshinskii-type incommensurate-to-commensurate (IC) phase transition when a magnetic field along the z axis exceeds 2 T. Subsequent theory predicted that the IC transition does not occur immediately, but is mediated by an intermediate phase [2], realized for 1.7 T < H < 2.9 T. Below 1.7 T, the ground state is a cycloid propagating along the x-axis, whose spin rotates in the xz plane. For H > 1.7 T the cycloid acquires a nonzero spin component along the y-axis and becomes a conical spiral, which degenerates into a spin-flop state at 2.9 T. New experiments have now confirmed that the intermediate phase occurs as predicted, but also observed an unexpected IC phase transition for a strictly in-plane field at 9 T [3]. This observation was explained by a nonzero weak-ferromagnetic component in the DM anisotropy [4]. $Ba_2CuGe_2O_7$ is the only system where DM-induced weak ferromagnetism and helimagnetism coexist. Here we anticipate the existence of unconventional domain walls in the intermediate phase, whose ground state is double-degenerate with respect to sign-inversion of the y-spin component. Here, domain walls are truly stable localized nonlinear excitations connecting two topologically distinct spatially modulated vacua. Their properties differ significantly from more conventional counterparts. For example, domain walls discussed here possess only discrete translational invariance. Note that domain wall depends on the ground states, whose properties, such as magnitude of the spin along the y-axis and the spiral period, can be tuned by changing the strength of the field. Finally, when an in-plane field is applied along x, the weak-ferromagnetic DM anisotropy lifts the ground-state degeneracy, and triggers the dynamics of driven domain walls via mechanism similar to that in ordinary weak ferromagnets.

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O-3 $Bi_{0.95}Mn_{0.05}FeO_3$ - $Ni_{0.5}Zn_{0.5}Fe_2O_4$ nanocomposites with multiferroic properties

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Nanoparticles of $Bi_{0.95}Mn_{0.05}FeO_3$ (BMFO) and $Ni_{0.5}Zn_{0.5}Fe_2O_4$ (NZFO), synthesized using sol-gel autocombustion method, were mixed with the chemical formula x.$Bi_{0.95}Mn_{0.05}FeO_3$ - (1-x).$Ni_{0.5}Zn_{0.5}Fe_2O_4$, where x takes the values of 0, 0.5, 0.6, 0.8 and 1 to prepare multiferroic composites. The sintering of the materials was done at 800°C/6h in air atmosphere. Dense and homogeneous compounds with fine grained microstructures were achieved in all the composite samples as evident from the obtained scanning electron micrographs thus indicating a better mixing of the two phases. Structural analysis of the composites, carried out using the X-ray diffraction data and FTIR data, reveals the existence of two phases i.e., perovskite and spinel in all the composite materials. Dielectric studies as a function of temperature reveals that there is a phase transition in the composites from ferroelectric to paraelectric around the Neel temperature in each case. Magnetic hysteresis loops were taken using vibrating sample magnetometer at room temperature. The saturation magnetization was found to be increasing /decreasing according to the constituent percentage of the ferrite content added to the composite samples. Superparamagnetic behaviour with zero coercivities was observed for all the composite samples. Polarization-electric field (P-E) loops, which were obtained using TF 2000 ferroelectric tester at room temperature, provides the evidence for the existence of spontaneous polarization in all the composite materials. The preservation of both the ferroelectric and ferrimagnetic phases with required interfacial coupling between them in these composite samples makes them an attractive choice for sensor and spintronic applications.

O-4 Planar Hall effect sensors with tunable properties for sensing magnetic nanoparticles

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Experimental and micromagnetic studies have been carried out on Permalloy based planar Hall effect (PHE) structures used to capture and detect super paramagnetic (SPM) nanoparticles employed as labels for biodetection applications. Disk-shaped structures, made from Permalloy, 1 mm diameter and 20 nm thick, were deposited on to oxidized Si substrate. No anisotropy axis has been defined. To control the sensor sensitivity and linearity, a DC biasing field has been applied along the driving current. In addition to this, different magnetisation states of the sensor layer can be well controlled. It has been shown that the strong localized stray field from domain walls can trap individual SPM beads [1]. In this way, the strong magnetostatic interaction between the magnetic beads and the sensor's magnetic layer can be responsible for the capturing of SPM particles and, in reverse, for complex changing of the magnetic moments orientation in the sensing layer due to the stray field produced by the particles. These aspects will be explained by means of micromagnetic simulations and revealed trough experiments. Using this method to capture the magnetic nanoparticles in some positions above the sensor surface can improve the signal stability and detection sensitivity. In previous studies we have discussed the experimental setups that offer the best detection performance using PHE sensors. From aqueous solution containing maghemite nanoparticles, 10 nm diameter, functionalised with PEG 6000 were placed droplets, 0.7 µl, over the sensor surface. Special field configuration has been used to capture the nanoparticles mostly on the sensor surface and not on his edges. In addition to biasing field, a magnetic field, used to magnetise the nanoparticles, was applied perpendicular to the sensors surface in order to avoid the saturation of the PHE signal. We used different methods to sweep the fields and the results of our experiments show that can be easily detected magnetic moments lower than $3.73x10^{-5}$ emu. This value of the detected magnetic moment corresponds to a mass of 8.77 µg of PEG 6000 maghemite powder. Lowering the sensor dimensions to micrometer scale, the detection sensitivity will be improved.

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O-5 Two-Step Transition in 1D Spin Crossover System Investigated by FORC Diagram Method

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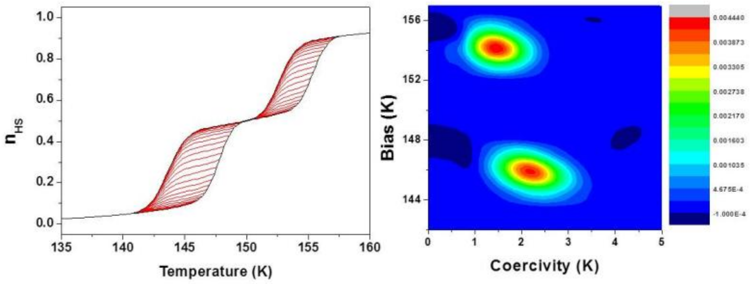
The two step ST behaviour is particularly interesting for the investigation of their influence through cooperativity/anti-cooperativity, intramolecular and intermolecular interactions on the metal centers lying in the neighbourhood [1]. Most of the compounds, which present two steps ST behaviour, are found in the cases of mono-, bi- and tri-nuclear compounds [2]. Only a few of the 1D, 2D and 3D systems present such characteristics. In this paper we use First-Order Reversal Curve (FORC) diagram method in order to study the role of the intramolecular and intermolecular interactions in the 1D spin crossover molecular complexes exhibiting two-step spin transition behaviour.



Simulated FORC (left) and the derived FORC diagram (right)

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O-6 Pressure hydrostaticity investigated by FORC diagram method

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Spin crossover (SCO) materials are of current interest in materials science due to their intrinsic properties and also to their potential applications as active element in sensors, memory, molecular switches or display devices. A spin transition may be physically induced by applying an external perturbation such as: temperature, pressure, light or magnetic field. Due to the change in the metal-ligand bond length when the SCO occurs, these materials are highly sensitive to an external applied pressure [1-2]. Over the last few years an important effort has been done by different laboratories to explain, experimentally or theoretically, different unusual behaviors of SCO complexes under an external applied pressure. Most of the experimental studies have been done by using clamp type or DAC pressure cells that use silicone oil, Flourinert FC70/77, NaCl, etc. as pressure transmitting medium which freezes at cryogenic temperatures and the hydrostaticity might be lost. Moreover, the hydrostatic character of the pressure cells, at cryogenic temperatures, of our knowledge, has been never rigorously discussed. In this paper we present a systematic study on the presence of a pressure gradient in a SCO system, investigated by First-Order Reversal Curve (FORC) diagram method.

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O-7 Compressible Ising-like model of spin crossover solids

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The molecular complexes of transition metals with the electronic configuration d4−d7 can have both high spin (HS) and low spin (LS) central ions and are called spin crossover solids. The compressible model of spin-crossover compounds we consider in simplest way. The deformations are homogeneous and isotropic. Magnetic ions occupied a cubic regular lattice. In mean-field approach the Gibbs free energy per spin is given by:

$$g=zJ\langle s\rangle^2+K\xi^2-p\xi-\ln[z(x)], \quad (1)$$

where z is the number of nearest neighbors of magnetic ion, J is the interaction integral upon homogeneous deformations, $\langle s\rangle=2n_H-1$, n_H is fraction of molecules in HS state, K is the bulk modulus of the lattice, p is the pressure, $z(x)=2\cosh(x)$, $x=(2zJ\langle s\rangle+h)/k_BT$, $h=-(\Delta-k_BT\ln g)$ is the uniform "magnetic field", Δ is directly related to the crystal field on site, T is the temperature. Values n_H and ξ are two coupled order parameters. If we take into account the explicit dependence of Gibbs free energy on the temperature (1), we obtain the entropy for this system:

$$S=k_B(\ln[z(x)]+(\ln g-x)\langle s\rangle), \quad (2)$$

where lng is the electrovibrational degeneracy ratio between the HS and LS states in our model. The obtained numerical results enable us to construct the energy diagram, which in turn confirm the presence of first and second order phase transitions in such compounds. The dependence of the critical temperature and the coefficients of Landau expansion of the Gibbs free energy on the external pressure are derived. Phase transition kind depends generally on the magnitude inter-ion interaction. Obtained results show that the increasing the strain of system lead to a forthcoming of first-order phase transition. Finally, the phase diagram which characterizes the system is examined numerically.

The possibility to address spin states (HS state and LS state in considering model) through external stimuli opens the perspectives to construct new kinds of switches and magnetic storage.

O-8 The particle size-distribution study of CuO nanocrystaline by the modified Warren– Averbach procedures

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In the present work, the particle size distribution in CuO nanocrystals investigated by the odified Warren–Averbach procedures from X-ray diffraction profiles. Assuming spherical ape and log-normal size distribution of crystallites and strain broadening of diffraction ıes due to the dislocations, the area and volume-weighted mean crystallite size distribution e obtained. The results confirm that the sizes of the crystallites are on a nanometer scale.

P-1 MgB_2 with addition of cubic BN and C_{60} obtained by Spark Plasma Sintering Technique

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Cubic BN (cBN) and C_{60} additions to MgB_2 obtained by ex situ spark plasma sintering enhance the critical current density Jc in high magnetic fields. A Jc (T = 20 K) of 100 A/cm^2 is obtained at 3.9 T in the pristine sample and at 5.65 T in the $(MgB_2)0.975(C_{60})0.025(cBN)0.01$ sample. The critical temperature decreases with the increase of the addition of C_{60}. Jc (20 K, H = 0) shows a small decrease from 5.5*10^5 A/cm^2 in the pristine sample to 4.25*10^5 A/cm^2 in $(MgB_2)0.975(C_{60})0.025(cBN)0.01$ sample. Carbon substitutes boron in MgB_2 and cubic BN does not.

P-2 Structural and magnetic characterization Fe(Co, Ni) – Sn – Ti mixed oxide nanoparticles obtaine by glycine-mediated solid state combustion

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Mixed oxide nanoparticles containing Fe_2O_3-SnO_2-TiO_2 or MFe_2O_4-SnO_2-TiO_2 (M = Co or Ni) were synthesized from iron acetylacetonate, nickel or cobalt acetates, tetrabutyl 1,3-diacetoxydistannoxane and titanium tetraisopropoxide (Fe:Sn:Ti atomic ratios = 1:1:1 and 0.5:1:1) precursors using the glycine combustion technique. The powders were analysed using TEM, XRD, EDX and TGA techniques. The Ni or Co ferrite-containig samples show a higher magnetization saturation than the corresponding samples containing only Fe (and also Sn and Ti). These complex oxides can have potential applications in the field of gas sensing and catalysis (in the presence or absence of the light).

P-3 Numerical investigation of the effect of the perpendicular spin-torque on the excitation of a spin-torque oscillator

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Spin-torque-induced magnetization dynamics currently receive a rapidly growing interest due to its potential applications to spintronic devices such as magnetic random access memories (MRAMs) and microwave spin-transfer oscillators (STOs). The operating principle of the STO is the transfer of angular momentum from spin polarized electrons to the local magnetization of a thin magnetic layer, which is equivalent to a torque acting on the magnetization, called spin-torque. The theoretical predictions [1] showed that the spin-torque has two components, one acting in-plane (aJ) and another, which is quadratic in applied voltage, acting perpendicular to plane (bJ). In metallic systems bJ is small and it has generally been neglected in past analyses. However, in magnetic tunnel junctions bJ becomes much larger and can reach 30% the value of aJ. Using numerical simulation, this report analyzes the effect of the perpendicular spin-torque on the dynamics of a STO consisting in a synthetic ferrimagnetic (SyF) and an in-plane magnetized free-layer. The simulations were carried out by solving the Landau-Lifshitz-Gilbert equation, including for aJ the Slonczewski's spin-torque term [2] in the frame of the macrospin approximation. bJ is considered proportional to aJ with the proportionality factor varying from 0 to 1. The numerically derived state diagram shows that regions of stable states and of steady state excitations are depending on the perpendicular spin-torque amplitude. Moreover bJ influences the evolution of the oscillation frequency of the STO.

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P-4 FORC diagrams for 1D and 2D longitudinal arrays of nanowires

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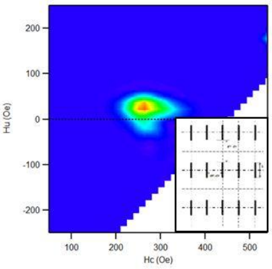
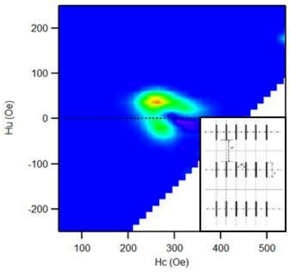
Macroscopic nanostructures with frustrated interactions are exceptional candidates for a number of applications [1] especially as materials used in high frequency devices due to their absorption properties dependent on the geometry of the structures. The systems of magnetic wires perpendicular to a plane have been extensively analyzed and a proper understanding of the interactions within these samples is now available [2]. In this case the interactions between wires are rather simple and it was shown that it is sufficient to use in simulations the field along the wires in their central point. When the wires are placed within the plane (longitudinal geometry) the two assumptions cannot be used. The interaction field has two components: one along the wire and one perpendicular to the wire and these components do not have the maximum value in the middle of the wire. In this presentation we show a technique developed by us to improve the accuracy of the interaction field evaluation in longitudinal systems. For the evaluation of interaction fields we have used the well-known FORC diagram technique [2].



1.



2.

We have simulated the switching of each wire with an Ising-Preisach model (the isolated wires have an intrinsic anisotropy and a symmetrical rectangular hysteresis loop). The switching between the two states is controlled by a classical Monte-Carlo-Metropolis algorithm. The energy barrier between the two states is dependent on the field along the wire and on the component perpendicular to the wire. Another important point in this study is to provide a systematic way to analyze how the geometry of the structure is influencing the interaction field distribution and their average effect (magnetizing or demagnetizing). Tuning the interactions using the geometrical properties of the array is in this case possible and this analysis is providing a method to design structures with different type of interactions. In a longitudinal system of magnetic wires the magnetostatic interactions between the wires can have a magnetizing or demagnetizing effect depending on the values of the distances between the wires along the wire's length and on the perpendicular direction.

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P-5 Studies regarding stability issues of [Fe(Htrz)2(trz)](BF4) spin crossover complex

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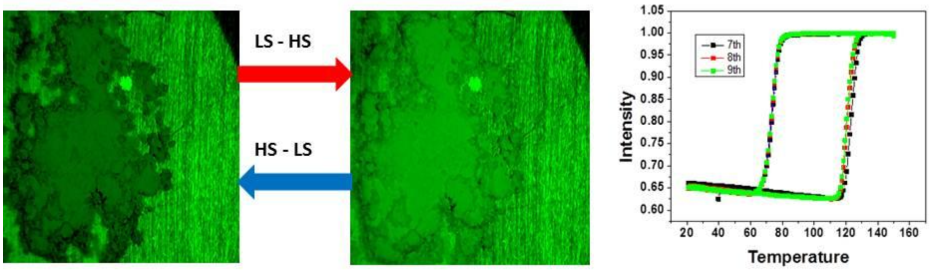
Spin crossover (SCO) materials are molecular materials or extended coordination networks containing a central 3d4 – 3d7 transition metal ions in a pseudo-octahedral configuration with organic ligands, which presents molecular bistability in their magnetic, optical, electrical and mechanical properties upon application of external stimuli. Thus, by applying an external perturbation (light irradiation, magnetic field, electric field, temperature variation or an external pressure) the SCO system can switch between the low spin (LS) state and high spin (HS) state [1]. In this work we present a number of studies regarding the stability of a selected SCO complex.



Images of the titled sample in LS and HS states irradiated with light at 550 nm (left) and the thermal hysteresis loops for 9 sequential measurements

The studies have been made on two different electrical devices [2], looking at the evolution of electric properties and respectively on powder form, concerning reflectivity measurements. Moreover we report a dehydration effect seen on high aspect ratio rods of our compound.

Acknowledgements: This work was founded by the joint French-Romanian project ANR-UEFISCDI, contracts nos. 9ROFR/01.02.2013 and ANR-12-IS07-0003-01.

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P-6 (NdFeB) – (MgB_2) pair-type bulk magnet

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We have studied the trapped magnetic field, Btr, in a pair-type sandwich-like magnet composed of a MgB_2 superconducting (S) bulk disc and a permanent axially magnetised magnet of NdFeB (PM, ~0.5 T). The superconducting (S) bulk discs of 20 mm in diameter and 3.5 or 3.3 mm thickness of MgB_2 (pristine or added with cubic BN, respectively) with density above 97% were prepared by Spark Plasma Sintering. Using a Hall sensor positioned at the centre of the arrangement between the superconductor and the permanent magnet we measured the trapped field, Btr, with temperature, time, and the reduction rate of the applied magnetic field. It is shown that the permanent magnet with certain polarity favours higher trapped field of the superconductor owing to suppression of flux jumps specific for high density MgB_2 samples. The Btr of the PM-S pair was 2.45 T (20 K) and 3.3 T (12 K).

P-7 Simulation of the fundamental processes involved in the heating process of magnetic nanoparticles used in hyperthermia

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The main mechanisms responsible for generating heat using a magnetic nanoparticle placed in a varying magnetic field are: hysteresis losses (Neél relaxation), damping losses (Brown relaxation) and losses from eddy currents [1]. Obviously, the process with the smallest characteristic time prevails. In a process governed by the Neél relaxation, the source of losses is the intrinsic mechanism which determines the hysteresis behavior of the nanoparticle. Energy is released during a Barkhausen jump, when the system “jumps” to its new local energy minimum[2]. Total energy absorbed, and in the case of thermal equilibrium, released, is equal to the area of the hysteresis loop. When we have a small nanoparticle and a relative small viscosity coefficient of the environment in which it is placed, then Brown relaxation is the dominant process.[3] The nanoparticle finds its way to the new energy minimum by changing its position or orientation, so the energy is lost due to friction.

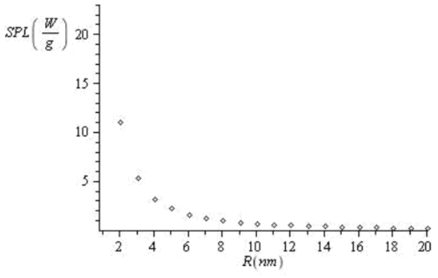

Figura 1

The main task of this work is to simulate the processes described above and to determine the correlation between the size, shape and composition of the nanoparticle, and characteristics important in hyperthermia: saturation magnetization, coercivity, Neel relaxation time and the blocking temperature. This is done by atomistic simulation of the nanoparticles. The second part of the work looks at the Brownian losses. Is studied energy dissipated as a function of the type of movements, frequency, size and the shape of the nanoparticles. The figure shows an example of our simulations concerning the dependence of specific power loss by a linear oscillating sphere, on the size of the nanoparticle

[1] S Dutz, R Hergt, J Mürbe,Magnetic nanoparticles for biomedical heating applications
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P-8 Optimized magneto-impedance effect in low-magnetostrictive amorphous wires

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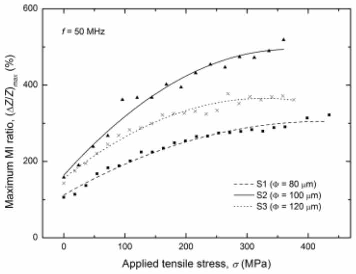
Amorphous wires with nearly zero magnetostriction, such as CoFeSiB ones prepared by in-rotating-water spinning, with diameters between 80 and 120 μm, exhibit good soft magnetic properties, which make them suitable for magneto-impedance (MI) based sensors [1]. Their MI response can be tailored for various sensing applications, including stress and vibration sensing. Here we report on the influence of wire diameter and applied stress on their MI response. Amorphous wires with the diameters of 80, 100, and 120 μm, respectively, have been investigated. MI measurements have been performed on samples subjected to mechanical tensile stresses ranging between 0 and 450 MPa, for various frequencies of the ac driving current: 1, 10, and 50 MHz, respectively. The amplitude of the ac driving current has been kept constant at 3 mA. To understand the effect of wire diameter and tensile stress on the MI effect, we studied the stress dependence of the maximum MI ratio, $(\Delta Z/Z)_{max}$, given by the maxima of the $\Delta Z/Z$ vs. applied field curves, with the sample diameter as a parameter.



Maximum MI ratio vs. applied stress for the samples with the diameters of 80, 100, and 120 μm, respectively

At 1 MHz, the samples with 100 and 120 μm in diameter display a large MI effect when subjected to applied tensile stresses on the entire range of values, however, the maximum MI ratio is only 150%. As the frequency increases to 10, and subsequently to 50 MHz, the microwire with 100 μm in diameter exhibits the largest sensitivity of the MI response. The maximum value of $(\Delta Z/Z)_{max}$ reaches over 500%. The origin of this important result is in the interplay between the large circumferential magnetic permeability [2] and the specific domain structure with a circumferentially magnetized outer shell. The optimum balance is achieved in the sample with 100 μm in diameter. Hence, its MI response under applied stress shows that suitably optimized samples can be employed to develop sensitive stress sensors.

Acknowledgments: Work supported by the Romanian Ministry of National Education through project PN-II-PT-PCCA-2013-4-0471 (SmartFlow).

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P-9 The effect of high-energy milling on Curie temperature of Fe-Nb-Cr-B glassy powders

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The potential of magnetic nanomaterials in different applications is growing significantly in the last years [1,2]. In this context, it is extremely important to understand how their reduced dimensionality is influencing the structural and magnetic behavior in order to make them useful for applications.

In this paper we report our most recent results on the $Fe_{79.7-x}Nb_{0.3}Cr_xB_{20}$ (x=11.5–13 at. %) submicron powders produced by high energy ball milling (Retsch PM 200) from glassy melt-spun ribbons precursors. High-energy ball milling, which for a long time has been used to produce nanocrystalline and amorphous materials, is employed for the synthesis of submicron particles with high aspect ratios. The synthesis conditions have been investigated for both the dry and wet milling conditions. The effect of post-milling heat treatment on the magnetic properties of the powders is also presented.

The structural properties have been investigated after each step of the milling process enabling to determine the effect of different milling conditions on the production of submicron powders. The magnetic properties of the powders: magnetization, coercive field, Curie temperature, have also been determined. Following the structural and magnetic characterization we have developed a protocol for wet/dry mechanical milling of $Fe_{79.7-x}Nb_{0.3}Cr_xB_{20}$ (x=11.5–13 at. %) glassy melt-spun ribbons which allows us to tailor the magnetic properties of the obtained submicron magnetic powders, and mainly the Curie temperature around 40-42^{0}C.

Acknowledgments: This work was supported by a CNDI–UEFISCDI grant, Project #148/2012 (HYPERTHERMIA).

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P-10 Complex analysis of LITH hysteresis in spin crossover compound

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The spin transition solids are molecular compounds, commutable between two states in thermodynamic competition: the low spin state (LS) and the high spin state (HS). The commutation is accompanied by hysteresis, property at the base of applications for information storage and numerical display. We can obtain various hystereses, such as thermal, light induced or pressure hysteresis. By irradiating the compound with a laser, one obtains the Light Induced Thermal Hysteresis (LITH). Because of the competition between the irradiation and the temperature dependent HS-LS nonradiative relaxation, this hysteresis is highly affected by the kinetics. In order to obtain more information about the intrinsic properties of the compound and also to disentangle between kinetic and static components of the LITH, we used the FORC (First Order Reversal Curve) method. Understanding kinetic aspects of the hysteresis reflected in FORC diagrams is important for a larger class of magnetic materials exhibiting kinetic effects. In the present magnetometry experiments, we have used a compound based on $Fe(Fe_{1-x}Zn_x(bbtr)_3(NCS)_2(H_2O))$, either in a pure state (x=0) or doped with Zn impurities (x=0.33). LITH was measured for different sweeping rates and irradiation intensities provided by a continuous laser. By overlapping the results of both, pure and diluted compounds, we can observe the influence of the impurities (narrow hysteresis due to weak interactions). By analysing the changes determined by impurities on FORC diagram, it can be equally noticed the effect of interactions. For a better understanding of the kinetic and impurities effects, we used a simple mean field model based on the Master Equation with distributions of activation energies and interactions.

P-11 Optimization of a spin-valve magnetoresistive structure for magnetic field sensing applications

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Nowadays, spin-valves magnetoresistive structures are widely used in magnetic field sensing applications due to their relative small size, low cost and high sensitivity [1], [2]. In order to obtain a magnetoresistive sensor with high sensitivity, it is mandatory to get a high magnetoresistance ratio while maintaining the soft magnetic properties of the free layer. In this work, the influence of the CoFe/NiFe composite free layer thickness on the MR ratio and on the coercive field was studied. Two series of spin valves with typical multilayer structure of Ta (5 nm)/CoFe (3 nm)/IrMn (20 nm)/CoFe (3 nm)/Cu (3 nm)/CoFe (x nm)/NiFe (x nm)/Ta (5 nm) were deposited by magnetron sputtering on glass substrates. In the first series, the NiFe layer thickness was kept constant at 5 nm and the CoFe layer thickness was varied as it follows: 0, 1, 2, 3, 5 nm. In the second series, the thickness of the CoFe layer was kept constant at 2 nm and the NiFe layer thickness was varied as it follows: 0, 1, 3, 5, 7 nm. The optimum characteristics of the spin-valves were obtained for the CoFe(2 nm)/NiFe(7 nm) composite free layer. By using the optimized thicknesses of the free layer a magnetoresistance ratio of 4.15 % and a coercive field of 18 Oe were obtained.

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P-12 Giant magneto-impedance effect in FINEMET type microwires with different diameters

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In this paper we report on the magnetic properties and magneto-impedance (MI) effect of $Fe_{73.5}Si_9B_{13.5}Cu_1Nb_3$ conventional wires with diameters between 90 μm and 25 μm. The sample where obtained by successive cold drawing of an amorphous wire with diameter of 105 μm, prepared by in rotating water melt spinning [1]. All sample where annealed using a vacuum furnace at temperatures between 300˚C and 600˚C for 1 hour and characterized from magnetic point of view using hysteresis loop and MI measurements.

When the diameter is reduced the permeability of the wire undergoes a significant decrease due to the high residual stress which is induced in the cold drawing process. The decrease of the permeability leads also to a decrease of the amplitude of the MI response. By annealing at proper temperature the wires go through a process of relaxation and nanocrystallization that leads to a permeability increase and consequently to a higher MI response. The obtained results show that the maximum axial permeability is obtained for an annealing temperature of 500˚C for all samples. The maximum value of the relative permeability ($4.5*10^5$) was obtained for the wire with a diameter of 35 μm. The coercivity decrease when the annealing temperature is increasing up to 550˚C due to nanocrystallization and increase for higher temperatures. The maximum values of the giant magneto-impedance (GMI) response were found also for the samples annealed at 550˚C. The amplitude of the GMI variation increase when the diameter decreases. For the wire with 25 μm in diameter we measured the highest impedance ratio ($\Delta Z/Z_{(H=max)}=(Z-Z_{(H=max)})/Z_{(H=max)}*100$) of 150% at a frequency of 10 Hz. The results are discussed with respect to the dimensions, microstructure and internal residual stresses.

A controlled decrease of the wires diameter produces a significant increase in GMI ratio, this kind of nanocrystalline wires having potential for development of new magnetic sensors based on GMI effect.

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P-13 Evaluation of the interaction field distribution in systems of ferromagnetic single-domain particles from first and second-order reversal curve measurements

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Romania

The experimental evaluation of inter-particle interactions in samples containing ferromagnetic single-domain particles is one of the most important problems to be solved in order to understand properly the complex behavior of such ensembles in various applications from sensors to recording media. For the moment, we know rather well to model the magnetization processes in single-domain ferromagnets but the mentioned interactions could dramatically change the magnetic response of the ensemble as compared to the superposition of the non-interacting entities under the same applied field. For many years, Henkel plot (or deltaM plot) were used to estimate the interactions as the deviations from the no-interaction Wohlfarth line. More recently, the first-order reversal curve (FORC) diagrams were used mostly to observe the interaction field distribution. We have shown previously that the main difference between the two types of experiments is the order of measurement [1-2]. The Henkel plot and the deltaM curve are obtained from second order reversal curves but they are also using one curve (Isothermal Remanent Magnetization – IRM) that starts from a demagnetized state (usually an AC demagnetization) that is ideally an infinite order magnetization curve, which is not very well defined in experiments [1-3]. Solutions to avoid the use of IRM measurement were proposed also a few years ago [4]. In this study we analyze the results given by various experimental techniques for two samples: one with clear positive deltaM (interpreted as a sample with magnetizing interactions) and one with a negative deltaM (with demagnetizing interactions). We show that in both cases the FORC diagram is clearly indicating demagnetizing interactions in contrast with the deltaM finding. We also analyzing and discussing the possibility to use other type of demagnetization in IRM measurement (like the DC demagnetization) with a well-defined order of the experimental curve.

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P-14 Magnetization processes in arrays of Stoner-Wohlfarth macrospins

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Most of the models used in the characterization of magnetic systems are essentially scalar in nature even if the magnetization processes are basically vectorial. As the complexity of the simulated processes is increased, in order to maintain the numerical manageability, the behavior of the magnetic systems is described by simpler fundamental models, like the Ising model . However, in some applications the vectorial characteristic is essential and the two-states Ising-type description of the system is not adequate. When a vectorial model for single-domain ferromagnetic particle is required the well-known Stoner-Wohlfarth can be used. Recently a generalization of this model was developed for pseudo single particles . In the present study we essentially show the results of the techniques developed for systematic characterization of Ising-Preisach-type systems when they are applied to arrays of Stoner-Wohlfarth macrospins (see in [1] typical magnetization processes). We are calculating not only the major hysteresis loop for these systems but also first-order reversal curves (FORC). This allows us to estimate the intensity of interactions and the relation between the calculated diagrams and the real interaction fields between the macrospins as a function of various magnetization processes. The use of vectorial models to calculate scalar magnetization processes (similar to the experimental data produced in usual VSMs) could provide a fundamental understanding in the so-called reversible components which could have a significant importance in the total moment measured as a projection along an axis. The use of a perfect array of SW macrospins could also provide a better understanding of the influence of the local structure symmetry on the overall interaction field distribution. By taking into account of possible experimental errors in producing the "perfect" network of macrospins we can also simulate these effects on real structures.

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P-15 Numerical approaches of all-optical ultrafast switching

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There are many aspects of all-optical ultrafast switching mechanism to be clarified, from physical perspective to the technological aspects which must be taken into account in order to achieve a reliable all-optical magnetization reversal device [1-4]. In the absence of relevant theories to explain all-optical switching phenomena, the numerical descriptions can provide valuable information with both theoretical and applied implications. In this respect, different numerical approaches, based on Landau-Lifshitz-Bloch equation and Metropolis Monte Carlo method, can capture some relevant characteristics of all-optical switching processes. Our numerical investigations based on Landau-Lifshitz-Bloch equation and Metropolis Monte Carlo methods of all-optical magnetization reversal could be fundamentally important in establishing physical switching conditions of magneto-optical device with important technological implications in computational and storage industry.

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P-16 Random numerical tools for classical and quantum materials characterizations - ferrites as a case study

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Random number generators are used increasingly in the simulation of various natural systems [1-2]. Often, standard random number generators versions from common programming libraries are unable to reproduce accurately the dynamics of these systems. Whether they are used to assign a realistic distribution of nanosystems, atoms, molecules, clusters and vacancies or are used effectively in describing the dynamics through classical or quantum Monte Carlos methods; the random number generators must be adapted properly. In the present study we analyze how the random number generators parameters are reflected in the numerical description of the ferrite materials properties [3-4] were are analyzed both magnetic and electrical characteristics.

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sensitivity, magnetic and electrical properties of barium hexaferrite, Superlattices and Microstructures 70 (2014) 46–53

P-17 The anisotropy of a system of interacting Stoner-Wohlfarth particles. Experiments and simulations.

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As most the devices using magnetic materials are produced from various structures of microscopic elements a central interest in the experimental characterization of these ensembles is to estimate the properties of the isolated entities from measurements performed on the global sample. Essentially, this is possible only if the effect of inter-particle interactions is properly understood. However, due to the long-range magnetostatic interactions, it is almost impossible to develop a theoretical model able to cover all the variety of structures. Simulation is offering a tool to find causal links between the behavior of the ensemble and the intensity of interactions. In this study we analyze the efficiency of vector-type magnetometry on the evaluation of anisotropy field distribution in systems of single-domain particles. We have considered measurements starting with the well-known rotational hysteresis experiment to more recent types of measurements like the rotational first-order reversal curves (FORC) and FORCs measured at different angles between the system easy axis and the applied field direction [1-2]. In the simulation area, the Stoner-Wolhfarth model is a good starting point with the recent improvements related to the concrete anisotropy-type of the measured samples. In order to have a simplified but still physical model we consider an ensemble of interacting SW macrospins with different packing ratios to evidence the effect of interactions on the experiment simulation. The role of the second order term in the series expansion of the magneto-crystalline anisotropy energy (as described in [3-4]) is also analyzed and discussed.

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P-18 The dynamics of Ising-like spin-crossover model with fluctuations

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[2]General Physics, Chernivtsi National University, Chernivtsi, Ukraine

The spin-crossover complexes have drawn a great interest in recent years due to their special switching properties and bistable behavior. These features make them potential candidates for practical applications in thermal and pressure sensors as well as optical devices. The spin-crossover compounds are characterized by high-spin (HS) and low-spin (LS) states which are determined by the distribution of electron spins on sublevels of d orbitals of transition metal ions. The spin-crossover compounds are characterized by $3d^4$-$3d^7$ electronic configuration. The switching may be induced by external field and is accompanied by changes of the magnetic, optical, and dielectric properties of the material. Because transition between spin states, involves the changes of ligand field action on metal ion it is important to study its variable nature.

In this work we have studied thermal induced spin transition in presence of fluctuations of external field. The spin-crossover system with fluctuating term $\xi_i(t)$ is described by Ising-like Hamiltonian in the following way [1]:

$$H=-J\sum_{\langle ij\rangle} s_i s_j + \sum_i[\Delta-kT\ln g+\xi_i(t)]s_i, \quad (1)$$

where $s_{i,j}$ are pseudospin variables taking the values +1 and -1 for HS and LS state respectively, J describes the ferromagnetic interaction (J>0) and represents the system cooperativity, Δ is energy gap between spin states, k is Boltzmann constant, T is temperature, and $g=g_{HS}/g_{LS}$ is the degeneracy ratio between HS and LS states. The stochastic process $\xi_i(t)$ reflects the local random field and becomes significant for critical temperatures. It was found that the presence of fluctuations move the spin crossover system in phase space from the region of second-order phase transition to the region of first-order phase transition.

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P-19 Magnetic fluid preparation, characterization and environmental application

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Soft magnetic material in the form of colloidal suspension of $CoFe_2O_4$ was prepared aiming applications to environment issues. Magnetic cores of submicron size were synthesized using adapted Massart's method [1]. Their surface modification with dilute perchloric acid was carried out by optimizing coating protocol to get final product consisting of stable suspension of core/shell nanosystems in deionized water, i.e. $CoFe_2O_4$ based ferrofluid. Structural and magnetic properties of colloidal particles were investigated: granularity (SEM), crystallinity (XRD), coercitivity and saturation magnetization (VSM) while rheological properties of the ferrofluid were assessed by measurements of density, capillary tension and viscosity. The results revealed typical spinel structure and slight coercitive field in accord with literature data. The application to the study of magnetic contamination of environmental microorganisms was developed by administration to Phanerochaete chrysosporium cellulolytic fungus with role in the wood waste decomposition. The oxidative stress induced in the cell cultures grown in the presence of various ferrofluid dilutions was revealed by specific enzyme activity assays. Possible problems related to magnetic nanoparticles influence on the wood waste natural decomposers were highlighted.

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P-20 Magnetic structure and transport phenomena in $La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$ manganites

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The doping of alkali-earth cations such as Ba, Sr, Pb at the A site of colossal magnetoresistive (CMR) manganites (ABO_3) is an interesting topic of study. The substitution with cations having a different radius than those of La^{+3} leads to an increase of the chemical disorder degree, a lowering of the Curie temperature (T_C) and implicitly to a decrease of the metal-insulator transition temperature. Some La manganites doped with Pb exhibit interesting transport characteristics near room temperature. We extend this type of compounds by a partial substitution of La with Pr and of Pb with Sr. The $La_{0.5}Pr_{0.2}Pb_{0.3-x}Sr_xMnO_3$ manganites (x = 0, 0.05, 0.10, 0.15, 0.20) were sintered in air and proofed for phase composition and microstructural parameters (lattice constants, microstrains, average size of coherent blocks) by XRD and ND methods. Data on magnetic and transport properties were obtained at temperatures between 77 and 400 K. We observed a spin glass

– metal transition at temperatures between 150 and 200 K. The substitution of Pb with Sr leads to important structural changes and we show that a transition from cubic to rhombohedral structure occurs for $x > 0.05$. A large magnetoresistance appears near room temperature. The most intriguing characteristic of magnetic behaviour is the transition from spin-glass to ferromagnetic state, which seems to depend on the ratio of Pb and Sr concentrations. There is a strong dependence of the resistance on the cooling and measurement conditions, which implies the presence of the spin-glass state. From magnetic measurements in magnetic field cooled samples we conclude that at temperatures lower as Curie temperatures there are three phases: a ferromagnetic phase, a spin-glass phase and a small amount of a nonmagnetic phase. These phases differ from each other only by the presence/absence of the magnetic moment.

P-21 SANS investigations concerning spin-glass to ferromagnetic state transition in some Cr substituted manganites

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Magnetoresistance is defined as a decrease of the resistance to the application of a magnetic field, observed for the manganese oxides with perovskite structures. A complete explanation of the magnetic and electric properties of manganites can be done taking account the spin and the carriers correlations to the lattice and its distortions. Concerning the variation of the resistance with the temperature and magnetic field intensity, an important role plays the appearance of spin-glass state at low temperatures and its transition to ferromagnetic state. The purpose of present paper is to study the influence of the substitution of Mn with Cr on the magnetic and crystalline structure of $La_{0.54}Ho_{0.11}Sr_{0.35}Mn_{1-x}Cr_xO_3$ manganites. The samples with the chemical composition $La_{0.54}Ho_{0.11}Sr_{0.35}Mn_{1-x}Cr_xO_3$ were prepared by means of sol-gel method, using as precursors rare earth oxides and the Sr, Mn and Cr acetates. The phase composition, structure, and lattice parameters were determined by powder X-ray diffraction using a DRON-4 diffractometer. The magnetic measurements were performed with a vibrating sample magnetometer between 77 and 600 K. The resistance variation with temperature and magnetic field were measured between 30 and 300 K, by using fields of maximum 5 kOe. The SANS measurements were performed by YuMO diffractometer, IBR-2 reactor, FLNP-JINR, Dubna, Russia. The samples contain only a perovskite phase, the volume of the lattice cell remaining practically unchanged with the increase of the Cr concentration in the samples. The cation distribution is given not only by the nominal chemical composition, but also by the oxidation degree of the manganites. The Curie temperature monotonously shows a maximum corresponding to x=0.15. At temperatures between 100 and 200 K a transition from the spin-glass to ferromagnetic state was observed. We discuss the dependence of magnetoresistance on the treatment conditions of the samples.

P-22 Annealing influence on the structural and magnetic properties of $Fe_{73,5}Cu_1Nb_3Si_{13,5}B_9$ powders

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Fe-based nanocrystalline alloys present a major interest in fabrication of soft magnetic cores [1,2]. The paper presents results concerning the thermal treatment influence on the structural and magnetic properties of $Fe_{73,5}Cu_1Nb_3Si_{13,5}B_9$ powders prepared by mechanical grinding. Ribbons with same composition, annealed 1 hour at 300°C, were milled with a planetary ball mill (SPEX SamplePrep 8000-series) for 1 to 4 hours in air/argon atmosphere. The powders were isothermally annealed in a vacuum furnace (10^{-6} Torr) at temperatures between 300°C and 550°C.

Scanning electron microscopy (SEM), X-ray diffractometry (XRD), and vibrating sample magnetometry (VSM) were used in order to analyze the shape and surface morphology, the structural evolution, and the magnetic behavior of the powders. The Curie and crystallization temperatures were determined from the thermomagnetic curves.

SEM images indicate that the shape of the powder particles is irregular and the size distribution is wide. For particles size of about 30 μm (obtained after 4 hours milling time, in argon atmosphere) the Curie temperature of the amorphous phase is approximately 340°C, while the crystallization process starts at about 500°C. For the annealed powders, the Curie of the amorphous phase increases. For samples annealed at temperatures higher than 490°C, the crystalline state is formed. The crystallization state indicated by the thermomagnetic curves was confirmed by XRD analysis of the powders.

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P-23 Monte Carlo simulation of field, time and temperature dependent magnetization processes in arrays of Ising-Preisach macrospins

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The accurate evaluation of the magnetization processes in systems of macrospins (single-domain ferromagnetic particles) is really important for many technological applications. The simulation techniques have evolved dramatically in the last decades especially due to the progresses in computer technologies. However, the numerical modeling of macroscopic devices containing a reasonable high number of macrospins (statistically significant) is still a difficult task. Especially when the simulation should include not only the response of the system to the externally applied magnetic field but also how this response is influenced by the sample temperature and the duration of the experiment the scientist should find creative modelling schemes in order to simplify sufficiently their model without losing the main physical characteristics of the system. Essentially, the model should be simple enough to be numerically tractable and in the same time to describe the fundamental attributes of the modeled physical system. For the magnetic nanostructures an ideal solution is the use of the concept of macrospins with two-states (up/down - Ising systems) with intrinsic anisotropy [1]. These macrospins have rectangular hysteresis loops (similar to the Preisach hysterons) and are interacting through dipolar fields. In this study we present the results of a Monte-Carlo simulation for complex magnetization processes (field, time and temperature dependent) in a network of Ising-Preisach macrospins. We start from 1D networks and gradually generate 2D systems (longitudinal and perpendicular). The results are compared with standard Ising simulations. We analyze and discuss the numerical efficiency of the implemented models.

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P-24 Effective Anisotropy In Heated Magnetic Core-Shell Nanowires

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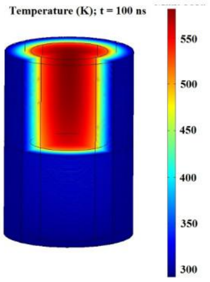
The temperature field is an important parameter to be known and controlled in the magnetization process of the core-shell nanowires. The paper analyzes the temperature dependence of a hysteretic process in a core-shell nanowire subjected to a dc Joule heating process. The spatial and temporal evolution of the temperature in system was done using a model based on time-dependent heat conduction equation. The stresses determined by thermal gradients and different expansion characteristics of core and shell materials were computed. A dc current determines a temperature field and thermal stress distribution in the system.



The spatial temperature in the core-shell system at time t = 100ns

The temperature and stress depend on the size parameters of the system, dc Joule current and the initial temperature of the system. The magnetic behavior of the nanowire was analyzed using the Micromag application. The magnetization process of the core is influenced by the thermal field induced by dc current subjected to the system.

Acknowledgment The work was supported by Romanian CNCS-UEFISCDI Grant Nos. PN-II-RU-TE-2012-3-0439 and Grant Nos. PN-II-RU-TE-2012-3-0449.

P-25 The synchronization study of the magnetic moments oscillations of the ferromagnetic particles system with magnetostatic interactions

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The synchronization is the process by which a group of interacting oscillators spontaneously lock to a certain frequency or phase. One of the most used models to study of the synchronization phenomenon is the Kuramoto model [1]. The synchronization studies using the Kuramoto model are performed in the systems with large number of oscillators nearly identical, with different natural frequencies and synchronization result is expressed by a global parameter called the order parameter. We have implemented the Kuramoto algorithm in the analysis of the magnetic moments oscillations of the ferromagnetic system particles with magnetostatic interactions both when the system is free and it’s subjected with two magnetic fields, alternating field (AC) and continuous field (DC) on perpendicular directions In the second case we have analyzed the forced oscillations synchronization of the magnetic moments projections on the AC field direction which acting on the center distribution of particles, only [2]. The oscillations of the particles become total synchronized when all magnetic moments oscillate at the same frequency (frequency synchronization) determined by the alternating field and when the phase difference between any two such oscillators remains time constant (phase synchronization).

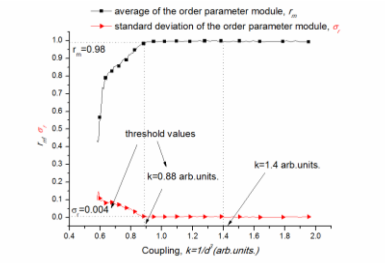

Fig.1

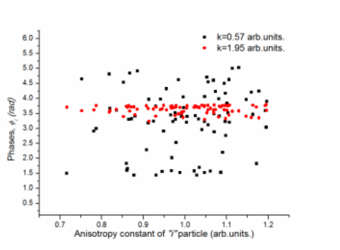

Fig.2

The phases of oscillations particles are considered the azimuthal angles between magnetic moments direction and easy axis direction for each particle. The azimuthal angles are determined by use of the Landau Lifshitz equation. In this paper we have used two distribution of the particles from system: a linear chain [2] and a 2D arrangement. The Kuramoto algorithm will be used for synchronization analysis of the particles by the order parameter and standard deviation calculus (fig.1), the phase's distributions determination (fig.2) and the coupling dependencies of these parameters. The limit of the Kuramoto algorithm is determined by the appearance of the chaotic oscillations.

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P-26

Drug release by chemical bond splitting of functionalized magnetic nanoparticles with core-type architecture

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The goal focuses on the synthesis of biofunctionalized hexagonal core-shell magnetic nanoparticles. Our recent strategy demonstrates the ability to functionalize, drug-load and well stabilize magnetic nanoparticles in suspension [1]. The ferrite magnetic nanoparticles are functionalized with a silica shell that possesses a MCM-41-type hexagonal arrangement of the cylindrical mesopores. Drug-like molecules are confined into the biocompatible mesostructured silica. For controlled drug release induced by an external magnetic field we used a Diels-Adler reaction of the organic shell. The structure and morphology were evaluated by X-ray diffraction (XRD), transmission electron microscopy (TEM) and dynamic light spectroscopy (DLS). The drug release has been evaluated using UV-VIS spectroscopy after heating the ferrofluid using a high frequency generator.

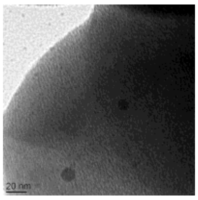

Figure 1. TEM micrographs of magnetic nanoparticles embedded in the silica architecture

ACKNOWLEDGMENTS: This work was supported by the German Academic Exchange Services (DAAD). The authors thank to Sylvia Kuhn for TEM measurements and Ph.D. Sandra Schäfer for fruitful discussion.

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TOPIC 5

Nanostructures and
Low Dimensional Systems

PL-1 Surface characterization of nanostructured silica based microspheres

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Silica based microspheres were prepared by combined sol-gel and spray drying methods. Spray drying is a very efficient method used to prepare particulate materials for a large diversity of applications as catalysts, pharmaceuticals, food additives, biomaterials. The specific applications of the microspheres are mainly imposed by their surface properties. On the other hand, these properties can be modulated by surface functionalization. Structural ordering of the amorphous spray dried microspheres was induced by heat treatments at different temperatures. Treatment parameters were chosen so as to obtain nanostructured microspheres because this architecture promotes enhancement of bioactivity and catalytic properties. The surface characterization of the spray dried microspheres subjected to heat treatments at different temperatures was achieved using X-ray diffraction, scanning and tunneling electron microscopy, Fourier transform infrared and Raman spectroscopies, as well as X-ray photoelectron spectroscopy.

PL-2 Structure charactariaztion of complex liquid dispersions by scattering methods

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The present day structural research of dispersed nanosystems are based on complex investigations involving various complementary methods. Each technique specifies to different extents unique features of the inner organization of systems under study. The given talk is intended to compare main possibilities and restrictions of various structural methods used in characterization of highly dispersed nanosystems with a special accent to applications of X-ray (including synchrotron radiation) and neutron scattering techniques including diffraction and small-angle scattering. Together with the general introduction the experimental examples are given for various classes of liquid dispersions covering colloidal solutions of magnetic nanoparticles (magnetic fluids), fullerenes and nanodiamonds. All of the considered systems are actively used in practice. The structural information is very important knowledge which helps to regulate their properties and stability in different conditions. The general question how to use the results of various structural methods is discussed with respect to dispersed systems. Non-equilibrium aggregation in these systems is a significant problem for interpretation of experimental data. The obtained structural parameters characterize not only basic structural units, but the thermodynamic stability of the system. As a rule, their use in the precise analysis of nanoparticles in multicomponent polydisperse systems requires a special consideration for each kind of the systems under study.

PL-3 Computational nanomechanics in search for new materials

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Mechanics at the nanoscale is a cross-disciplinary area where the traditional concepts of mechanics overlap with the fundamentally different aspects of quantum chemistry and solid-state physics. In our studies of graphene nanostructures, ZnO nano-wires, and Si nano-particles, we have encountered situations when this overlap gives rise to new and useful phenomena. This talk will concentrate on three such examples: (i) Graphene is intensely researched for electromechanical applications. I will discuss how simulations carried out with a new microscopic technique called objective molecular dynamics, reveal the electromechanical response of twisted graphene nanoribbons. I will show that a microscopic effective strain concept provides the key for understanding the electromechanical response. From the effective-strain perspective, the twist-induced bandgap modulations in graphene nanoribbons appear strikingly similar to those exhibited by the seamless carbon nanotubes in tension. (iii) Twisted zinc oxide nanowires and nanotubes were recently synthesized by screw-dislocation growth. We show, based on objective molecular dynamics simulations, that once their diameter increases above a critical size of the order of a few atomic spacings, the existence of these structures can be rationalized in terms of the energetics of surfaces and veritable Eshelby's twist linear elasticity mechanics supplemented by a nonlinear core term. For Burgers vector larger than the minimum allowed one, a twisted nanotube, rather than a nanowire, is the most stable nanostructure. (i) Recently, our colleagues discovered that although silicon nanoparticles are superhard, they stick to a substrate when colliding at 1-2 km/s. Molecular dynamics simulations explain this puzzling result in a surprising way: Although the contact force is relatively low by macroscopic standards, the impact pressure causes the high speed particle to change its crystalline structure and soak up so much energy that the particle can't bounce away. This understanding may help develop wear-resistant coatings created by many such impacts.

PL-4 Chemical synthesis and properties of ferroelectric nanostructures and nanoceramics

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Ferroelectrics are functional materials characterized by a switchable spontaneous polarization. The most important class of ferroelectrics is represented by oxides with perovskite or perovskite-like structure with general formula ABO3. Ferroelectrics show several technologically important properties, such as piroelectricity, piezoelectricity, second harmonic generation and high dielectric constant. Therefore, compounds such as BaTiO3 and Pb(Zr,Ti)O3 have found application in transducers and actuators, biomedical imaging, diesel injection systems and multilayer ceramic capacitors. Ferroelectricity is a long-range cooperative phenomenon corresponding to the alignment of the elementary dipoles of the unit cells in domains with uniform macroscopic polarization. Consequently, the properties of ferroelectrics are significantly affected by the characteristic size of the system (thickness for thin films, diameter for wires, grain size for ceramics, etc.) when this size is reduced to the nanoscale. Surface and interface effects as well strain and depolarizing field can become very important when the system is confined in a small volume. The study of size effects in ferroelectric ceramics requires the availability of high quality, non agglomerated very fine powders (particle size of 10-20 nm) and suitable sintering methods to obtain dense nanostructured materials. High quality nanoparticles of BaTiO3, SrTiO3 and LiNbO3 can be obtained by wet chemistry methods, such as hydrothermal and solvothermal synthesis. The surface of these particles can then be modified by coating with a different compound. Densification by spark plasma sintering and related techniques results in dense nanoceramics and nanocomposites. In barium titanate nanoceramics (grain size <100 nm), a decrease of the dielectric constant, shift of the Curie temperature, suppression of polarization switching, strongly reduced tunability and thermal conductivity are commonly observed. This suggests a progressive loss of ferroelectric properties with decreasing grain size. The high density of grain boundaries typical of nanoceramics is the main responsible for these effects.

PL-5 SiGe superstructures towards light emision

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Silicon which is the headlight material in microelectronic industry offers unequalled physical features in terms of oxidation, doping (both P- and N-type), electronic transport and abundance presence in the nature. Nevertheless, since decades the microelectronic industry faces the technological bottleneck of integration of opto-electronic devices in CMOS technology. Moreover, light emission from Si nanostructures would be of great interest owing to the need for silicon-based light sources for applications in silicon photonics. In this quest of the Grail, several studies tried to associate Silicon with other materials and in particular with Germanium which forms with Si a perfectly miscible alloy. Both Si and Ge possess indirect band gaps, which makes them very inefficient light emitters. Band gap engineering has been proposed as one way to overcome this limitation and although light emission with greatly improved efficiency has been obtained at low temperatures the emission at room temperature is still very weak, because of exciton dissociation. Recently, through employing novel band gap engineering computations, entirely new Si/Ge and Si supercell structures possessing direct gaps have been proposed. For instance, according to d'Avezac et al., a $SiGe_2Si_2Ge_2SiGen$ superstructure should have a direct and dipole-allowed gap of 0.863 eV, which is ideally suited for optical fiber data transmission applications. Here we report on several kind of superstructures fabricated either by epitaxial deposition or by dewetting of Si/Ge heterostructures. We also describe their electronic and optical properties. In this framework we will report some original processes for the self-organization of Si based nanostructures using high resolution liquid Metal alloy ion source focused ion beam (LMAIS-FIB).

PL-6 Photoemission spectromicroscopy of lead zirco-titanate (001) and (111) thin films

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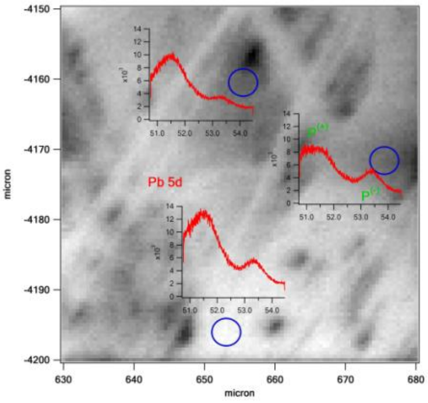
It has been recently demonstrated that photoelectron spectroscopy is an appropriate tool to derive surface band bendings of free ferroelectric thin layers [1,2] and for interfaces formed by metals deposited on these layers [3-6]. Thus, binding energy contrast may be used in spectromicroscopic techniques in order to investigate areas with different out-of-plane ferroelectric polarization, and also with different degrees of charge compensation of the depolarization field. This Contribution will outline recent photoemission experiments performed by using synchrotron radiation at Elettra, combined with sub-micrometer spatial resolution, on the Spectromicroscopy beamline. Experiments are performed on lead zirco-titanate Pb(Zr,Ti)O3 (PZT) thin layers prepared by pulsed laser deposition, resulting in highly (001) or (111) oriented layers. Samples are analyzed as introduced and after a cleaning procedure in ultrahigh vacuum, up to the achievment of good low energy electron diffraction (LEED) patterns. Binding energy contrast was identified as an useful tool to assess domains with different polarization orientation.



Example of spectromicroscopic data obtained on PZT(111). The image represents the integral over all individual photoemission points in the data cube, eith some selected spectra outlined for the areas represented by blue circles.

Also, after the cleaning procedure, contaminants are removed and the layers become highly insulating; thus, the available charge carriers in the layers do not suffice in some cases to create the mobile charge sheets of sufficient surface density such as to screen the depolarization field inside the layers. Therefore, layers with relatively high internal electric fields are obtained, and these layers might be useful for a wealth of new applications of ferroelectics in surface chemistry, catalysis, photocatalysis and photovoltaics. Another effect put in evidence was the partial surface reduction of the PZT, delivering metal Pb aggregates, whose degree of mobility on the surface is relatively elevated at room temperature. Moreover, in some cases it was found that this photoreduction process might be reversible. Piezoresponse force microscopy and high resolution transmission electron microscopy investigations are also discussed, in order to support the spectromicroscopic investigations.

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I-1 Formation and growth of clusters in fullerene solutions: experimental and theoretical aspects

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Solutions of fullerenes C60 in various liquids present an interesting system from both fundamental and practical points of view. The most promising practical applications are connected with perspectives for biomedicine of fullerene-water solutions. A number of peculiar effects in C60 solutions keeps up the pure scientific interest. Among most interesting are the kinetic effects observed in fullerene solutions. These are, namely, solvatochromic effects in polar fullerene solutions and cluster formation and growth. An intensive study of these effects in various solvents, including water, carbon disulfide, CS2, a biomedically compatible solvent N-methyl-pyrrolidone (NMP) and its mixtures with water and non-polar solvents has been performed in Frank Laboratory of Neutron Physics of the JINR for the last few years [1]. The present report covers current progress of this research. The experimental investigation of fullerene solutions of different polarity where made via small-angle neutron scattering (SANS), UV-Vis spectrophotometry, mass-spectrometry and dynamic light scattering (DLS). In low-polar fullerene solutions, the effect of non-linear dissolution and excess value of the gyration radius in C60/CS2 system was addressed. Presently, the main interest is concentrated on polar C60/NMP and high-polar fullerene water solutions (FWS). The C60/H2O solutions of two concentrations where studied by neutron scattering. In FWS fullerenes are present in form of stable colloids with average size of 70 nm. Basing on SANS data, a model of C60 aggregate as a densely packed crystallite covered by a thin shell of hydration water is proposed. The slow growth of large stable fullerene aggregates in C60/NMP has been observed by DLS and SANS. Theoretical modeling of cluster growth via a system of kinetic equations has been performed. The developed approach allows to obtain the modeled SANS and UV-Vis curves at each stage of C60 cluster state evolution in solution. This modeled data is compared with experiment. An interesting effect of cluster state reorganization is discovered in C60/NMP when a polar (water) or non-polar (toluene) solvent is added to the solution. A complex experimental study of this phenomenon is presented.

1. M. V. Avdeev, V. L. Aksenov, T. V. Tropin, // Russ. J. Phys. Chem. A, V. 84 (8), pp. 1273–1283, 2010.

I-2 Exploiting the full potential of dip-coating to prepare nanostructured coatings with original properties.

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Complex hierarchical nano structures can be achieved when combining chemical advanced bottom-up strategies, such as self-assembly and sol-gel chemistry, together with liquid solution processing, such as dip-coating. It will be demonstrated that dip-coating is an extremely versatile tool to prepare thin nanostructured and mesoporous metal oxide films from liquid solutions and that it has been used for many decades without taking advantage of its whole potentiality. Many types of oxide can be prepared and will thus be mentioned, but the present communication will focus mainly on SiO_2 (from amorphous to epitaxial alpha-quartz), photoactive TiO_2, and on other state-of-the-art nanostructured thin films.

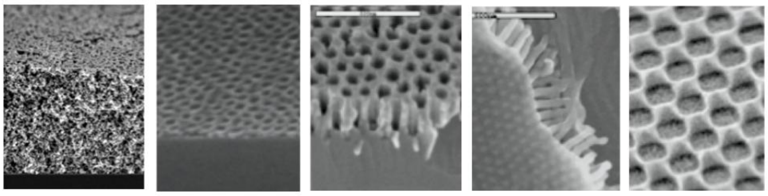

Fig.1

Their interests in optics, in microelectronic, in photovoltaic, in photocatalysis, in nano fluidics, or in nano construction will also be discussed. The usefulness of the ellipsometry analytical techniques in determining thin films optical properties, porosity characteristics, mechanical properties, photocatalytic activity, or thermal and chemical stabilities will also be presented all along the presentation. Finally, we will show that the described “bottom-up” approaches can be combined with conventional “top-down” technologies, such as reactive ions etching or optical and nano imprint lithography, to construct even more complex morphologies with multi scales features and motifs (Fig.1).

1) D. Grosso et al. special issue 25th years anniversary of Chem Mater. 2014 2) M. Faustini et al. J. Mater. Chem. 2011

I-3 Fabrication of core-shell nanowires composed of silicon and germanium

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Experimental results of core-shell fabrication processes are reported. The core-shell structure is fabricated by a combination of growth, milling and oxidation-condensation steps. The growth is realized by the VLS method using gold as a catalyst. The impact of the growth parameters on the final morphology of the nanowires is studied. The milling is done in a dual beam FIB using germanium ions. The density of defects, morphology, abruptness of the core/shell interface, Ge concentration in the case of SiGe, and thickness of the shell layer are analyzed and compared as a function of the fabrication process. Special attention is paid to the impact of initial surface of the nanowires without the shell on the final core/shell interface.

I-4 Interface polarized charge transfer in core-shell half-metal magnetic nanoparticles coated with semiconductors

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Different types of magnetic nanoparticles composites can be designed as multifunctional platforms with controllable magnetic properties, thus being able to facilitate their use in different applications. Moreover, the interface interactions between different components can greatly improve the performance of the multi-components system and even generate new synergetic properties. In this work new nanocomposite systems based on magnetic nanoparticles of half-metallic type coated with semiconducting materials are presented. In case of half metallic ferromagnets, the spin–up (majority) and spin-down (minority) conduction bands are split such that the Fermi level is situated in the upper unfilled minority band. This splitting is generally due to intense low symmetry crystalline fields or intense spin-orbit couplings. Two types of half-metal magnetic nanoparticles like Fe_3O_4 and FePt ($L1_0$) alloy were coated with semiconductors like ZnS, TiO_2 and poly(3 hexylthiophene) (P3HT). By ZnS coating of Fe_3O_4 nanoparticles the saturation magnetization significantly increases while by TiO_2 coating a reversed process take place. Due to the interface energy band alignment electronic spin–down dominant states are transfer from ZnS valence band into magnetite conduction band leading to the polarization of semiconductor. In case of TiO_2 coating the transfer goes in the reversed sense namely into the band gap of TiO_2. Inside the semiconductor the spin polarization coherence is lost and being extended band states the coherence is also lost in magnetite conduction band, thus decreasing the saturation magnetization of Fe_3O_4. When FePt ($L1_0$) nanoparticles were coated with P3HT a significantly reduction of the coercivity was observed. The spin-down polarized transfer goes from the semiconductor into the half-metal conduction band determining the magnetic polarization of the semiconductor polymer. The process can be described by using the RKKY model. Additionally, the magnetically polarized P3HT semiconductor becomes partially exchange coupled to the hard magnetic FePt ($L1_0$) phase.

I-5 C_{60} aggregation, between modeling and realization

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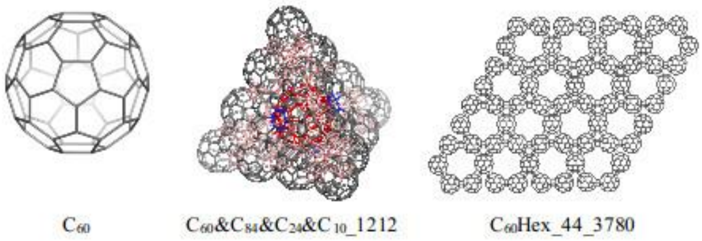
Fulerene C_{60} can aggregate with itself or with other cages to fill a given space [1,2]. Aggregation can happen randomly or following a well-defined geometry, of which energy trends to a minimal value. In this work we present the „co-habitation“ of C_{60} with C_{84} and the smaller cages C_{24} and C_{10} in 3D-structures (see figure) or in 2D-structures, called hyper-graphenes.



C60 and some of its aggregation structures

Design and energetic study of some hypothetical aggregates of C_{60}, with well-defined geometry is presented in terms of map operations. Calculations were made at the HF, DFT and DFTB level of theory. The design of nanostructures was performed by original software packages. Pre-experimental facts are discussed.

Acknowledgements: This work was partially supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-RU-TE-2012-3-0202 and by the strategic grant POSDRU/159/1.5/S/133652, co-financed by the European Social Fund within the Sectorial Operational Program Human Resources Development 2007 – 2013.

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2. M. V. Diudea, C. L. Nagy, *Periodic Nanostructures*, SPRINGER, Dordrecht, 2007.

O-1 Structural and impedance spectroscopic studies of CuO based nanoparticles

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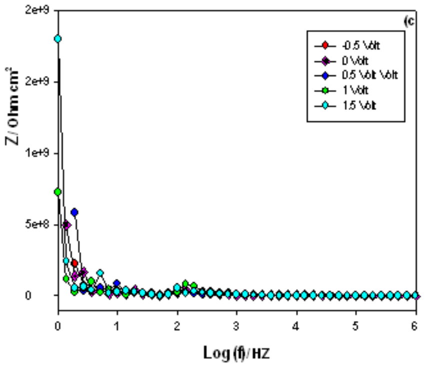
CuO nanoparticles with an average size of 22.04 nm have been successfully prepared by sol-gel method. The CuO nanoparticles are characterized by using techniques such as X-ray powder diffraction and impedance spectroscopy. The X-ray plot confirms the formation of the CuO with space group C2/c and monoclinic phase with the preferential orientation along the [101], [002] direction. Dielectric properties of nanocrystalline CuO thick films were studied using ac impedance spectroscopy under different conditions through capacitance –frequency measurements in a wide frequency range from 1Hz to 1MHz and bias voltage range from -0.5V to 1.5 V.



The Bode plot of total impedance versus frequency

Increasing of the capacitance with decreasing frequency demonstrates that interfacial polarization has very strong influence on dielectric properties.

[1] Li X, Chen G, Po-Lock Y, Kutal C. J Chem Technol Biotechnol 2003; 78:1246-51. [2] Hemissi M, Adnani H A. DIG J NANOMATER BIOS 2007; 2: 299-305. [3] Reddy KM, Manurama S V, Reddy A R. Mater Chem Phys 2002; 78: 239-45. [4] Kumar S A, Lo P H, Ming Chen S. Nanotechnology 2008; 19:255501. [5] Xu X, Zhao J, Jiang D, Kong J, Liu B, Deng J. Anal Bioanal Chem 2002; 374:1261- 6. [6] Harizanov O, Harizanova A. Sol Energy Mater Sol Cells 2000; 63:185-95. [7] Li B, Wang X, Yan M, Li L. Mater Chem Phys 2002; 78: 184-8.

O-2 Crystalline and electronic structure of supported gold catalysts determined by EXAFS, XRD and XPS methods

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The gold nanoclusters as supported catalysts were analyzed by extended X-ray absorption fine structure, X-ray diffraction and X-ray photoelectron spectroscopy in order to determine their local, global and electronic structure. The present study has pointed out a strong deformation of the local structure of the metal, due to its interaction with oxide supports. The average particle size, the mean squares of the microstrain, the probability of the faults, the particle size distribution and microstrain functions of the supported Au catalysts were determined by X-ray diffraction method. The method is based on Fourier analysis of the experimental X-ray line profiles (111), (200), (220) and (311). The global structure is obtained with a fitting method based on the generalized Fermi function facilities for the approximation [1]. The local and global microstructures of the catalysts are modified by the strong interaction between the metal clusters and oxide supports. As a result, the chemisorptions and catalytic processes, which occur at the Au-support interface, are also changed. The both types of measurements were performed on Beijing Synchrotron Radiation Facilities. The Au/MO catalyst samples were investigated, where MO: LaOx/Al2O3, ZnO/MgO/Al2O3, CuO/Al2O3, CeOx/Al2O3, ZnO/Al2O3, TiO2, MnOx/Al2O3, Al2O3, CeOx/ZrOx/Al2O3, Li2O/CeOx/Al2O3, and Rb2O/CeOx/Al2O3. One of the main purposes of the present paper is to focus on understanding the specific role of the gold particle size determined by X-ray diffraction and that of the oxide (MO). The most active catalyst in CO oxidation is the multicomponent catalyst Au/ZnO/MgO/Al2O3 with MgO being a stabilizer for the Au particle size and MnO being the co-catalyst [1]. Based on X-ray absorption fine structure spectroscopy analysis we consider that the whole local structure of the investigated systems are strongly distorted concerning the atomic number but the distances between atoms are practically the same as for standard Au foil. Due to the strong modifications of the gold cluster local structure, the metal-support interface may influence the electronic properties of metal clusters and thus their reactivity for absorption of the reactant molecules.

1. Ruud Grisel, Kees-Jan Weststrate, Andrea Gluhoi and Bernard E. Nieuwenhuys, "Catalysis by Gold Nanoparticles", Gold Bulletin 35/2 45,(2002).

O-3 Molecular dynamics simulation of a Gold nanodroplet in contact with graphene

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[1]*Physics, University of Zanjan, Zanjan, Iran*

The liquid Gold (Au) Nanodroplet spreading on a graphene substrate is studied by molecular dynamics (MD) simulation technique. The EAM interatomic potential and Tersoff many body potential have been used for Au-Au and C-C interactions respectively, and Lenard–Jones potential has been employed for Au-C interaction. The temperature of nanodroplet and substrate were controlled by Nose-Hoover thermostat in canonical (NVT) ensemble. The cross-section snapshots of the nanodroplets are used to study contact angle and wettability of nanodroplet. The size of nanodroplet is changed and no obvious effect on the contact angle is seen in the nanodroplet on the graphene surface. Moreover, we changed temperature of graphene to obtained effect of temperature on the contact angle. Our MD results show that the contact angle increase with increasing temperature and nanodroplet trend more spherical shape. It means that, the wettability of Au nanodroplet is independent of nanodroplet size and dependent on substrate temperature. Our computed results are in reasonable agreement with the experimental data where they are available.

O-4 Investigation of Irradiation influence on graphene in electron – beam lithography process using raman spectroscopy

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The development of the nanoelectronics devices based on graphene sheets requires the use of various techniques involving an electron beam in both imaging such as scanning electron microscopy (SEM), transmission electron microscopy (TEM) and fabrication of nano-devices using Electron Beam Lithography (EBL). Electron beam irradiation of graphene layers can generates defects, lattice disorder and can changes the electronic transport properties depending on electron kinetic energy and the exposure dose. Raman spectroscopy methods are capable of detecting small changes in the crystal structure by examination of the evolution of Raman D, and G bands (ID/IG) and the broadening of the G band line width (FWHM) function on dose and e-beam accelerating voltage.

In this paper we present the results of a study regarding the effect of e-beam exposure on the electron-sensitive resist (Polymethylmethacrylate, PMMA) coated single layer graphene by using Raman Spectroscopy (LabRAM HR800) in order to determine the conditions corresponding to minimal influence on graphene properties. A sample containing a large flake of single layer graphene (SLG) on SiO2/Si substrate was coated with PMMA and the pattern on the e-beam resist then is printed on the graphene, Fig.1(inside). These graphene layer was placed in a scanning EBL system (Raith e_Line , high vacuum (10-6 torr) and exposed to e-beam with following characteristics: acceleration voltages in the range: 200 V - 20 kV ; exposure doses: 100 - 100.000 μC/cm2. In figure 1 are presented Raman spectra acquisitioned with red laser (633 nm) corresponding to PMMA coated graphene irradiated at 1kV and one corresponding to high quality SLG and in Fig. 2 is plotted D band amplitude function of doses at different accelerating voltages. The minimal modifications of graphene after e-beam exposure are found for 1kV acceleration voltage and exposure doses of 200 μC/cm2 and 500 μC/cm2. In the case of irradiation by using doses larger than 10000 μC/cm2 acceleration voltages lower than 500 V and larger than 10kV the graphene is rendered useless.

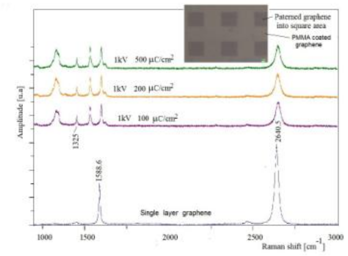

Fig. 1

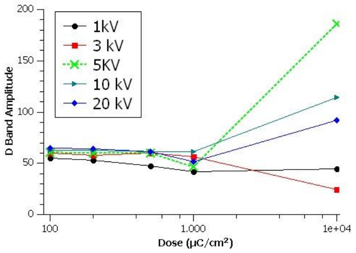

Fig. 2

Acknowledgments. This work has been supported by Romanian Ministry of National Education, project PN-II-PTPCCA-2013-4-2104-D1.

P-1 Structural, optical, fluorescence and magnetic properties of Ni doped SnO_2 nanoparticles

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In the last few years, the interest in the optical and physical properties of metal oxide has significantly increased due to their potential applications in optical and electronic fields, especially when they are doped with magnetic components. Tin oxide with the rutile structure is a promising functional n-type semiconductor material with a wide band-gap (Eg = 3.65 eV at 300 K), has been investigated for various applications such as gas sensors, solar cells, transparent conductive electrodes, spintronics and biosensor etc. [1, 2]. In this work the influence of Ni doping on the structural, optical and magnetic properties of SnO2 nanostructures were studied. All the samples were prepared using coprecipitation method. The room temperature ferromagnetism was found in Ni doped SnO2 powder samples. Fig. 1 Properties of Ni doped SnO2 nanoparticles: (a) TEM microstructure of powders prepared by coprecipitation method; (b) Hysteresis curves at room temperature; (c) PL spectra of Ni doped SnO2 nanoparticles at λex=300 nm. The X-ray diffraction data reveal that all samples have a pure tetragonal crystalline phase characteristic to tin oxide and the Ni nanoparticles does not change the tetragonal structure of SnO2.

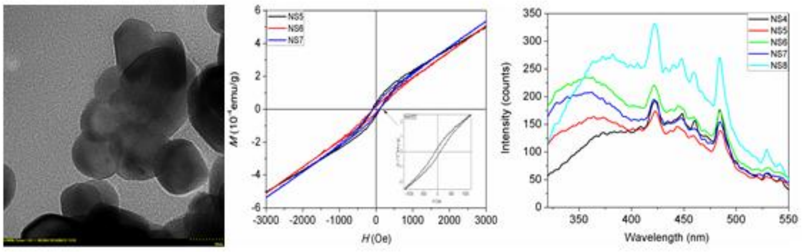

Fig. 1 Properties of Ni doped SnO2 nanoparticles: (a) TEM microstructure of powders prepared by coprecipitation method; (b) Hysteresis curves at room temperature; (c) PL spectra of Ni doped SnO2 nanoparticles at λex=300 nm.

TEM results depict the formation of tetragonal shaped and small sized nanoparticles of the diameter of about 10-40 nm. The estimated values of the saturation magnetization (Ms) and the coercive field (Hc) are found to be 5·10-4 emu/g and between 83 ÷ 96 Oe (depending on the amount of Ni in the sample). The emission spectra of the SnO2 and Ni doped SnO2 nanoparticles present three main regions, described by following characteristics: the first part consist from a broad emission band located between 320 and 395 nm blue to the free exciton recombination; a second part includes four emission bands at about 412, 438, 450 and 475 nm, respectively; and the last region with the low intensity (green emission bands at 520 and 533 nm).

Acknowledgements: This work was financially supported by the project POSDRU/159/1.5/S/133652.

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P-2 Synthesis and characterization of iron/mesoporous silica core-shell nanostructures

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Magnetic iron nanoparticles have attracted an increasing attention due to their properties and potential application in the field of magnetic resonance, magnetic recording, magnetic carriers and catalysis [1,2]. The instability toward oxidation and natural tendency of aggregation limits the technological application of iron nanoparticles. The most effective way to control the oxidation and aggregation is the coating of iron nanoparticles with a protection layer such as metals, metal oxides, carbon and mesoporous silica [3]. The deposition of uniform mesoporous silica shells on iron particles has been successfully carried out by different procedures [3] based on sol-gel technique. However, in the sol–gel process the agglomeration of iron nanoparticles lead to the degradation of the core–shell nanostructure properties. Recently,have been a few reports on the preparation of core–shell nanostructures using the sonochemical technique [3]. In this paper, we report the synthesis and characterization of core-shell nanostuctures consisting of spherical iron nanoparticles coated with mesoporous silica shell. The coating of spherical iron nanoparticles with mesoporous silica layer was performed using the sonochemical technique. The ultrasonic irradiation was used to accelerate the formation of the mesoporous silica framework and to prevent the agglomeration of iron nanoparticles. The obtained iron/mesoporous silica core-shell samples were characterized by powder X-ray diffraction (XRD), focused ion beam- scanning electron microscopy (FIB-SEM), vibrating sample magnetometer (VSM), ferromagnetic resonance (FMR) and nitrogen adsorption-desorption isotherms measurements. The X-ray diffraction result suggests that the structural characteristics of iron are maintained after mesoporous silica-coating under ultrasonic irradiation. The room temperature magnetic analysis shows that the spherical iron nanoparticles and core-shell sample are superparamagnetic in nature. The discrepancy observed in magnetization value between uncoated and coated iron particles suggests that a small amount of silica is bonded on the surface of iron particles.

Acknowledgement: This work was supported by the Romanian project IDEI–EXOTIC 185/2011.

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P-3 Structural, optical and photoelectric properties of GaSe-CdSe lamellar nanostructures

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GaSe is a typical representative of layered III−VI semiconductor group, composed of flat Se-Ga-Ga-Se elementary packings, perpendicular to its hexagonal crystallographic axis. The links between packings are of Van der Waals type, much weaker in comparison with those between four monoatomic sheets inside a package, accomplished by ionic-covalent (predominant) forces. The specific structural features of ε-GaSe (relative arrangement of elementary stratified packings) enable formation of a subnanometric gap between neighbouring packings, favorising intercalation of divers atomic (molecular) ions between chalcogen planes and thus formation of lamellar structures. In this work structure of composite obtained by 10 min−24 h intercalation of GaSe single crystalline lamellas with Cd from vapor phase at 750 K is primarily investigated. X-ray diffractometry and combined diffusion spectroscopy studies revealed that actual preparation technology leads to GaSe−CdSe lamellar composites, containing hexagonal CdSe and GaSe crystallites with average size of ~ 30 nm. CdSe crystallite size is increasing together with heat treatment temperature and duration. By short-duration heat treatments (10−40 min) a layer composed of CdSe flat islands is formed at the surface of GaSe lamellas. Absorption spectra of intercalated samples have been obtained from transmission and reflection measurements of composite lamellas prepared by short treatments, as well as from diffuse reflection spectra of microcrystalline composite resulted from 24 h Cd intercalation. Spectral characteristics of photoconductivity for 24 h intercalated composite and of photoelectromotive force for GaSe−CdSe heterojunctions formed on the (0001) and (1000) GaSe surfaces have been also examined. Structure of photoconductivity and photoelectromotive force spectra is strongly influenced by surface state concentration in intercalated GaSe lamellas.

P-4 Anisotropy of photoelectric and luminescent properties of GaSe:Eu−CdSe and GaSe−CdSe lamellar nanostructures

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[4]*Faculty of Physics, Alexandru Ioan Cuza University of Iasi, Iași, Romania*

Lamellar nanocomposites have been prepared by 10 min−24 h intercalation of GaSe and GaSe:Eu (0.49 at. % and 1.00 at. %) single crystalline lamellas with Cd from vapor phase at 750 K. These have been obtained by splitting (along the cleavage planes) respective ingots, grown by Bridgman-Stockbarger technique. Hole concentration at 300 K was of 2.0×10^{14} and 3.8×10^{15} and 9.0×10^{15} cm^{-3}, in undoped and Eu-doped (0.49 at. % and 1.00 at. %) GaSe single crystals, repectively. Lamellar nanostructures have been obtained from single crystalline undoped and Eu-doped GaSe plates, displaying 3 natural surfaces, one of which was parallel to the C_6 crystallographic axis. Thin In films, vacuum deposited and heat treated for 1 h at 430 K, have been used as electrodes in photoelectric and photovoltaic measurements. Structure of photoconductivity spectra in a direction parallel to the C_6 crystallographic axis, and of photoelectromotive force of CdSe−GaSe and CdSe−GaSe:Eu heterojunctions (with nanometric CdSe layer) in both parallel and perpendicular directions to the C_6 axis has been analyzed. Kinetics of photoconductivity and photoelectromotive force in CdSe−GaSe and CdSe−GaSe:Eu nanolamellar structures upon excitation with light pulses corresponding to the depth and the edge of fundamental absorption band, of 10^{-5}–10^{-6} s and 10^{-8} s length, has been also investigated. Both relaxation curves are characterized by 2 distinct relaxation processes with time constants of $\sim10^{-7}$ s and 10^{-3} s. GaSe:Eu based heterojunctions were found to exhibit a third relaxation time of the order of atleast 10^{-1} s. From the analysis of spectral characteristics of photoelectromotive force and optical absorption spectra, the mean free path of minority charge carriers in CdSe−GaSe and CdSe−GaSe:Eu heterojunctions has been determined. On the basis of registered spectral and relaxation curves of photoconductivity and photoelectromotive force a energy band diagram showing recombination levels of nonequilibrium charge carriers has been proposed.

P-5 Crystal structure and anisotropy of photoelectric and luminescent properties of GaTe−CdTe lamellar nanostructures

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By Cd-vapor heat treatment, at temperature 653 K, of GaTe single crystalline plates, displaying 3 natural surfaces, one of which is parallel to the C_2 crystallographic axis, flat GaTe−CdTe heterojunctions and nanocrystalline CdTe−GaTe composites have been obtained. Short-duration (10−40 min) heat treatments led to planar heterojunctions with submicrometric CdTe layer at the GaTe surface, while long (24−60 h) treatments resulted in a nanocomposite material containing CdTe and GaTe nanocrystals. Spectral characteristics of photoconductivity of the composite and photosensitivity spectra of GaTe−CdTe heterojunctions with a CdTe layer grown on the GaTe surface, perpendicular and parallel to the C_6 crystallographic axis, have been studied. From the combined analysis of the absorption spectrum in the domain by vicinity of the fundamental absorption edge of GaTe and of spectral dependence of photoelectromotive force, the free mean path of nonequilibrium charge carriers in GaTe layer from GaTe−CdTe heterojunctions has been estimated. Its value was found to be ~30 μm for heterojunctions with CdTe layer perpendicular to the C_6 axis, while in heterojunctions with CdTe layer parallel to the C_2 axis of GaTe, it was about 2 orders of magnitude lower. This difference was explained by quite distinct surface state density values for GaTe surfaces parallel and perpendicular to the C_2 axis. Photoluminescence spectra and kinetics for CdTe−GaTe heterojunctions and composites have been also examined. From the analysis of spectral dependences of photoluminescence and photoelectromotive force a energy band diagram for the recombination levels active in these processes is proposed.

P-6 X-ray characterization of iron-based oxide nanoparticles made by laser pyrolysis and combustion techniques from organo-metallic precursors

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Iron based oxide nanoparticles have been studied intensively due to the large number of applications, from biomedical to magnetic nanofluids. Maghemite-based nanoparticles were synthesized from the vapors of iron-pentacarbonil Fe(CO)5 in different oxidizing conditions and at different power densities using the laser pyrolyses method. To extend the range of nanoparticles, precursors like Fe(acac)3 containing different divalent metal compounds (Zn , Ni , Co , Cu , Ba , Sr) in the presence of PVP (polyvinyl pyrrolidone) or glycine have been used in the synthesis processes. The crystallographic phases and the average size of crystallites have been determined by X-ray Diffraction measurement. The dimensions of crystallites have found to be in the nanometer range. Their properties are discussed in relation with the nanometric dimensions.

P-7 Colloidal gold nanoparticles: synthesis, characterization and size control

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The synthesis techniques of metallic nanoparticles have been continuously evolving, leading to improvement in the control over their size and shape [1]. Particularly, gold nanoparticles situated in the range of 2-300 nm are classified function on their size in three classes having different properties and applications [2]. Most of the size depending applications refer to the 10-300 nm gold nanoparticles class, which represent an excellent substrate in developing of analytical methods for biosensing and chemical sensing [3]. We present here the results of a photo-chemically induced direct writing (DW) process to generate metallic particles by patterning within a solid matrix. Parameters as reactants concentration and fluence were investigated for the same system in different conditions to control the size of particles. Optical spectroscopic investigations revealed a specific surface plasmon resonance response and optical microscopy evidences a higher density of the small particles in the centre of the written patterns. The bigger particles, situated at the outer side of the patterns, strongly scatter the light in the visible range, and can be used to adjust the localized SPR extinction from visible to near infrareds range. Also, the AFM measurements of the nanostructured patterns indicate a uniform size distribution of the particles characteristic to the 10-300 nm class.

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P-8 DC Magnetization relaxation and the frequency dependent AC magnetic response of $YBa_2Cu_3O_7$ films with embedded nanorods and nanoparticles

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The increase of vortex pinning efficiency in the high-temperature superconductors is a field of intense activity, where the appropriate determination of the characteristic pinning energy is necessary. Vortex pinning is widely investigated at present using DC magnetization relaxation measurements over a relaxation time window of the order of 10^3 s, as well as by analyzing the frequency f dependent AC magnetic response, involving short relaxation time $t = 1/f$ scales. The results are discussed in the framework of the general vortex creep equation with logarithmic accuracy. The AC measurements offer a simple method for the extraction of a vortex activation energy $U_{AC}(T, H)$, based on the Arrhenius relation. Large U_{AC} values at high temperatures have been reported and interpreted in terms of vortex creep, leading to the conclusion that some pinning centers “remain very effective even in the vicinity of the irreversibility line”. We compared the magnetic relaxation at long and short t in the case of $YBa_2Cu_3O_7$ films with embedded $BaZrO_3$ nanorods and Y_2O_3 nanoparticles. Our results indicate that the AC magnetic response at usual frequencies is not in the flux creep regime, and the high U_{AC} values in the vicinity of the irreversibility line are essentially related to the pinning enhanced viscous drag and significant vortex velocities.

P-9 Glycerol-derived mesoporous carbon: N_2-sorption and SAXS data evaluation

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Mesoporous carbons have been synthesized from a glycerol solution using mesoporous silica as template and a dehydrating acid. The effect of the glycerol concentration and pyrolysis temperature on the microstructure and morphology has been analyzed. The pore size and volume can be readily and independently controlled by the glycerol concentration and pyrolysis temperature [1,2]. The synthesized carbon samples were characterized with nitrogen sorption, small-angle X-ray scattering and electron microscopy. SAXS data reveal a mesoporous structure resulted upon template removal. As the mesopores are accessible for nitrogen, the mesoporosity of the carbon samples have been also proven by nitrogen sorption. SAXS and electron microscopy indicate the μm sized carbon structure with a nanoscaled substructuring. The parameters - such as surface area, pores volume and size - deduced from sorption and SAXS experiments were compared.

[1] C. Scherdel, G. Reichenauer, Carbon 47 (2009) 1102–1111 [2] M.Ignat, C.J.Van Oers, J.Vernimmen, M.Mertens, S.Potgieter-Vermaak, V.Meynen, E.Popovici, P.Cool, Carbon 48 (2010) 1609-1618

P-10 Morphology and behavior of solid state metal complexes of Cu(II) with flexible ligands

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Three copper complexes with organosiloxane ligands consisting in bis-azomethines derived from 1,3-bis(3-aminopropyl)tetramethyldisiloxane and 2-hydroxybenzaldehyde (1), 5-nitro-2-hydroxybenzaldehyde (2) and 3,5-di-tert-butyl-2-hydroxybenzaldehyde (3) have been prepared. Their thermal stability was evaluated by thermogravimetric analysis and correlated with supramolecular structure. Due to the presence in structure of the polar (-OH, -NO2, -CN) and nonpolar (1,3-bis(propyl)tetramethyldisiloxane) moieties, the aggregation of the molecules in solution occurs at certain concentrations. The morphologies of the films formed on solid substrate as solvents of different polarities slow evaporate from diluted solutions of the complexes were investigated by Atomic Force Microscopy (AFM). Contact angle measurements were also performed on the surface of the films formed from different solvents.

1. N. Lanigan, W. Xiaosong, Chem. Commun. 49 (2013) 8133-8144. 2. S.S. Soni, N. V. Sastry,V.K. Aswal, P.S. Goyal, J. Phys. Chem. B 106 (2002) 2606-2617.

P-11 Electrohydrodynamic filtration of flue gas by nanoparticle trapping in microfluidic devices

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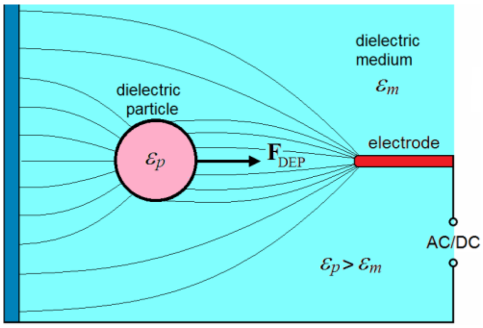
In recent years, many new methods for increasing flue gas filtration efficiency, particularly focusing on particles in the nanometer size range, have been proposed. Among these, the methods based on electrohydrodinamics (EHD) proved to be the most promising. EHD in general refers to the movement of particles suspended in fluids due to the action of electric fields. The interaction of a non-uniform electric field, i.e. one that has a spatial variation in magnitude, with the induced moments of the particle produces a movement termed dielectrophoresis (DEP). The DEP force depends on the magnitude of the electric field and its gradient, the particle size and the Clausius Mossotti factor, which is a measure of the polarisability of the particle in the suspending medium and importantly varies with the frequency of the applied potential. All these features make DEP force an important tool in manipulation of submicron particles in fluid suspensions. This work investigates the behavior of particles suspended in flue gas subjected to non-uniform AC electric field created by a electric potential difference applied to interfacial microelectrodes having a periodic, interdigitated configuration.



Electrically neutral particle in the presence of a spatially non-uniform electric field

The numerical solutions of the electric potential, electric field, DEP force, gas flow field and particle trajectories for a 3D geometry corresponding to a typical DEP-based microfluidic separation device are calculated using the COMSOLMultiphysics finite element solver. The study focuses on nanoparticles having radii ranging from 50 to 200 nm, particles that cannot be filtrated by classical techniques and have a harmful effect for environment and human health. All the presented results show that the dielectrophoresis can be exploited as one of the leading mechanisms for driving and controlling the movement of suspended nanoparticles. Based on the proposed mathematical model and corresponding numerical simulations, an optimal set of parameters can be find, in order to improve the filtering process of flue gas in a microfluidic device.

[1] M. Lungu,, A. Neculae, and M. Bunoiu, J. of Optoelectronics and Advanced Materials 12 2423-2426 (2010) [2] R. Pethig, Biomicrofluidics, 4 022811-1 – 02281-34 (2010)

P-12 Topological symmetry of multi-shell clusters

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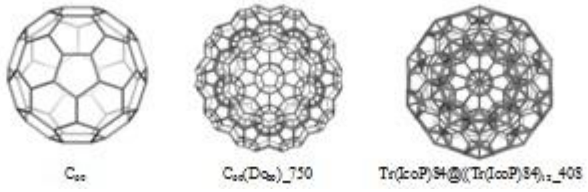
Topological symmetry is referred to the maximum possible symmetry achievable by a given molecular structure; it can be performed either by permutations on the adjacency matrix [1] or by calculating the value of some topological indices. The equivalence classes of vertices/atoms, edges/bonds and faces of the multi-shell nanostructures in figure were solved by using a topological index computed on the layer matrix of distances and compared with the results of matrix permutation.



Polyhedral multi-shell nanostructures

A centrality order of vertices in multi-shell clusters is given. The design of nanostructures was performed by map operations as implemented in our original software package CVNET.

1. M. Diudea, in Diamond and Related Nanostructures, eds. M. V. Diudea and C. L. Nagy, Diamond and Related Nanostructures, Springer, Dordrecht, 2013, Chap.19, p. 335-385.

P-13 Magnetoplasmonic nanorods for theranostic applications

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In the last two decades the application of nanostructured materials in medicine has progressed rapidly. Among the most hot topics are magnetic hypethermia, contrast agents for nuclear magnetic resonance imagery and targeted drug delivery. When nanoparticles can play a double role as heating and contrast agents they are called theranostic agents. Experimentally was demonstrated [1] that iron oxide nanoparticle doped with 10-hydroxycamptothecin drug nanorods with an organic conducting polymer coating outside can be used for cancer diagnosis and chemo-photothermal therapy. In our work the effort were focused on simulating the heating process in such kind of structure. Placed in an external alternating magnetic field the nanorod ferromagnetic core act as localized nano magnetic hyperthermia heater of the tissue. Conducting capping material (gold or conducting polymer) eliminates the toxicity of iron nanoparticle, can be functionalized for drug delivery or enable by influencing the rotational dynamics of nanoparticle the imaging of the cancer by longitudinal plasmon resonances. A computer model based on the finite element method and using COMSOL Multiphysics software was used to simulate the electric field scattering through the calculation of the cross sectional properties and proved that the nanostructure can be used heating and contrast agent. The heat dissipation in and around the nanoparticle generated by both magnetic core and gold shell exposed to the laser and magnetic field was investigated taking into account the properties of suitable core-shell for nanostructure with different sizes.

[1] Y. Yang, X. Zhang, C. Yu, X. Hao, J. Jie, M. Zhou, X. Zhang, Smart nanorods for highly effective cancer theranostic applications, Adv. Healthc Mater. 2014 Jun;3(6) p. 906-15

P-14 The influence of concentration of coprecipitation agent on structural and magnetic properites of Zn ferrite nanoparticles

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The influence of concentration of NaOH coprecipitation agent in synthesis process of zinc ferrite nanoparticles were investigated by systematic studies of X-ray diffraction, Fourier transform spectroscopy, transmission electron microscopy and vibrating sample magnetometry. Variation of NaOH concentration lead to particular sizes and shapes of particles, resulting different magnetic properties due ratio of surface and volume anisotropy.

Zinc nanoferrites were synthesized with NaOH concentration varying between 1÷5M in solution containing zinc chloride (II) and iron chloride (III). The patterns from X-ray powder diffraction showed in Figure 1 were found to match well with those of cubic spinel crystalline structure without secondary metal oxide phase. Pure compounds are obtained at any concentration of NaOH (precipitate agent) between 1÷5M. Precipitation agent plays an important role on particles morphology.

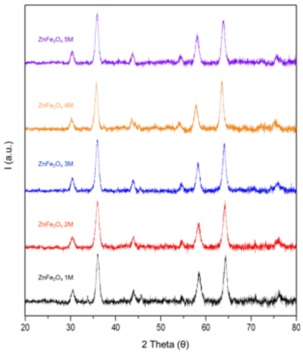

Figure 1 XRD pattern for cubic spinel ZnFe2O4 nanoparticles obtained with 1÷5M NaOH coprecipitation agent.

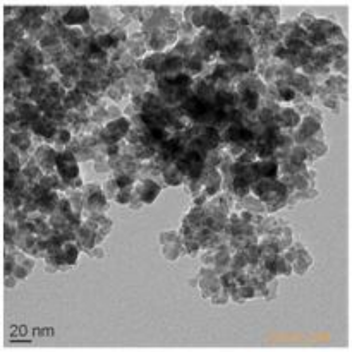

Figure 2 TEM images for ZnFe2O4 nanoparticles synthesized at 4M NaOH concentration

TEM micrographs for zinc ferrites obtained with 4M NaOH concentration presented in Figure 2 demonstrate well spherical shaped particles with the average size of 8nm. Magnetic properties at room temperature demonstrate that in this case the surface anisotropy plays an important role and determine ferrimagnetic properties for Zn ferrite. The properties are interpreted starting for possible cations' distribution among A and B site.

E.V. Gafton acknowledge the support given by the strategic grant POSDRU/159/1.5/S/137750, Project “Doctoral and Postdoctoral programs support for increased competitiveness in Exact Sciences research” cofinanced by the European Social Found within the Sectorial Operational Program Human Resources Development 2007 – 2013.

P-15 The influence of doping concentration on the properties of $Ga_{2-x}Cr_xO_3$ powders as seen by EPR

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The doping of different diluted magnetic semiconductors by 3d transition metal ions (TM) has been of great interest in the last years due to the potential formation of a ferromagnetic phase with a high Curie temperature. The data reported in literature show that there is a strong dependence of their magnetic properties on both the annealing temperature and doping content. It is believed that oxygen vacancies and substitutional incorporation are important to produce ferromagnetism in semiconductor oxide doped with transition metal ions. The present paper reports detailed electron paramagnetic resonance investigations (EPR) of $Ga_{2-x}Cr_xO_3$ powders (x = 1%, 3%, 5%) in order to investigate how Cr ions are incorporated into the Ga_2O_3 lattice and their interaction with environment. The EPR results are correlated with Raman and UV- VIS experimental data.

P-16 $Co_xMn_{1-x}Fe_2O_4$ nanoparticles with possible applications in theranostic

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Scientists increasingly speak more often about theranostic and medical applications of magnetic nanoparticles with very complex structures. Mentioned applications are magnetic cell separation, detection of biological entities, drug delivery, diagnosis, gene delivery, hyperthermia, phototherapy, chemotherapy, contrast of the medical images, magnetic hyperthermia, etc. [1]. In theranostic as examples, apart from the acquisition of good magnetic properties for the heating process in alternating magnetic field is also equally important the shape and the volume of the nanoparticles and theirs availability for functionalization and biocompatibility. These can be quantified by the ultrafine nature of the particle size, shape, mono dispersity in liquid media and surface properties. The main objective of the study was to synthesize a mixed manganese cobalt ferrite series of nanoparticles with the chemical formula CoxMn1-xFe2O4 ($0 \leq x \leq 1$) by a simple co-precipitation method and to investigate their structural and magnetic properties to find their suitability as potential agents in hyperthermia, drug delivery and diagnostic.

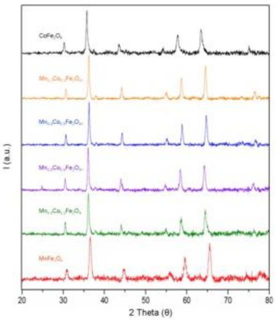

Fig. 1 XRD patterns of $Co_xMn_{1-x}Fe_2O_4$ nanoparticles

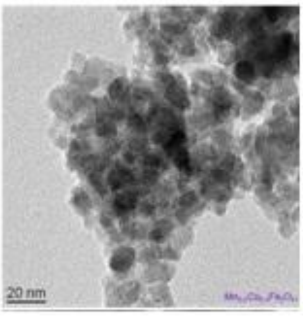

Fig. 2 TEM micrograph of sample $Co_{0.5}Mn_{0.5}Fe_2O_4$

Using X-ray diffractometry (fig.1) and transmission electron microscopy (fig.2) the crystallite size and average particles size were studied. Vibrating sample magnetometer (VSM) was used for magnetic properties characterization and FTIR measurement to observe theirs suitability for functionalization. The specific absorption rate was determined by a calorimetric method and obtained values are interpreted in correlation with microstructure and magnetic data. The preliminary data proved that member of the series are ready for use in theranostic. Study of the possible use as contrast agents is under way.

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P-17 Band structure of CdTe quantum dots capped by thioglycolic acid: Investigation through cyclic voltammetry

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Quantum dots (QDs) have generated tremendous interest due to their unique size-dependent chemical and physical properties. Such nanoparticles have direct applications in developing biological nanosensors and optoelectronics. Behavior of quantum dots can be described as oxidation and reduction of the core of the QDs. One of the basic electrochemical methods of the analysis of redox processes is cyclic voltammetry (CV). Band structure of CdTe QDs stabilized by thioglycolic acid has been investigated using the method of CV. The purpose of our study was to determine the band structure of the particles for instance the band gap (Eg), conduction band edge and valence band edge as a function of quantum dot size. Three-electrode system with platinum counter electrode, an Ag/AgCl reference electrode and the flat platinum electrode as the working electrode, was used for the measurements. Scan rate were 10, 20, 50, 100 and 200 mV/s. All experiments were carried out at room temperature (22-24 °C). This work demonstrates that the difference between the potentials of cathodic and anodic peaks in cyclic voltammograms corresponds to the band gap (Eg) which is consistent with spectroscopic data. CV for different samples show the presence of similar cathodic and anodic peaks that corresponding to the electrochemical activity of CdTe QDs. Also, the effects of scan rates were studied. Therefore, it was found that distance between the oxidation and reduction peaks increases with decreases QDs sizes. Band gaps (Eg) diagrams for different particle sizes were plotted on the base of the obtained results.

P-18 Peierls structural transition in Q1D crystals of TTF-TCNQ for different values of carrier concentration

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Earlier the Peierls structural transition in quasi-one-dimensional (Q1D) organic crystals of the tetrathiofulvalene-tetracyanoquinodimethane (TTF-TCNQ) type was investigated in a 1D physical model of the crystal. The aim of this paper is to present the study of the Peierls transition in a more complete 2D physical model. Two electron-phonon interactions are considered: one is of the polaron type and the other is similar to that of the deformation potential. The method of temperature Green functions is applied and the analytic expression for the polarization operator is obtained in the random phase approximation. The polarization operator as a function of temperature is calculated numerically for different values of the ratio d of the transfer energy in the direction transversal to conductive chains to the transfer energy along the conductive chains. The Peierls critical temperature T_p was determined for different values of the parameter d in two cases: 1) when the conduction band is half filled and the dimensionless Fermi momentum $k_F = \pi/2$, and 2) when the conduction band is filled up to slightly more than a half of the Brillouin zone and $k_F = \pi/2 + \delta$, where δ represents the increase of the Fermi momentum, determined by the increase of carrier concentration. It is found that in the first case the T_p strongly decreases with the increase of the parameter d and for a certain value of the parameter d the Peierls transition does not take place on the whole. In the second case, the T_p with the increase of carrier concentration n also decreases and for a given value of n the transition disappears too. In both these cases the physical interpretations of such behavior of the Peierls transition are presented and discussed.

P-19 Scientific Data Analysis Applied in Physical and Chemical Spectroscopy

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©NAldea is a small private company dedicated to Scientific Data Analysis formed by researchers with huge scientific performances. It is focused on scientific and technological transfer activities resulted from various measurements provided from physical, chemical and engineering spectroscopy. By the mutual collaboration you can also obtained scientific reliable results, professional quality documents presentations and custom interactive computational results in the complete package programs environment developed in different computer languages such as Fortran, Turbo Pascal and C or symbolic algebra all implemented in friendly Windows interface . Beside on those activities we can develop numerical and analytical models based on theoretical concepts that have provided from physics, chemistry, engineering and Life sciences. The input data for our data analysis can also provides from optical, structural, magnetic behaviour and electronic measurements of the general and local structure of modern materials, such as Me/support catalysts, high Tc superconductors, vitro/ceramics, solid films, etc. The main data can also be furnished by XRD, XAS (EXAFS, and XANES) spectroscopy

P-20 Effects of interactions on the switching fields observed in FORC diagram of nanomagnet arrays

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In 1935 Ferenc Preisach has proposed a powerful model that describes magnetic hysteresis (Classical Preisach Model – CPM). This phenomenological model is based on the bi-dimensional distribution of coercive and interaction fields supposed to be uniquely associated to the magnetic entities within the ferromagnetic sample [1]. These fields define a Preisach hysteron that in the same time designates switching fields between two equilibrium positions of the magnetic moment.

Magnetic characterization of the ferromagnetic samples based on FORCs becomes an extensively used method after 1999, when Pike and coworkers have used for the first time this technique [2], decoupling the FORC method from the Preisach model. A grate challenge is the understanding how Preisach hysterons (switching events) are accounted in the FORC diagram especially in the case of strongly interacting systems as arrays of nanomagnets (nanowires or nanopillars) in axial applied field. The advantage of these magnetic systems lies in the fact that each isolated element has a rather well established simple hysteretic behaviour described by a rectangular symmetrical loop. The interactions are changing the loop symmetry and the loops are like in the fundamental image described by the Preisach model in its simplest form. Unfortunately, in the complex protocol of the FORC method in which a large number of magnetic states are reached, switching fields are state dependent on the reversal curves and consequently Preisach hysterons have not a unique representation in the FORC diagram. We observe essentially two categories of effects of the interactions: nanoelements with the loop shifted along the interaction field axis without a significant change in the coercivity and nanoelements with the increased coercivity without a significant change in the loop symmetry [3]. In the full presentation a complete analysis of the switchings contributions will be performed showing how Preisach hysterons associated to the nanomagnets are contributed in the FORC diagram. We assess in this case the limits of the usual interpretation of the experimental FORC distribution directly in terms of Preisach hysterons.

[1] F. Preisach, Z. Phys. 94, 277 (1935). [2] C. R. Pike, A. P. Roberts, K. L. Verosub, J. Appl. Phys. 85, 6660 (1999). [3] C. I. Dobrotă, A. Stancu, J. Appl. Phys. 113, 043928

P-21

Nanostructured WO_3: Synthesis and characterization

M. Suchea[1,2], I.V. Tudose[1,2], A. Kougias[2], D. Manica[1], C. Tinica[1], C. Varlan[1], F. Iacomi[1], E. Koudoumas[2]
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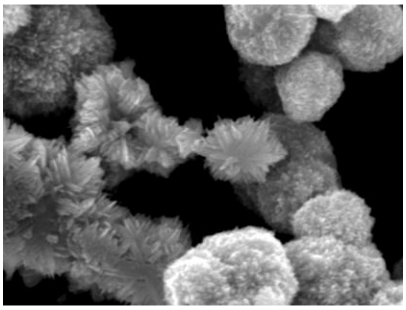
Metal oxides are the key ingredients for the development of many advanced functional materials and smart devices. Nanostructuring is one of the best ways to exploit their properties. Tungsten oxide (WO3) is a material that have been mostly studied for its electrochromism, photocatalysis, and sensing capabilities. Metal oxides can be prepared in various sizes and geometries, but one of the greatest challenges remains the precise control of the particle size, shape, crystalline structure and processing properties. The present contribution presents preliminary results of chemical synthesis and chacterization of nanostructured WO_3 for potential applications in organic solar cells application as a charge injection layer.



Chemically synthesized nanostructured WO3

Acknowledgements: Part of the work was partially supported by the strategic grant POSDRU/159/1.5/S/133652, co-financed by the European Social Fund within the Sectorial Operational Program Human Resources Development 2007 – 2013 and by the grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-RU-TE-2012-3-0202.

P-22 Investigations of $CoFe_2O_4$-ferrofluid magnetisation curves

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[4]Faculty of Physics, Moscow State University, Moscow, Rusia

The magnetic properties of ferrofluid systems are interesting both in the development of a large spectrum of applications and from a theoretical point of view In this work results of CoFe2O4 ferrofluid magnetization curves investigation at low temperatures are presented and analyzed. For the theoretical treatment the magnetogranulometric methods based on Langevin model and on the hypothesis of a log-normal distribution for the magnetic diameters of particles were considered. According to the Langevin model of paramagnetism, the ferrofluid is considered as composed by non interacting spheres with a permanent dipolar magnetic moment rotating together with the particle when applying an external magnetic field. The macroscopic magnetization is obtained as a result of the combined action of an orientation induced by the external field and a destabilization produced by the Brownian motion. The magneto-granulometric analysis for the ferrofluid sample performed at T=300K, where the Langevin model is applicable, gives the parameters of the size distribution. The experimental results obtained for temperatures below 100K cannot be treated using the Langevin model.

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P-24 Multifractal analysis of $CoFe_2O_4$/ 2DBS/H_2O ferrofluid from SANS and TEM Measurements

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Morphology and structure of CoFe2O4/ 2DBS/H2O ferrofluid is investigated from SANS and TEM measurements. TEM analysis was carried out on a LEO 912 AB OMEGA transmission electron microscope with an accelerating voltage of 120 kV (Advanced Technology Centre, Moscow). One droplet of water dispersion of CoFe2O4 nanoparticles was dropped on a carbon-coated copper grid and then dried naturally before recording the micrographs. Small angle neutron scattering (SANS) experiments were performed at the time-of-flight YuMO spectrometer in function at the high flux pulse IBR-2 reactor, JINR Dubna. The experiments were carried out at a sample-to-detector distances of 5.28 m and 13.04 m, resulting in a Q range of 0.007÷0.3 A-1. The sample diameter and thickness in the beam were 14 mm and respectively 1 mm. The measured neutron scattering spectra were corrected for the transmission and the thickness of the sample, background scattering on the experimental cuvette and on vanadium reference sample using the SAS software, providing a neutron scattering intensity in absolute units of cm-1. A statistical analysis of the particles diameters is made using the log-normal distribution. The 3-dimensionally reconstructed images show the characteristic morphology of the spatial dispersion of nanoparticles and nanoparticle conglomerates in the liquid suspension. A multifractal analysis of the two TEM images representing portions of the same sample using two different enlargement is made. The multifractal spectra of the studied images reveal universal multifractality. A comparison with fractal approach applied to SANS data is presented.

P-25 $Fe_{67,7}Cr_{12}Nb_{0.3}B_{20}$ powders prepared by DC arc discharge method

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$Fe_{67,7}Cr_{12}Nb_{0.3}B_{20}$ powders have been prepared by DC arc discharge method. This method allows the preparation of amorphous and crystalline nanoparticles with dimensions of hundreds of nanometers, depending on the amount of depression of the inert gas and the parameters of the electric arc. The parameters which used for the preparation of the $Fe_{67,7}Cr_{12}Nb_{0.3}B_{20}$ powders are: temperature enclosure of 0 ºC to -17ºC, working gas pressure of -0,85 bar He to -0,5 bar He, discharge current of 40 to 100A, time discharge of 3 minutes to 15 minutes, and powders were collected from different areas of the enclosure. The magnetic properties have been investigated by vibrating sample magnetometery (VSM) and thermomagnetic mesurements and dimensions of the particles was estimated from scanning electron microscopy (SEM). On an area not exceeding 15mm wide of the 50 mm diameter cylindrical chamber we have obtained amorphous powder (confirmed by the thermomagnetic measurements) and above and below this area the obtained powders are crystalline. This difference in the powder's structure is determined by the temperature gradient carrying metal clusters from the surface of the molten alloy to the wall and by the time of flight (while the particle size increases). The flight time increase due to the increase in the particles velocities towards the wall results in a almost continuous layer of particles deposited on the chamber wall, almost impossible to collect without altering the structure. The magnetization of powders decreases with decreasing the working gas pressure from -0.6 to -0.85 bar. If the discharge current is increased the magnetization increases. Increasing the discharge time the amount of powder increases proportionally, but for a discharge time higher than 15 minutes the powder looses the amorphous character. Thus $Fe_{67,7}Cr_{12}Nb_{0.3}B_{20}$ powders with diameters between 100-150nm have been obtained for the temperature range of the enclosure between -17ºC and -13ºC, a DC current of 50A and He depression of -0,7 bar.

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TOPIC 7

Metamaterials. Applications

O-1 Metamaterials lens for optimization of carbon fibers-PPS composites electromagnetic testing

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Carbon Fiber Reinforced Plastics (CFRP) are multilayered composite materials with applications among most different from aeronautic industry to sport goods. The principals' factors that recommend the use of CFRP are low density, high elastic modulus along the carbon fibers, high ultimate strength along the same direction, no fatigue phenomena and the expansion coefficient is small. The disadvantages are low strength at impact even at low energies (1÷10) that can lead to delaminations without and with fiber breaking, matrix deterioration due to chemical action of adsorbed water, the impossibility to use CFRP at temperature exceeding glass transition temperature [1]. CFRP is a paramagnetic composite ($\mu r \approx 1$), having electrical conductivity relatively high in the fibers plan, 10^2-10^4S/m[2]. From this reason, the using of electromagnetic methods for characterization is perfectly justified. Samples from CFRP with matrix from PPS reinforced with 12 layers of woven carbon fibers 5 harness satin fabrics have been studied. The volume ratio of carbon fibers is 0.5±0.03, the total thickness of composite being 4.2mm. The samples have been impacted using a hemispheric bump head, 20mm diameter, with energies between 2 and 12J. Due to the plastic deformation following the impacts, the transversal electrical conductivity is modified [3], allowing electromagnetic procedures for evaluation. For the detection of delaminations, an electromagnetic transducer with metamaterials lens has been used [4]. The transducer is connected to the equipment developed in this purpose. The surface of each sample is scanned on 60x60mm2 area, with 1mm steps on both directions using a X-Y motorized stage Newmark USA. The command of the modular equipment and recording of data is made by means of codes developed in Matlab 2011b. The signal received by the reception part of the transducer is used for assessment of complex CFRP structures. The sensor based on metamaterials lens assures the manipulation of the evanescent waves that appear between the carbon fibers. This method has been applied for investigation of CFRP impacted with low energies in order to determine their influence over the area of delaminated surface.

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O-2 The evanescent waves in metallic strip gratings complex structures in subwavelenght regime

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The interaction of electromagnetic field with periodical structures consists an interesting domain from both theoretically and applicative point of view. The diffraction limit is the one that restricts the dimensions which can be distinct on the image at half of wavelength and it can be exceeded using metamaterials. Metamaterials can provide solutions which exceed this limit by the ability to control and manipulate the interactions electromagnetic wave - materials. The metallic strip grating (MSG) is the one of most studied due to a multitude of reasons: it represents the basis element of printed circuits, from feed to signal transmission and presents special properties when are "illuminated" by plane electromagnetic polarized wave. The recent researches have shown that evanescent waves can appear in the space between the conductive traces of metallic strips and also inside the open surface cracks from metallic pieces. The evanescent waves are exponentially attenuated in medium so that, in order to manipulate them, the use of transducer with metamaterials lens is proposed [1-4]. In this paper, we focus on the study and obtaining of metallic strip gratings and complex structures, with thick Ag strips, deposited on different substrates by vacuum thermal evaporation by modifying the evaporator-substrate distance, the deposition time and strip and slit width with applications as sensors/ biosensors. The investigation of the structural characterization of the study structures by XRD and SEM methods emphasized that a thickness of Ag strips in the range of micrometers can be obtained only when certain depositions and a certain mask is used. m order is comparable with the depth penetration of electromagnetic wave in radiofrequencies, so that evanescent waves could appear at the edge of strips. We proved that transducers with metamaterials lens can be used in amplitude evaluation of the evanescent waves formed at the edge of strips.µThe Ag strip grating thickness of

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P-1

About the optimization of acoustic metamaterials in the audible frequency range

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The use of acoustic metamaterials represents one of the most innovative and effective way to achieve sound control emission. Within this context a problem of particular interest relates to the absorption of sound and noise emission at very low frequencies ranging, in particular, in the audible frequency range. In fact, in this range, the commonly used porous absorbers show an important lack of performances making so necessary the use of subwavelenght resonant absorbers as, primarily, Helmholtz resonators based membranes. Acoustic metamaterials are able to overcome, if adequately designed, this difficulty. In this paper we'll analyze, by implementing suitable numerical methods, the absorption and control performances of acoustic metamaterials in the audible frequency intervals, comparing the results with those offered by traditional techniques.

P-2

Glass-coated amorphous microwires metastructures for GHz shielding applications

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In the last years, the high frequency properties of magnetic glass-coated amorphous microwires (GCAWs) are investigated in order to develop artificial structures based on specific GCAWs that exhibit left-handed behavior in narrow microwave frequency band. [1-3]. Combination of different type of GCAWs with similar high frequency properties could be a strategy in order to enlarge the frequency domain with metamaterial behavior of such metastructures. The aim of this work is to propose new structures based on Co-, CoFe- and Fe- GCAWs systems with parallel arrangements that can be used as broadband frequency shielding metasystem for microwave range.

Experimental results of the free standing systems based on $Co_{72.5}Si_{12.5}B_{15}$ GCAWs with metallic nucleus diameter D_m= 6 μm and glass layer thickness t_g=8 μm parallel arranged at b=3 mm interwire distance, shows left-handed properties between 8.5 and 13.2 GHz while the free standing system based on $Fe_{77.5}Si_{7.5}B_{15}$ GCAWs indicates the presence of left-handed properties between 6.2 and 10.5 GHz.

The combined structure developed by alternating Co- and Fe- GCAWs at 3 mm interwire distance presents a broader frequency domain with left-handed behavior between 6.5 and 11.7 GHz with a narrow transmission window around 9 GHz. In order to supplementary expand the left-handed frequency domain of the metasystem, the individual $Co_{40}Fe_{40}Si_{12}B_8$ GCAWs with the same geometrical characteristics having the left-handed behavior between 5.5 and 9.1 GHz, were added by alternation in the mixed structure.

The metastructure with all types of GCAWs shows the left-handed behavior between 5.5 and 13.2 GHz as superposition of common frequency domain with the transmission window between 8.3 and 9.5 GHz which can be fine-tuned in the presence of an external magnetic field. The experimental results are in agreement with the calculated ones using LLG equations.

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TOPIC 8

Polymer Materials and Composites

PL-1 High-throughput manufacturing of polymer-ceramic nanocomposite dielectric capacitors designed for energy storage

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Two material properties define the energy density of a dielectric layer: the dielectric constant and the breakdown as derived from the definition of capacitance. There has been significant of work over the past ten years trying to maximize either the breakdown field or the dielectric constant in order to increase the total energy density, however, these improvements still fall short of the energy density requirements and methods that address both properties are needed. Former research that tries to increase both dielectric constant and breakdown field through nanocomposites consisted of mixing high dielectric nanoparticles with known high breakdown polymers with the assumption that, although both the dielectric constant and breakdown field will reduce below the pure materials, there will be an overall increase in energy density. However the interface of the nanoparticle and polymer matrix creates a void which acts as a charge concentrator, greatly reducing the breakdown field. Elimination of this gap greatly increases the breakdown field of the nanocomposite film. By designing a thermally and electronically stable polymer that is cured through UV processing, functionalized high dielectric constant nanoparticles can be directly bonded into a high breakdown polymer matrix. The design of a high breakdown material requires the control of the structure and chemistry to increase cross-linking, crystallinity, dipole traps, and dipole interactions. Thiol alkene click chemistry, combined with precise curing techniques (such as xenon flash curing), offers the control necessary to design a polymer to create a high breakdown dielectric. Although the material design is the most significant aspect to meet the energy demands, the processing techniques must be scalable and energy efficient to gain industrial acceptance. During the design of the high energy density materials, fluid properties are characterized and optimized so that they can be printed by roll-to-roll processing, making them amenable to large-scale production. Thiol-alkene based polymer-ceramic nanocomposites are inkjet printed and photonically cured to produce high-energy, high-power density dielectric capacitors.

I-1 Experimental design, modeling and optimization methods for materials preparation and applications

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Design of experiments (DoE), response surface methodology (RSM) and artificial neural networks (ANN) are valuable tools of applied mathematics and statistics employed to solve multivariate regression problems for modeling and optimization of experimental processes related to materials preparations and their applications in chemical engineering. The models, constructed based on RSM and ANN, have proven to offer good predictions of process responses as the functional relationships of input variables. For instance, such models have been developed to predict and improve the performances related to preparation of polymeric membranes and their applications in separation and purification technologies, such as membrane distillation (i.e. direct contact membrane distillation DCMD, air gap membrane distillation AGMD and sweeping gas membrane distillation SGMD), reverse osmosis RO, pervaporation PV and polymer assisted ultrafiltration PAUF [1-3]. Also, multivariate regression models have been constructed for modeling, response surface analysis and optimization of adsorption and electroplating processes using different types of materials. The model-based optimization has been performed using single-objective optimization algorithms (such as, random searching, pattern-search, gradient method, genetic algorithm, etc.) or multi-objective optimization algorithms (i.e. desirability function approach, NSGA-II).

In this work, the basic concepts of design and modeling tools, i.e. DoE, RSM and ANN, are discussed, as well as, it is pointed out their implementation to solve the real problems regarding the optimization of materials preparation and maximization of their efficiency in various applications related to chemical environmental engineering.

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I-2

Viscoelastic phase separation process and the development of micro and nanomorphologies in epoxy based blends for super toughness

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Phase separation in general could be by diffusion or by diffusion and hydrodynamic flow. A new model has been suggested to follow the phase separation process in asymmetric mixtures composed of fast and slow components. This new model is often called the viscoelastic phase separation process due to the fact that viscoelastic effects play a dominant role in the phase separation process. The dynamic asymmetry can be induced by either the large size difference or the difference in Tg between the components of a mixture or blend. The mol.wt difference often exists in complex fluids, such as polymer solutions, polymer blends, colloidal suspensions, emulsions, and protein solutions. In dynamically asymmetric mixtures, phase separation generally leads to the formation of a long-lived `interaction network' (a transient gel) of slow-component molecules, if the attractive interactions between them are strong enough. Because of its long relaxation time, it cannot catch up with the deformation rate of the phase separation itself and as a result the stress is asymmetrically divided between the components. This leads to the transient formation of network like or sponge like structures of a slow-component-rich phase and its volume shrinking [1]. In the present talk we present our new results on the viscoelastic phase separation process in epoxy/SAN and epoxy/ABS blends. Epoxy resin is often blended with high mol.wt. thermoplastics to generate micro structured morphologies for the better impact performance. These systems are very ideal to follow the viscoelastic phase separation process on account of their mol.wt and Tg differences. We have looked at the phase separation process in these blends by various techniques such as optical microscopy, scanning electron microscopy, TEM, AFM and SALLS. The dynamics of phase separation has been followed by POM and laser light scattering. In most cases the system undergo SD and the viscoelastic phase separation was prominent at higher conc. of the thermoplastic phase where phase inversion occurs. The particle in particle morphology (secondary, ternary and quaternary phases), IPN type of structures and unusual shrinkage have been examined as a result of the phase separation process.

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O-1

New design of antimicrobial membranes based on polymers colloids/MWCNT hybrid materials and silver nanoparticles

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Abstract The aim of this study is to obtain membranes with antimicrobial activity presenting a complex sandwich type structure. The outer layers are comprised of PMMA membranes, whereas the inner - active layer consists of a modified commercial membrane in order to achieve antimicrobial properties. This characteristic results from the presence of silver nanoparticles (AgNps) in a material with a hybrid composition deposited on a commercial membrane. This hybrid material consists of polymer colloids and multiwall carbon nanotubes (MWCNTs) used for both the stabilization of the active layer by the interconnections of the polymer particles. The filtration tests revealed a good stability of the materials and an increased hydrophilicity of the hybrid membranes. The antimicrobial properties have been evaluated using Staphylococcus aureus and have been correlated with the migration rates of silver ions.

O-2 Optical properties of silane copolymer doped with fullerene C_{60}

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Polysilanes belong to a class of σ-conjugated polymers. They exhibit intrinsic electric conductivity, broad photoluminescence, and transparency in the visible region. Being doped with fullerene, they are known to form complexes and to exhibit photoinduced electric conductivity. Based on this phenomenon, fullerene-doped polysilanes seem to be a promising material for thin film solar cells.

We synthesized a highly soluble diphenylsilane/methylsilane copolymer (PSHDF). For optical research, we prepared PSHDF and C_{60}-doped PSHDF samples in the form of solutions and films. We varied the fullerene concentration in the PSHDF samples from 0.07 to 1.92 wt%.

In the UV-vis spectra of the PSHDF sample, the characteristic σ—σ* electron transitions lead to the wide specific band within the 300-400 nm region. In the spectrum of the C60-doped polymer (1.85 wt%), it spreads to longer wavelengths and its maximum shifts from 345 to 380 nm. This batochromic shift indicates that intermolecular charge transfer complex (CTC) is formed. The C_{60} concentration equal to 0.8 wt% was found to be critical. Exceeding this concentration guarantees PSHDF/C_{60} complexation. Also we investigated the photoluminescence intensity of the PSHDF/C_{60} complex as a function of C_{60} concentration. Since in the PSHDF/C_{60} complex the polymer is an electron donor and fullerene is an electron acceptor, the excitation energy absorbed by the PSHDF may be transferred to the acceptor molecule C_{60} as a nonradiative process. This leads to decreasing of the photoluminescence intensity of C_{60}-doped PSHDF. Hereby the photoluminescence quenching in C_{60}-doped PSHDF confirms the CTC formation.

The research leading to these results has received funding from the Russian Foundation of Basic Research (Project No 13-03-00033) and the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement No 264115 - STREAM.

O-3 Organic-inorganic membranes for desalination of biological liquids

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N+ groups are placed. The aggregates, which have a negative impact on functional properties of the membranes, are practically absent. It is very important, since the aggregates stretch pore walls providing increase of swelling, decrease of surface charge density, deterioration of membrane permittivity towards cations or anions. The aggregates form secondary porosity, which enhances electroosmosis. No significant transformation of porous structure of the matrices was found with a method of standard contact porosimetry. The nanoparticles block penetration of large organic species into the membranes (fouling prevention).–SO3H or R4–Organic-inorganic materials were obtained by modification of ion exchange heterogeneous membranes with nanoparticles of zirconium hydrophosphate and hydrated zirconium dioxide, into cation- and anion-exchange matrices, respectively. As found by means of TEM and SEM methods, the inorganic constituent exists in a form of non-aggregated nanoparticles (4-20 nm). They are located in nanosized transport pores of the polymer, where functional R 10 нм, this is in accordance with the data of standard contact porosimetry.≈The membrane-solution systems were investigated using impedance spectroscopy. The membrane conductivity increases within a wide interval of NaCl concentration in the solution. Modification was found to increase a contribution of gel phase into the conductivity due to participation of counter-ions of functional groups of the inorganic constituent in charge transport. The field of concentrations, which corresponds to domination of surface conductivity was identified. The domination is due to overlapping of diffusion parts of intraporous electrical double layers. Radius of transport pores of the membranes calculated according to Debay formula is As found using voltammetry, modification prevents concentration polarization of the membranes, if the current is lower than a limiting value. This allows us to avoid deposition of insoluble compounds on the membrane surface, which deteriorates the efficiency of electromembrane separation and enhances the energy consumptions. The modified membranes were used for electrodialysis desalination of whey and distillers grains.

O-4 WAXS/SAXS/USAXS investigation of orientation induced by deformation in semi-crystalline polymers

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During the industrial transformation, most polymers are involved in specific processes resulting in the macromolecular chain orientation. Such orientation is appearing from the local phase to the mesophase and sometimes even up to the macroscopic phase. Small Angle X-Ray Scattering (SAXS) is a technique well suited for investigating nano-materials and nano-structures of polymers. Information is collected on sample structure parameters such as particle shape or size, size distribution, orientation, surface to volume ratio… in the range from 1 nm to beyond 100 nm. Moreover, orientational functions can be derived from 2 dimensional x-ray patterns. Length-scales down to 0.1 nm can also be investigated in combination with Wide Angle X-ray Scattering (WAXS). In the case of samples with internal structures larger than 200 nm, USAXS (Ultra Small Angle X-Ray scattering) experimental conditions are required. USAXS allows to access heterogeneities about some hundreds of nanometers while providing the opportunity to investigate the large-scale structure evolution during the deformation of polymeric materials [1].

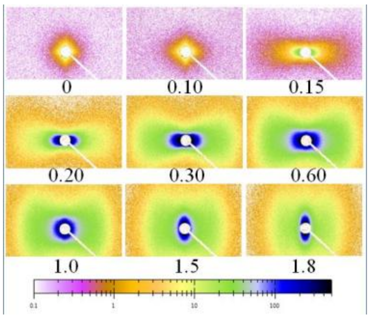

Figure 1: 2D-USAXS patterns of PB-1 crystallized at 60°C stretched at 30°C as a function of engineering strain - 50s exposure time. Stretching direction horizontal. Data courtesy of Pr. Men and Y. Wang

The progress in the performances of x-ray components and subsequent assembly offers such characterization methods in the laboratory. Hence, investigation of an injected semicrystalline polymer has been performed, emphasizing the nanostructure orientation and processing relationships. Further, recent results obtained on in-situ stretched Polybutene-1 (PB-1) [Figure 1] illustrate the capability to perform lab measurement equivalent to Synchrotron USAXS [2] highlighting microscopic structural evolution and macroscopic strain-whitening phenomenon correlation.

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O-5 Preparation of novel composite materials via CO-Coagulation of NPs

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Since the term ‘nanocomposites’ has been proposed for the first time by Theng in 1970, the science dealing with these materials has arisen at the border of different areas of knowledge. Numerous procedures for the preparation of nanocomposite materials have been investigated in order to generate materials with controlled features, which is still one of the great challenges in nanotechnology. The purpose of this work is to use the extended and large knowledge of self-assembly behavior of spherical nanoparticles and its dependence on interparticle interactions for the preparation of various polymeric nanoparticles and the investigation of their self-assembly, to generate hybrid nanostructured composites. The nanocomposite comprises different concentrations of hard silica nanoparticles (20 nm diameter) blended with a colloidal dispersion of soft poly(butyl acrylate/methyl methacrylate) copolymer particles (80 nm diameter). In order to investigate the specific role of the interparticles interaction on the final structure and mechanical properties of the materials, the nanocomposites have been synthetized following three different assembly stategies: mixing of stable particle suspensions with same surface charge, aggregation/gelation of the filler particles inside the matrix particle stable suspantion, hetero-aggregation of particle suspensions with opposite surface charge. The different hetero particle suspensions have then been precipitated and subsequently annealed, giving rise to a nanostructured polymeric composite, which has been characterized in term of structure and mechanical properties using different techniques (SAXS, AFM, SEM, tensile test).

O-6 Aromatic Polyamide-Imide modified by hydrosilicates nanoparticles of different morphology

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Development of organic-inorganic materials for advanced technologies, including membrane technology, is an actual problem of modern material science. In this study physical-chemical and morphology of composites based on PAI matrix, containing Na-Mg hydrosilicate nanoparticles of fibrous structure, $Na_2Mg_4Si_6O_{16}(OH)_2$ are investigated comparable with those filled by $Mg_3Si_2O_5(OH)_4$ nanotubes - NT. The obtained results showed that the nanotubes embedded in the polyamideimide matrix form aggregates, irrespective of the degree of polymer filling. Consequently, the PAI-NT films should rather be considered as micro-composites, then nano-composites, with the thermal properties (thermal stability and glass transition temperature) considerably exceeding those of the polymer matrix. The optimum mechanical properties of PAI-NT composites (high Young modulus in combination with high plasticity), were attained when the NT content do not exceed 2 wt.%. AFM investigations of the polymer and composite films revealed considerable transformation of the surface’s morphology by introduction of the inorganic nano-filler aggregates. When the content of NT reached 5 wt.% the nanoparticles are pushed out of the surface layer, leading to failure of adhesive contact between polymer and nanotubes. This process can be the reason for micro-defects formation and was accompanied by decreasing of mechanical properties of films. PAI films and composites based on PAI possess anisotropy of mechanical properties, related with the polymer structure and introduction of fibrous hydrosilicates leads to the decreasing of mechanical properties, compared with neat PAI and composites with nanotubular particles. Investigation of the nanocomposites films cross-section by SEM and AFM allows us to explain the decreasing of physical-mechanical properties of composites as consequence of the non-uniformity of nanoparticles distribution and bad adhesion between polymer matrix and nanofillers.

O-7 Study of muzeal textile materials, artificial ageing, by AFM, dynamometry and WAXD

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In this study we analyze some parameters that influence the conservation conditions of materials like wool, cotton, silk in museum enclosures. It is ascertained that textile materials inside closed enclosures (shop windows, glass cabinets, boxes), abide a degradation process in time, which can not be explained by UV radiations, temperature changes, microclimate conditions connected with great number of visitors, etc. We take in account the influence of wood emanation of acetic acid vapors in museum rooms. The samples have been analyzed by: - WAXD – Wide Angle X-Ray Diffraction, in order to see the changes in the crystalline structure; - AFM – Atomic Force Microscopy, in order to study the changes in the surface morphology; - dynamometry on single fiber in order to see the influence of treatment over stress-strain curve, ultimate strength and young modulus.

O-8 Polymer-dispersed liquid crystals: preparation, electro-optical properties and applications

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Research publications of last years reveal an increasing interest to polymer-dispersed liquid crystals (PDLCs). They are already used for manufacturing flat-panel displays, switchable windows, holographic films, etc. Nowadays PDLC displays with a very high resolution, near a laser printer quality, are produced. PDLC is a mixture of liquid crystals (LCs) and monomer, in which phase separation is induced by either thermal/UV curing or solvent evaporation. The resulting two-phase system contains LC domains, which are surrounded with a polymer matrix. The nematic structure within a LC domain is randomly oriented, so that incoming visible light is scattered, and the PDLC appears milky white. Application of an external field orients domains in the preferred direction, and PDLC becomes transparent. There are two principal methods of PDLC preparation: encapsulation and phase separation. In the first method, an LC is mixed with a polymer dissolved in water. When the water is evaporated, the LC is encapsulated by a polymer matrix. In the second method, an LC first is mixed with polymer/monomer. Consequently, LC domains are formed by the phase separation of the components. Phase separation during the PDLC formation can be realized by monomer polymerization, thermal action, and solvent evaporation. Polymerization-induced phase separation occurs immediately when LC is mixed with a monomer solution. Thermally-induced phase separation happens when the mixture of LC and a melted polymer is cooled. Solvent-induced phase separation occurs when dissolved mixture of LC and a polymer is subjected to the solvent evaporation. Three types of the characteristics are shown to affect the electro-optical behavior of PDLCs: i) the structure, the size, the shape, the packing, and the content of LC droplets embedded into the polymer matrix; ii) the flexibility/rigidity of the polymer matrix; and iii) the components compatibility. The recent results of the kinetic study of the nematic phase growth across the thermally-induced phase separation during the PDLCs preparation are presented.

P-1 Elaboration and characterization of m-Cresol Polyamide12/ Polyaniline composite films

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Fabrication of thin film capacitors on multi-chip modules is essential to reduce circuit's size in electronic systems of very high speed. To produce such films from intrinsically conducting polymers (ICPs) is not only complicated because of the difficulty of processing, but also because the ICPs are generally strongly coloured because of their conjugated system. The present work deals with the preparation of transparent antistatic films from an extreme dilution of an ICP with not coloured polymers. Our approach is based on the chemical polymerization of a very thin layer of the intrinsically conducting polymer (PANI) around particles of a transparent polymer (PA12). This particulate structure allows achieving low conduction thresholds and high dielectric constant. Transparent conducting films are then obtained by dissolving the synthesized core-shell particles in m-Cresol. The structure and dielectric property relationships were investigated by using X-ray diffraction, micro-Raman spectroscopy and dielectric relaxation spectroscopy. X-ray diffraction data show broader and lower intensity of PA12 peaks when increasing PANI content, probably due to the remove of additional doping effect of m- cresol. The doping of PA12/PANI films with Dodecyl benzene sulfonic acid (DBSA) was unequivocally verified by Raman spectroscopy. Composite films exhibited a well established dc conductivity over all the frequency range for 10 wt. % of PANI concentration related to the conductive properties of the PANI clusters. It was shown that the conductivity can be enhanced by heating m-Cresol solution when preparing films. High dielectric constants were obtained at 5 wt. % of PANI allowing their use as dielectrics compatibles with organic printed circuit boards. Relaxation phenomena were also observed and related to the interfacial polarization. The results are consistent with Raman spectroscopy and X-ray diffraction data concerning PANI particles dispersion in the polyamide films.

P-2 Metal – polymer nanocomposites based on polythiophene and Ni nanoparticles obtained by electrochemical method

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Much attention has been paid in recent years to understanding mechanical, thermal and electrical properties of nanocomposite materials (such as polymer films, nanorods, nanotubes or nanowires), which exhibit interesting electrical properties. Nanocomposites based on metal-polymer are especially attractive for nanoscience studies as well as for nanotechnology applications. These nanostructures have a deep impact on both fundamental research and potential applications in nanoelectronics or molecular electronics, nanodevices, nanocomposite materials, bio-nanotechnology and medicine [1-3]. The influence of Ni content on the structure and electrical properties of polythiophene-Ni composites prepared by electrochemical oxidative polymerization of thiophene in the presence of nickel nanoparticles was analyzed. Firstly, the method consists of the chemical synthesis of Ni nanoparticles of 6 ÷ 20 nm diameter having a narrow size distribution, and secondly, the encapsulation of the nanoparticles in a conducting polymer matrix. Pure metallic nickel nanoparticles, rectangular and spherical in shape, have been successfully synthesized by the chemical reduction of nickel chloride with hydrazine at 100 – 130 °C. The synthesis of nickel nanoparticles was carried out using poly (N-vinilpyrrolidone) (PVP) as protective agent. TEM, SEM, XRD, FTIR, XPS and TGA studies are performed for the morphological, structural and thermal characterization of the polythiophene (PT) nanocomposites. Composites on the basis of PT with a low Ni content (0.6 at 1.3 wt% from XPS measurements) possess both the good thermal stability and high electrical conductivity response to be considered as a conducting polymer. Electrical conductivity was studied as a function of temperature. Change in electrical conductivity of the polymer nanocomposites depends on the conductivity of the filler particles into conducting polymer matrix. The conductivity of the composite decreases from 0.0125 Ω·cm-1 to 0.0045 Ω·cm-1 as the amount of nickel was increased from 0.43 % up to 1.3 %.

Acknowledgements: This work was financially supported by the project POSDRU/159/1.5/S/133652.

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P-3

Hematite / Polymer composite fibers - magnetic properties depending on the process parameters

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Electrospinning has been considered the most effective technique for the fabrication of polymer nanofibers and composite nanofibers. The physico-chemical properties of nanofibers are intensively studied in the last decade [1-4]. In the present study we have attempted to show how the process parameters influence the formation of composite nanofibres and what effect they have on ferromagnetic properties. For this purpose we used for three different solutions in electrospinning process one needle (0.5 mm diameter for polymer pump) and three different distances between the needle and deposition support. Analyzing histograms performed on SEM images of prepared samples we observed that with decreasing distance needle - deposition support, appear two maxima distribution of fiber diameters. Since the used particles do not have a spherical shape and in addition they forms clusters along the fiber, during the electrospinning process in the area of this agglomerations is forming secondary Taylor cones and composite fibers are splitting (Fig.1).

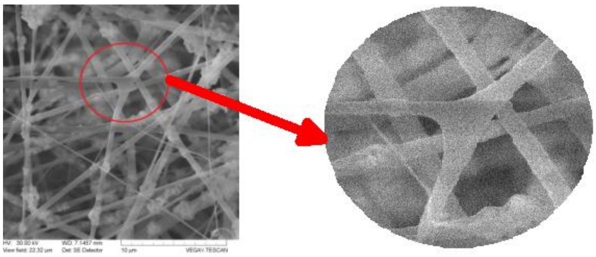

Fig. 1

Fibers splitting phenomena Taking into account that the higher the amount of particles embedded in the polymer matrix, which agglomerate along the fiber, may arise significant changes in the interaction field of the particles, and also modifying the coercive field distribution by the system. The interaction fields of the magnetic nanofiber assemblies were investigated using First Order Reverse Curves (FORC) diagram method. The decreasing interaction fields for growing α-Fe_2O_3 concentration of nanofiber are sustained by FORC diagram investigation.

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P-4 Poly(ethylene glycol)-block-poly(ε−caprolactone) methyl ether copolymer coating potential for bio-applications

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In this work, we explore the feasibility of using the Poly(ethylene glycol)-block-poly(ε−caprolactone) methyl ether copolymer as potential coatings for testing osteoblast adhesion. The films were deposited using Matrix Assisted Pulsed Laser Evaporation technique that allows good composition control and controlled thickness. The films were examined using Fourier transform infrared spectroscopy, contact angle measurements, atomic force microscopy, and cell adhesion studies. The Fourier transform infrared spectroscopy data demonstrated that the main functional groups in the MAPLE-deposited films remained intact. Characterization and evaluation of the coated substrates was carried out using different techniques. Scanning Electron Microscopy and Atomic Force Microscopy images showed the coatings to be continuous, with low surface roughness.

P-5 Electrocatalytic properties of composite films based on conjugated polymers with electrochemically reduced graphene oxide

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Graphene materials (GMs) – graphene, graphene oxide (GO), partially reduced GO (RGO) – are known to possess unique properties and are attractable considerable attention as a starting materials for the preparation of various GM-based composites with metal, semiconductor nanocrystals, polymers etc. Nanocomposites based on organic conducting polymers and GMs are a relatively new subject of research, but already are estimated as promising materials for electrochemical applications, such as electrocatalysts, supercapacitors and sensors. We have shown that the hybrid nanocomposite films based on conjugated polymers (poly-o-phenylenediamine – POPDA, polyaniline – PANI, poly-o-aminophenol – POAP) and RGO can be formed via several electrochemical approaches. It was established that composite films, when deposited onto glassy carbon (GC) or Au electrodes, have higher electrochemical activity in 0.05 M H2SO4 and provide better reversibility of redox system $[Fe(CN)_6]_3$-/$[Fe(CN)_6]_4$- compared with the individual polymer films. It was found that such composites exhibit sufficiently high electrocatalytic activity, in particular, in the processes of oxygen reduction (POPDA/RGO, PANI/RGO), oxidation of NADH and ascorbic acid (POPDA/RGO, POAP/RGO). The effect of conditions of composite films preparation on their electrocatalytic activity was shown.

P-6 Study of chitin fragmentation induced by high energy deuteron beam irradiation

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Chitin is a polysaccharide of N,N-acetyl-D-glucosamine and the second most predominant biopolymer in nature, after cellulose, found mainly in the exoskeleton of crustaceans and in the cell walls of fungi. Chitin and its primary derivative, chitosan, have several biological proprieties that make their study relevant, the most important being biocompatibility, biodegradability and nontoxicity. Chitin's biological proprieties are related to certain characteristics of the polymer macromolecule, like the degree of deacetylation (DD), molecular weight, viscosity. The influences of physical factors over these proprieties have been carried out for exposures to gamma rays, microwave and ultrasound. The aim of this study was to reveal the interaction processes of a deuteron beam with chitin powder. In this respect, chitin powder (provided by Sigma-Aldrich) was irradiated with a 2 GeV deuteron beam at the JINR Dubna (Russian Federation) facilities. Measurements were performed in order to establish the exposure dose. After irradiation, chitin solutions were obtained using a DMAc/LiCl system as solvent, with concentrations in the range of 0.31-0.026 mg/mL. Viscosimetric measurements were carried out using an Ubbelohde viscometer, with constant K=0.01004, and yielded a viscosity-average molecular weight of 6.9 x 105 g/mole for non-irradiated chitin and 5.7 x 105 g/mole for the irradiated one. The results showed that chitin is modified by the deuteron beam, which can break long molecules and create new chemical bonds. These aspects will be confirmed by thorough investigations.

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P-7 Chitin morphology modification after exposure to 2 GeV deuteron beams

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Chitin is a long-chain, natural aminopolysaccharide, having unique structure and multidimensional properties. Together with its derivative, chitosan, chitin is used in a wide-ranging applications in biomedical and other industrial areas. The positive properties of these polymers are biocompatibility and biodegradability, low toxicity and versatile biological activities. Despite its advantages and easy availability, chitin still remains underutilized because of its intractable molecular structure and its non-solubility to all common solvents. Modifying its molecular structure may allow new chemical bonds and new opportunities of use. One of the methods used for modifying chitin is the exposure to ionizing radiation at high doses, especially to gamma rays. Recently, chitin modifications under hadron irradiation are investigated, in terms of molecular weight and physiochemical properties. The aim of this work is to study the morphological modification of chitin after interaction with a deuteron beam. Chitin powder (provided by Sigma-Aldrich) was irradiated with a 2 GeV deuteron beam at the JINR Dubna (Russian Federation) facilities. The differences in morphological structure were studied by Atomic Force Microscopy and Scanning Electron Microscopy techniques. Also, the degree of fragmentation and the variations of molecular weight were measured using high performance liquid chromatography – mass spectrometry technique.

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P-8 Evaluation of layer thickness dependence of exposure and resin type in DLP 3D printers

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3D printing has become increasingly popular over the last few year due to the appearance of the Maker movement and the RepRap community in 2005. 3D printers exist from the 80' but RepRap movement was the one that offered the public the opportunity to own and use a 3D printer at affordable costs.It hasn’t been until the last five years, though, that personal 3D printing has begun to make such an impact—where objects made on a machine that might cost $30,000 in the industry can now be made with nearly the same quality on a machine that fits at home on your desk for less than $2,000.[1] 3D printing is a manufacturing process in which material (plastic, metal, or other) is laid down, layer by layer, to form a 3-dimensional object. (It is deemed an additive process because the object is built up from scratch, as opposed to subtractive processes in which material is cut, drilled, milled, or machined off.) 3D printers employ a variety of techniques and materials, but they share the ability to turn digital files containing 3-dimensional data—whether created on a CAD (computer-aided design) program or from a 3D scanner—into physical objects.[2] Stereolithography (SL) is one of several methods used to create 3D-printed objects. It's the process by which a uniquely designed 3D printing machine, called a stereolithograph apparatus (SLA) converts liquid plastic into solid objects. Stereolithography is an additive manufacturing or 3D printing technology used for producing models, prototypes, patterns, and production parts up one layer at a time by curing a photo-reactive resin with a UV laser or another similar power source.[3] In this study I experimented with different resins and time exposures of UV light. The goal of the study was to obtain a DLP 3D printer that is first of all cost effective while obtaining better results than a clasic RepRap FDM printer (Fused Deposition Modeling).

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P-9 Effect of Iodine Doping on Absorption Edges of Polysilanes

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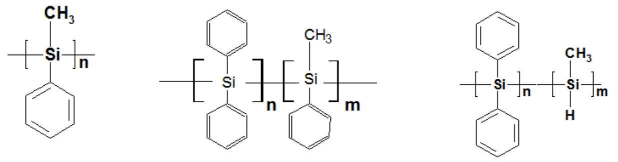
Polysilanes represent a special class of polymers containing Si-Si backbones and organic groups on each silicon atom. They behave as one-dimensional systems with weak intermolecular interaction and are characterized by σ conjugation that leads to interesting optical and semi-conductive properties [1]. In this work, polysilanes copolymers with structures depicted in scheme 1 were synthesized and their opto-electronic properties were investigated. The chemical nature of the side groups attached to the Si backbone was found to have a strong influence on the photophysical properties.



Polymethylphenylsilane

Polymethylphenyl-co-diphenylsilane, n=7, m=1

Poly[methyl(H)-co-diphenyl]silane, n=7 , m=1 or n=1 , m=1

Scheme 1. The chemical structure of the studied polysilanes

The energy gap and other energies describing the absorption edge were determined using the method proposed by Tauc for amorphous materials [2]. The effect of iodine doping on these optical parameters is discussed. On the basis of the obtained values, the influence of polysilane chain structure and of the structural disorder on the optical properties and electronic transitions has been ascribed.

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P-10 Composite biodegradable biopolymer coatings of Silk Fibroin – Poly(3-Hydroxybutyric-acid-co-3-Hydroxyvaleric-acid) for biomedical applications

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Composite biopolymer SF-PHBV biodegradable coatings were obtained by Matrix Assisted Pulsed Laser Evaporation (MAPLE), studying their physico-chemical and particularly the degradation properties, as a first step of applicability in the local controlled release for tissue engineering or regeneration. Silk fibroin (SF) and poly(3-hydroxybutyric-acid-co-3-hydroxyvaleric-acid) (PHBV) are both natural biocompatible polymers, with different degradability and tensile strength properties, combined for attending targeted biomedical uses. MAPLE is a recent method allowing the functional transfer of various organic or complex molecules, mixed or as multilayers. MAPLE composite coatings with different SF:PHBV weight ratios, or, comparatively, with simple coatings and chloroform, as solvent, have been deposited on titanium, silicon or glass substrates, using a KrF* excimer laser source operated at low fluences. The FTIR analysis revealed the same chemical composition of the MAPLE films with that of the constituent materials, suggesting that the stoichiometric transfer was accomplished. XRD confirmed the partial crystalline PHBV polymer phase and, as FTIR spectra, suggested the amorphous presence of SF. The static water-immersion and the wettability measurements showed very hydrophile coatings, notably the SF ones, while the PHBV films are the most resistant. The composite films are hydrophilic, among them the SF1:PHBV3 being the most stable. The hydrophilic behaviour increases when the laser fluence decreases. Degradation studies in SBF in a bioreactor also showed that adding PHBV to the SF slows down the degradation of SF. The simple SF coatings undergo a more rapid and enhanced degradation. These results provide supportive information for release applications, where degradation rate may be controlled for various applications by obtaining different composite material characteristics, mainly adjusting the mixture ratio, the crystalline status and/or the thickness of the coatings.

P-11 Comparative study on MAPLE and Dip Coating techniques for fabrication of biodegradable polymer thin films with medical applications

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Thin films of polycaprolactone (PCL)-polyethylene glycol (PEG) were deposited on titanium and <100> double side polished silicon substrates by both conventional matrix assisted pulsed laser evaporation (MAPLE) and dip coating (DC) techniques, using chloroform ($CHCl_3$) as a matrix solvent. In order to obtain that, PCL known for its excellent tensile properties, flexibility and biodegradability, but with a slow degradation rate, was blend it with the more soluble PEG, with purpose to obtain a biodegradable polymeric material with a medical application in tissue engineering. In the case of MAPLE method, in order to find the optimal parameters, we conducted a study of laser fluence: 0,2 mJ/cm^2 , 0,3 mJ/cm^2, 0,4 mJ/cm^2 and 0,5 mJ/cm^2 and for further experiments we selected the highest value of 0.5 J/cm^2, as being the most sensitive laser fluence for which the films are deposited stoichiometric and without any decomposition or polymer denaturation process. On the other hand, in the case of DC method, we varied the withdrawal velocity in order to analyze the variation of the thickness and the uniformity of the thin films. Two velocities were used for each solution: 10 mm/min and respectively 60 mm/min. One notices that faster withdrawal gives thicker thin coatings, so for further studies we selected the 60 mm/min velocity. The physico-chemical properties of the composite coatings were investigated by Fourier Transform Infrared spectroscopy (FTIR), XRD and Scanning Electron Microscopy (SEM). The results proved a stoichiometric and functional transfer of the deposited polymeric systems. For composite films, we noted a summation of PEG and PCL diffraction peaks, indicating that both polymers can crystallize and form distinct crystals. Wettability studies proved that the composite films exhibit highly hydrophilic surfaces and these first results provide evidence for controlled protein release applications, where degradation rate may be tuned.

P-12 Matrix Assisted Pulsed Laser Evaporation deposition of silk fibroin/poly(sebacic acid) diacetoxy terminated composite coatings for biodegradation medical applications

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We have analyzed the physical properties and degradability of poly(sebacic acid) diacetoxy terminated (PSADT) coatings reinforced with silk-fibroin (SF) for biomedical applications (local drug delivery). PSADT/SF composite coatings were grown by Matrix Assisted Pulsed Laser Evaporation (MAPLE), using a KrF* excimer laser source operated at low fluences. The composite coatings were deposited on titanium, silicon and glass substrates from solutions based on mixtures of SF with PSADT in different weight ratios (1:4, 1:1 and 4:1), as active compounds, and chloroform as solvent. The structural, morphological, and wettability properties of the SF/PSADT composite coatings were optimized with respect to the laser fluence up to 500 mJ/cm2. The stoichiometric transfer as composite thin films was demonstrated by FTIR spectra, which showed that all MAPLE films contain specific bands of both constituent materials, suggesting in the mean time the slight crystalline, predominantly amorphous presence of SF. As for the PSADT, the XRD indicated its partial crystalline phase. The SEM micrographs of the mixed coatings revealed mainly flower-like aspect uniform films, deriving as characteristic to PSA polymer, with large specific area, appropriate for low wettability contact angle. The wettability studies on SF/PSADT coatings also proved a superhydrophilic behaviour, with contact angle < 10°. Moreover, simulated body fluid-degradation and water-degradation proved that the copolymers composite films are highly hydrophilic surfaces, with the SF1-PSADT1 composition conferring a more degradable behaviour. The results of the physico-chemical and degradability tests sustain further studies for release applications, confirming that the degradation may be adjusted by the control of the mixture ratio and of the deposition parameters, modifying surface morphology, crystalline status and/or coating thickness.

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P-13 Plasma Polythiophene Films At Interface With Biological Medium

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Polythiophene (PTh) is a heterocyclic polymer that attracts particular attention because of its special physico-chemical and biological properties. Due to a unique combination of these properties it can be used in a wide range of applications, such as solar cells, sensors, also in medicine. Each biomedical application requires specific properties related to the biocompatibility, conductivity, surface stability etc.

The scope of this study is to obtain stabile pPTh films by polymerization reactions under the plasma conditions aiming to use these samples at interface with biological medium e.g., water, saliva, PBS, HCl and iodine solution.

Under the plasma conditions it is possible to obtain plasma polymerized thiophene (pPTh) films with specific properties by changing the working parameters, respectively composition of gases, flow rates, geometrical and electrical parameters of discharge. In our experiments we developed a method of pPTh film preparation based on a dielectric barrier discharge with plane–parallel geometry, working at atmospheric pressure in a mixture of helium and Th vapors with rates of 3 l/min and 103 μl/min respectively. Duration of deposition was 2 and 5 minutes, 6 kV applied voltage and 2 kHz frequency.

Characterization of pPTh films was performed by FT-IR, UV-Vis, XPS spectroscopy, AFM and contact angle measurements. Analysis of pPTh films showed a hydrophobic character, and the presence of functional groups corresponding to Th monomer.

Acknowledgment: This work was supported by the strategic grant POSDRU/159/1.5/S/137750, ”Project Doctoral and Postdoctoral programs support for increased competitiveness in Exact Sciences research” cofinanced by the European Social Found within the Sectorial Operational Program Human Resources Development 2007 – 2013.

P-14 USING NANOSTRUCTURES POLYMER AS REINFORCING AGENTS FOR ZOE MATERIAL

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Specialized studies revealed that zinc oxide eugenol (ZOE) paste can be used for temporary restoration, namely permanent teeth. The calming effect on tooth pulp given by this ZOE cement, make this material to be preferred by patients which may present tooth sensitivity after a cavity filling procedure. Commercial ZOE materials are presented in different compositions which influence physical and clinical characteristics of the pastes. Adding polymers as reinforcing agents can transform ZOE into a final cement and intermediate restorative material with an improved compressive strength. This paper sought to improve physical and clinical properties of ZOE materials by adding in their composition polymer nanostructures as reinforcing filler. The polymer nanofibers and nanoparticles investigated in this paper were obtained by electrospinning technique using cellulose acetate as starting polymer, the obtained nanostructures being deacetylated. The resulted cellulose nanofibers and nanoparticles were used as reinforcing filler for ZOE materials. Physical and clinical characteristics of these pastes were studied.

P-15 SHEAR ALIGNMENT OF CARBON NANOTUBES IN LIQUID CRYSTAL POLYMER MATRIX

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Cellulose derivative are high performance materials characterized by high thermal and mechanical resistance and excellent electrical properties. Their physical characteristics can be enhanced by embedding nanofillers, like carbon nanotube. This work is focused on preparing some new nanocomposites using hydroxypropyl cellulose (HPC) as liquid crystalline matrix, in which are incorporated different percents of multiwall carbon nanotubes. The preparation procedure consists in solution compounding in an organic solvent, followed by ultrasonication and magnetic stirring. The orientation of the nanofillers inside the HPC polymer is achieved by shearing the solution since it is well known that HPC in lyotropic phase unidirectionally deformed presents a ordered texture.The results are confirmed by atomic force microscopy and rheological tests. The obtained data are promising for obtaining complex materials with enhanced thermophysical properties, making them suitable as substrates for power electronics.

TOPIC 9

Biomaterials and Healthcare Applications

I-1 Structure and properties of silicate composites for thermoradiotherapeutical applications

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Silicate systems containing iron and neutron radioactivable isotopes like yttrium, dysprosium, holmium, samarium or renium can generate localized therapeutic hyperthermia, above 43°C, when injected intratumorally. By radioactivation these systems can be considered for brachytherapy and at the same time for simultaneous hyperthermia and brachytherapy, i.e. for thermoradiotherapy in cancer [1]. On the other hand, the iron containing particles can be used as contrast enhancement agents in magnetic resonance imaging. The structural changes induced in these systems by thermal treatments applied to develop the desired magnetic phases for hyperthermia applications influence the surroundings of the radioactive isotopes that are expected to be highly immobilized in order to impede the radioisotopes release at least during the time of their decay. After heat treatments, the iron preponderantly crystallises as magnetite, but hematite and maghemite are also developed [2, 3]. Spectroscopic studies evidenced that the potential radioisotopes are bound to interconnected SiO_4 structural units [4].

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I-2 Magnetic core/shell systems for biological applications

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Nanosized magnetic materials with various applications in life sciences are studied more and more aiming to improve their physical properties for increased efficacy and for developing new domains of utilization. In medical procedures magnetic nanoparticles suspended in the form of biocompatible colloidal fluids could be of great help in MRI diagnosis as contrast agents, in cancer therapy through tumor hyperthermia and in magnetically assisted drug delivery. We focused on the possible side effects of magnetic nanoparticles during their interaction with human body where microorganisms are present in low levels under critical thresholds; in the same time some aspects of environmental microorganisms responses to magnetic nanoparticles released in the water, air and soil from numerous natural and artificial sources are of increased interest nowadays from the viewpoint of magnetic contamination concept. The results obtained in our laboratory are based on magnetic core/shell systems prepared mainly from iron salt precursors and organic acids for the administration in the culture media of several bacterial species – at concentrations similar to those used in medical procedures. Physical characterization of biocompatible magnetic colloids was carried out by specific methods including XRD, TEM, SEM, AFM, VSM and rheological properties assays. Biological response was investigated at the level of bacterial proliferation with high attention on the side effects that possible develop following interaction with nanoparticles. Measurements of biological media turbidity and fluorescence were carried out to evidence the changes in the microorganism behavior. Mathematical model was proposed to explain the biological response to various compositions of the core/shell systems studied in laboratory experimental work.

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O-1 Toxicity study of water transferred graphene-based nanostructures for cell culture substrate

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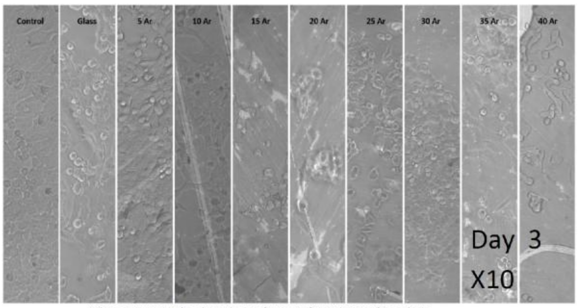
Graphene has attracted enormous attention due to its unique physical and chemical properties. Whilst early researches had focused on it electrical properties for device applications, graphene has now attracted increased interest in a wide range of fields including bio-medical applications, such as cell culture substrates. [1,2] These substrates are critical for: (1) investigations into the early stage development of cells and/or diseases, (2) the testing of new drugs and (3) scaffolds for tissue engineering. One of the benefits of GRM for these applications is that they can be produced with desired structural morphology (i.e. horizontal, vertical, hybrid) each having different useful properties. Additionally, the surface properties of graphene can be modified and tuned via plasma or chemical treatment, which decorate the surface with specific functional groups. Furthermore, these materials can be produced on (or transferred to) a plethora of substrates, an important feature as it has been demonstrated that the properties of substrates has a strong influence on the fate of cells. [3-5] Successful applications of graphene-based materials found in literature for bio-med applications, are predominantly produced via chemical methods, generating flakes that can be used to coat glass.



Microscopy control and graphene after transfer 72 hours after culture.

Microscopy control and graphene after transfer 72 hours after culture

When produced via Thermal Chemical Vapour Deposition, the transfer to the desired substrate involves chemical treatment, potentially contaminating the graphene. In this work, we use a unique plasma produced graphene transferred to glass via a chemical-free process as cell culture substrates. Before it can be used as a cell platform for biological applications, the graphene films must undergo a range of tests, specifically bio-toxicity, which is the objective of this work. Their biocompatibility was tested using lung cancer fibroblasts cells, cultured on the films for 5 days. It is shown that our films are non toxic, regardless the graphene structure. Cells morphology and proliferation were examined by Optical Microscopy on the first and third days, and indicates similar growth among all samples and the control. There appears to be some organization related with the amount defects and edges found on the sample surface.

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[5] Y. Zhang et al, Nanoscale, 4, 3833, 2012

O-2 A new Fe-Mn-Si alloplastic biomaterial as bone grafting material: In vivo study

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Designing substrates having suitable mechanical properties and targeted degradation behavior is the key's development of bio-materials for medical application [1]. In orthopedics, graft material may be used to fill bony defects or to promote bone formation in osseous defects created by trauma or surgical intervention [2]. Incorporation of Si may increase the bioactivity of implant locally, both by enhancing interactions at the graft–host interface and by having a potential endocrine like effect on osteoblasts [3]. A series of Fe-Mn-Si alloys was obtained as alloplastic graft materials for bone implants that need long recovery time period. The surface morphology of the resulted specimens was investigated using scanning electrons microscopy (VegaTescan LMH II, SE detector, 30 kV), X-ray diffractions (X'Pert equipment) or X-ray dispersive energy analyze (Bruker EDS equipment). This study objective was to evaluate in vivo the mechanisms of degradation and of adsorption / resorption for the proposed Fe-Mn-Si alloys, the physiological pathways by which the degradation products are stocked or expelled by the body and the effects of their implantation over the main metabolic organs. Biochemical, histological, plain X radiography and computed tomography investigations showed good compatibility of the subcutaneous implants in the rat organism. The implantation of the Fe-Mn-Si alloys, in critical size bone (tibiae) defect rat model, did not induced adverse biological reactions and provided temporary mechanical support to the affected bone area, allowed osteoid deposition, facilitated vascularization and bone tissue growth, promoted osteoinduction and osteointegration. Also, there was no evidence for local toxicity due to corrosion products. The degradation products were hydroxides layers which adhered to the substrate surface. Fe-Mn-Si alloys assured an ideal compromise between degradation and mechanical integrity in rat tibiae defects during bone regeneration.

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O-3 In vivo degradation behavior and biological activity of some new Mg-Ca alloys with concentration's gradient of Si for bone grafts

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Magnesium based alloys, especially Mg-Ca alloys are biocompatible substrates with mechanical properties similar to those of bones. The biodegradable alloys of Mg-Ca provide sufficient mechanical strength in load carrying applications as opposed to biopolymers and also they avoid stress shielding and secondary surgery inherent with permanent metallic implant materials [1]. The main issue facing a biodegradable Mg-Ca alloy is the fast degradation in the aggressive physiological environment of the body. The alloy's corrosion is proportional with the dissolution of the Mg in the body: the reaction with the water generates magnesium hydroxide and hydrogen. The accelerated corrosion will lead to early loss of the alloy' mechanical integrity [2]. The rate of degradation of an

alloy can be improved mainly through tailoring the composition and by carrying out surface treatments [3]. This research focuses on the ability to adjust degradation rate of Mg-Ca alloys by an original method and studies the biological activity of the resulted specimens. A new Mg-Ca alloy, with a Si gradient concentration from the surface to the interior of the material, was obtained. The surface morphology was investigated using scanning electron microscopy (VegaTescan LMH II, SE detector, 30 kV), X-ray diffraction (X'Pert equipment) and energy dispersive X-ray (Bruker EDS equipment). In vivo degradation behavior, biological compatibility and activity of Mg-Ca alloys with / without Si gradient concentration were studied with an implant model (subcutaneous and bony) in rats. The organism response to implants was characterized by using radiological (plain X rays and computed tomography), biochemical and histological methods of investigation. The (blood serum, urine and bones) analysis of the main biochemical markers has recorded different variations (but in normal limits) for the lot with the implant of Mg-Ca and concentration's gradient of Si compared to the lots with other implants. The results highlights that Si gradient concentration can be used to control the rate of degradation of the Mg-Ca alloys and for the enhancement of their biologic activity in order to facilitate bone tissue repair.

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O-4 Antimicrobial activity of biopolymeric thin films containing with natural compounds and antibiotics fabricated by maple

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Antimicrobial resistance has become a key issue affecting the public health throughout the world. One approach that has rendered traditional antimicrobial treatments ineffective is the formation of bacterial biofilms, which impart resistance to many types of antimicrobial substances. Prevention of biofilm-associated infections frequently requires high concentrations of antimicrobial agents for biofilm penetration and microbial eradication; however, the use of high concentrations of antimicrobial agents is commonly associated with a higher incidence of undesired side effects, including allergic reactions (e.g., skin reactions, anaphylactic shock, and serum sickness), dysbiosis, diarrhea, and superinfections. The purpose of this study was to investigate the interactions between the planktonic and adherent microorganisms and biopolymer (polyvinylpyrrolidone), flavonoid (quercetin dehydrate/resveratrol)-biopolymer, antibiotic-biopolymer, and flavonoid-antibiotic-biopolymer composite thin films that were deposited using matrix assisted pulsed laser evaporation (MAPLE). A pulsed KrF* excimer laser source ($\lambda = 248$ nm, $\tau = 25$ ns, $\nu = 10$ Hz) was used to deposit the aforementioned composite thin films, which were characterized using Fourier transform infrared spectroscopy and Raman spectrometry. The antimicrobial activity of the thin films was quantified using a novel antifungal assay involving culture-based methods, including spectrophotometric measurements to determine the density of microbial cell cultures and the viable cell counts assay. Amphotericin B and voriconazole agents served as positive controls in these studies. Scanning electron microscopy confirmed that MAPLE may be used to fabricate thin films with chemical properties corresponding to the input materials as well as surface properties that are appropriate for medical use. The antimicrobial activity of flavonoid-containing

films against both Gram-positive and Gram-negative bacteria demonstrated the potential use of these hybrid systems for the development of novel antimicrobial strategies.

P-1

SEM characterization of artificial teeth subjected to microwave disinfection

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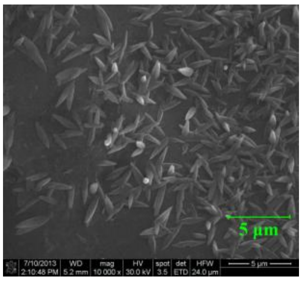
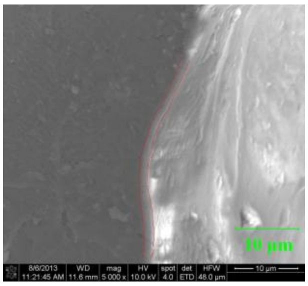
The purpose of this study was to evaluate the surface and cross-section alterations of acrylic artificial teeth subjected to domestic microwave wet disinfection. Using the same polymeric material and identical molds, two sets of specimens were fabricated according to the manufacturer's specifications and nine disinfection protocols were elaborated. We investigated the cumulative effects of microwave irradiation in comparison with previous designated controls, not subjected to decontamination procedure. For sample preparation we used a product based on methacrylate copolymerisates, with no subsequent surface processing or polishing, and polymethacrylate prefabricated artificial teeth. For sample irradiation we employed a generic microwave household oven with typical commercial specifications and capabilities.



Salt crystal deposits on polymer surface



Surface porosification visible in cross-section

The disinfection method was elaborated according to literature data and general accessibility for average denture wearers. Therefore, the irradiation procedure consists in variation of power over time: 500 - 650 - 750 W for 2, 3 and 5 minutes, respectively. The morphological characterization was conducted with a high-resolution FEG-SEM, after sample metallization. SEM investigations revealed various crystalline deposits on the surface - with no structural or functional impact - and insignificant polymer surface modifications. In cross-section, we observed a thin superficial layer of polymer alteration due to water presence which will increase the material porosity.

P-2

One step preparation of carbon-coated iron oxide nanoparticles for biomedical applications

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Nanostructured materials are largely considered as ones of the most suitable building blocks for new emerging technologies and innovative applications. Among them, metal oxide nanoparticles (e.g. γ-Fe_2O_3, Fe_3O_4) functionalized with carbohydrate-derived coatings have started to attract consistent research since their application potential has been evaluated as promising. The advantages provided by the inclusion of hydrophilic coatings onto metal oxide nanoparticles translated into increase of surface area, hindering of the oxidative processes at the surface of air-sensitive metal oxides, and decreasing of the magnetic coupling induced by reciprocal magnetic attraction. Also, due to their low toxicity, they can be successfully used in the biomedical field. To date, different strategies have been developed to synthesize magnetic nanoparticles functionalized with carbohydrate-derived ligands.

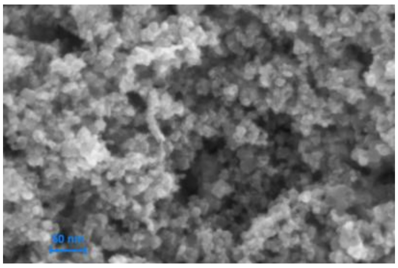

Fig. 1. SEM image of magnetic nanoparticles

However, many of them are complicated, energy consuming, and require special equipment. Therefore, in order to prepare iron oxides functionalized with carbohydrate-derived compounds, other strategies that avoid these drawbacks become of valuable interest. We report here a new and efficient approach for one-step synthesis of water-dispersed, carbon-coated, non-agglomerated iron oxide nanoparticles with a mean size of 10 nm. Fig. 1. The biocompatibility of both uncoated and carbon-coated magnetic nanoparticles was evaluated through a cancer cell line.

Acknowledgements: The authors wish to acknowledge the financial support from CNDI–UEFISCDI grants, Projects no. 8/2013.

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P-3 Topographical cues for modulating Mesenchymal stem cells fate

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Surface topography represents one major issue in cell-surface interfaces dictating the biological reactions. This work presents polymeric surfaces microstructured using excimer laser processing technique, and used as model surfaces to answer the question in how far anisotropy in defined surface microstructuring affects and steer stem cell behaviour. The structures (pits similar to those of a bone transversal section) with various depths in the range of 200 nm-7 micrometers were produced by an ablation process of polycarbonate on a large surface exposure set-up and a consecutive titanium coating process (magnetron sputtering). The response of human mesenchymal stem cells (hMSCs) was analysed and quantified. Cell growth and adhesion were depending on the topography of the substrates. The cell proliferation was apparently not affected for depths below 2 um after 72 h, but slightly decreased for those in the range of 3-7 um. The cell shape modifications induced by interaction with microtopography were analysed by SEM and immunofluorescence microscopy following actin filaments labelling. Data were correlated with osteogenic differentiation potential quantitated by mineralization assay. The results presented here indicate that substrate depth features play a key role in hMSCs spreading response and contact guidance. Our results demonstrate potential use of laser micropatterned substrates to modulate cell fate during bone implantation.

P-4 Screen printed electrodes sensors based on single wall carbon nanotubes functionalized with porphyrins for neurotransmitter sensing

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This paper investigates the electrochemical response of screen printed electrodes with gold-working electrode (SPE-Au) enriched with single wall carbon nanotubes (SWCNTs) functionalized with metalloporphyrins in the presence of neurotransmitters (dopamine, serotonin, and epinephrine). Both SWCNT capability as transducers and porphyrin immobilization supports are evaluated. SWCNTs were functionalized with three metalloporphyrins and then separately deposited by dropcast method on SPE-Au. SWCNT-porphyrins added on SPE-Au have changed the original SPE-Au sensing characteristics by both decreasing the oxidation potential with 50% and increasing neurotransmitter concentrations up to micromolar. The novelty of this work consists of using SWCNT as transducers in order to amplify the porphyrin sensitivity under the presence of neurotransmitters (dopamine, serotonin and epinephrine). This SPE-Au functionalized with SWCNT-porphyrins could be utilized in the diagnosis of different disease that implies neurotransmitter activity.

P-5 Composites for food freshness assessment: chemically modified graphene – polypyrrole gas sensor

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Gas sensors are important for fast detection of degraded food. When degradation occurs, C&N-containing gases are released; those volatile organic compounds (VOCs), produced by microorganisms developing inside the products, can be effectively evaluated by gas sensors based on graphene composites. Graphene is represented by a single layer of carbon atoms, arranged in a honeycomb lattice; their properties (excellent electronic conductivity, high surface area and increased mechanical resistance) create a support material perfect for immobilizing active molecules. This study reports the fabrication of two interdigitized sensors designed on modified graphene & polypyrole composites, obtained by electrochemical polymerization of pyrrole on the surface of gold microsensors. The electrical response of the sensors to several VOCs (including commercial meat samples, fresh and degraded) was measured by means of I-V characteristics. The sensors revealed a high sensibility towards N-containing gases (NH_3 and volatile amines).

P-6 A novel colorimetric sensor for meat freshness assessment

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Chromogenic sensors are a major research direction in health and security since they provide fast and simple food evaluation. Basely, a colorimetric sensor is represented by a sensitive dye, immobilized on an inert support which changes color when exposed to an analyte. In this study, a sensor array for meat freshness is proposed. The sensor array contains color-changing dyes (both natural occurring & synthetic), immobilized on polyacrylamide, silica and Al_2O_3 substrates via physico-chemical methods. The colorimetric sensor was tested to typical volatile organic compounds and biogenic amines released during microbial growth and to commercial available meat samples. The tests were conducted in a tight gas chamber. The sensor was coupled with a digital camera to accurately record the color shift and a mass spectrometer to analyze the gases in the chamber. The result indicate an irreversible, fast and reproducible response to a matrix of analytes typically occurring in spoiled meat, opening new pathway towards fast and cheap control instruments.

P-7 Microwave resonant methods for bone replacement biomaterials testing

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The paper deals with microwave resonant methods used for non-destructive testing of biocompatible materials using for bone replacement. The numerical and experimental results are done. The results showed the possibility of microwave resonant methods frequency using for finding inhomogenities in biocompatible metal samples not only on the surface but also in the volume of investigated material. Nowadays the significant need for the development of quantitative non-invasive and non-destructive test methods to measure bone implants stability and homogeneity is connected with exponentially increasing of biomaterials which are used for improving the life of people. Our work was directed to the investigation of microwave resonant methods possibility using both for in vivo and in vitro testing of homogeneity of biocompatible materials. Metallic implants interact with the surrounding biological environment. This interaction depends on chemical properties of bone surface and the shape of bone. The numerical simulation of reflected were done for biocompatible material – stainless steel in the case when the properties of surrounding area was changed. Numerical result showed that the defect presence in the volume of investigated material and its depth can be find from resonant frequency, which varies with the depth of defect. The experiments were done on flat stainless steel sample. And showed the defect acts like the lossy waveguide and reflected signal amplitude is strongly dependent on the depth of defect [1]. The depth of defect in the volume of investigated biocompatible material can be calculated from the resonant frequency to which is defect capable and reach the maximum of reflected signal.

Acknowledgements: This work has been supported from projects VEGA 1/0846/13 and 1/0743/12 and was done in the frame of bilateral project Slovak Research and Development Agency under contract SK-RO-0008-12.

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P-8 Inflammatory response of laser micro- structured surfaces

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Current strategies to improve implant biomaterial osteointegration and inflammatory response for rapid bone regeneration focus on nano- and micro- surface structuring that mimic natural occurring biological architecture. Using excimer laser processing technique, polymeric surfaces used as substrate were structured and investigated for the potential inflammatory effect and for topography induced cell viability, morphology, and spreading changes. The number of viable cells determined by colorimetric non-radioactive cell proliferation assay performed for 18 hours revealed no cytotoxic effect onto THP-1 cells treated or untreated with LPS, but endotoxin addition led to a decrease of viability irrespective of surface patterning. Immunofluorescent microscopy studies of actin and vinculin proteins implicated in cellular adhesion show that cells respond to nano and microscale grooved substrate. Thus THP-1 cells adhere and exhibit spread morphology on

the three-dimensional scaffold with surface architecture. Using ELISA method the TNF-α secretion from THP-1 cells differentiated to macrophages, revealed no detectable levels of proinflammatory cytokine compared to the cells treated with lipopolysaccharide (LPS) used as a control.

P-9 Surface Plasmon Resonance: a useful technique for studying bacteria adhesion on menthol-functionalized surfaces

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Surface Plasmon Resonance (SPR) is a label-free technique by which biomolecular interactions may be measured in real time. The research studies reported in the recent years, demonstrate the capacity of SPR system for application in the field of medicine, biotechnology and environmental monitoring. For example, SPR biosensors have been developed to determine the human growth hormone (hGH) in serum (Treviño *et al.*, 2009) or morphine-3-glucuronide (Dillon *et al.*, 2003), for the monitoring of pesticides in natural water samples (Mauriz *et al.*, 2006) or to investigate the angiogenic process in intact carcinoma living cells (Mauriz *et al.*, 2014).

The aim of our study is to investigate the effects of menthol previously immobilized onto SPR biosensor surfaces (gold- and graphene-based SPR sensors) against UTI 89 (uropathogenic *Escherichia coli* strain). The measurements were carried out using the Sensia Indicator system (Spain), a dual channel SPR instrument, which permits a parallel and separately detection in each sensing channel in real time. In the case of gold based SPR sensor, the immobilization procedure occurred via the formation of a thiol (RS-H) self-assembled monolayer (SAM) with terminal amine (-NH2, 6-amino-1 hexanthiol hydrochloride) or carboxyl (-COOH, 11–mercaptoundecanoic acid) groups. The coatings were characterized by X-ray Photoelectron Spectroscopy (XPS) measurements. The adsorption of *E. coli* bacteria to menthol-functionalized surfaces was monitored by SPR and compared to non functionalized surfaces. Our results indicated that menthol immobilization on various surfaces can be an alternative solution to prevent bacteria colonization and biofilm development and SPR is a useful technique for bacteria detection.

P-10 Platform for DNA analysis base on impedance spectroscopy

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Medical diagnostic of infectious vectors in humans have now been commuted from single detection to multiplexed detection, in order to gain relevancy in terms of time and quality. The diagnostic tests have to solve both specificity and speed on the condition that the detection of the presence of many sub-types of the same viral target have relevancy both for treatment and medical care approach. In this perspective, the platforms capable of multiplexed detection of viral agents become a necessity for diagnostic, reducing the time and resources involved to obtain the correct detection and increasing the overall quality of medical act. This paper report a platform used for DNA analysis base on impedance spectroscopy (Fig.1). This platform was design with an array of gold electrodes, each electrode being addressed individually, and a reference electrode. Gold electrodes were prepared by electron-beam evaporation on Si (100) wafers of Cr film used for adherence and followed by Au. In order to obtained an improvement of electrical answer the gold electrodes were nano-structured to permits a great number of molecules to be captured on its.

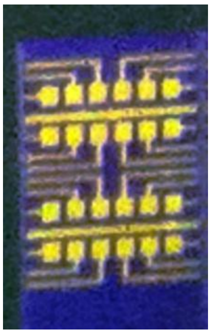

Fig. 1 Optical image of microarray electrodes

Deposition of probe molecule 5’-HS-ss-DNA with different concentration was realized using a microarray plotter in a controlled position on the electrodes. After 24h incubation time at 40 °C the structures was wash for eliminated un immobilized molecules and a step of blocking process of unused surfaces was perform. Hybridization with target DNA was carried out by incubation at 370 °C for 1 h. Hybridization experiments and impedance spectroscopy measurements were all performed in a standard hybridization buffer (HB) consisting of 0.3M NaCl, 0.02M Na_3PO_4, 0.002M ethylenediaminetetraacetic acid, and 0.2% sodium dodecyl sulfate. Hybridization of DNA was confirmed by florescent spectroscopy. The impedance spectroscopy measurement (IS) determined change in impedance answer between electrodes and correlation of this signal with concentration of ss-DNA immobilized on the surfaces.

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P-11 Synthesis and structural characterization of copolymer embedded magnetite particles

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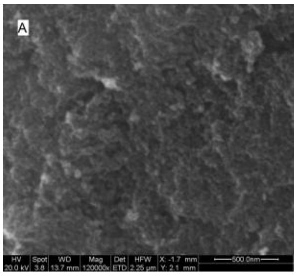
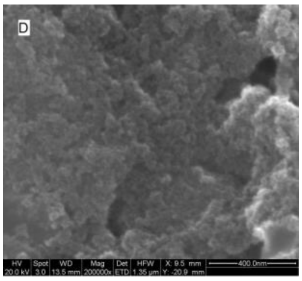
This paper shows synthesis by emulsion polymerization of magnetite particles coated with poly(methyl methacrylate-co-acrylic acid) (PMMA-co-AAc), polymer that creates surface functional groups. X-ray diffraction, Fourier transform infrared spectroscopy and electron spin resonance spectroscopy was performed in order to highlight the physical and structural properties. The influences of monomers and surfactant layers on interactions between the magnetite particles by varying their concentrations were also analyzed.



uncoated magnetite



coated magnetite

Analysis of these results it follows that thickness of the polymer has a significant effect on stability of the suspension of particles in a liquid by increasing the distance between them and reducing the dipole-dipole interactions that can occur. It is shown that to ensure a good dispersion of particles throughout liquid volume certain concentrations of surfactant were used, its role being to reduce interactions between magnetite particle and polymer layer.

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P-12 Comparative analysis over some archwires behavior used in esthetic orthodontology

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In the past few decades, the demande for esthetic orthodontic has increased rapidly. There are many commercial device on the market. Many of them gained popularity and become competitive because of her characteristics and mechanical, physical-chemical properties and biocompatibility. The purpose of this comparative analysis is to investigate the behaviour in bucal cavity of some different archwires based on stainless steel or NiTi with different cross-sections, before and after intra-oral exposure (from 4, till 18 weeks). The aim of this paper is to observe what kind of differences appear over this archwears capt under in mouth during 4 till 18 weeks. In order to expose the mechanical properties tensile strength analysis are performed on Instron facility. Corrosion analysis aspects and morphology of the surface alloy are identified by SEM.

P-13 Antimicrobial and degradable biohybrid substrates with controlled surface architecture

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For many applications within tissue engineering, the challenge is no longer one of the passive biocompatibility requirements previously considered acceptable for biomedical implants, but a high demand on patterning and processing of advanced multifunctional biomaterials as scaffolds. Therefore, one important goal is the generation of scaffolds with defined structuring/architecture and biofunctionalization in order to control processes like cell adhesion and differentiation. Within this context, this work outlines the study of texturing by excimer lasers (193 nm and 248 nm) and characterization of chitosan-collagen based structures with the goal of determining the optimal morpho-chemical characteristics of these structures for in vitro tailoring protein adsorption and cell behavior. Surfaces with different geometries (foams, roughness gradients) were obtained by varying wavelength, pulse number and sample tilting; and tested with various cell lines (i.e. L 929 Fibroblasts, HEP G2 hepatocytes, OLN 93 oligodendrocytes, M63 osteoblasts). Atomic force microscopy (AFM), scanning electron microscopy (SEM) and spectro-ellipsometry (SE) were used for morphological characterization. The structural changes induced by laser irradiation were shown by FTIR measurements. SE and AFM studies revealed different degradation behavior depending on the type of the laser modified surface compared to the control samples. Optical and fluorescence microscopy were used for analyzing cell morphology on the substrates.

P-14 Emerging Healthcare Applications Of Conductive Polymers

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Conductive polymers (CP) are a class of organic polymers that have unique electrical and optical properties similar to those of metals and inorganic semiconductors, while retaining attractive polymer characteristics such mechanical flexibility, high thermal stability and ease of processing and synthesis. Beyond the multitude of technical

applications (in microelectronics industry, photovoltaic devices, organic light-emiting diodes, electro-chromic displays, rechargeable batteries, electrodes for supercapacitors, etc.), conductive polymers have also emerged as versatile materials for a broad range of biological and medical applications. Some tissues respond to electrical stimuli and biocompatible CPs have been shown to modulate activities of the nerve, bone, muscle and cardiac cells. They can stimulate cell growth, adhesion and migration, enhance DNA synthesis and protein secretion [1]. CPs have the ability to entrap and controllably release biological molecules or can transfer charge from a biochemical reaction, thus making them particularly suited for biosensors applications, tissue engineering scaffolds, neural probes, drug delivery devices and bio-actuators (artificial muscles) [2]. This contribution provides snapshots of recent biomedical developments around CPs and their potential impact and implications on healthcare. A recently reported electrochemical DNA hybridisation probe based on polypyrrole films offers great promise for its translational use in early diagnosis, prognostic assessment and monitoring response to therapeutic agents [3]. Electrodes for electroencephalography based on conductive polymer PEDOT:PSS have been shown to outperform dry Au electrodes. This opens the possibility for long-term recording of brain activity in a non-invasive manner useful in the diagnostic of epileptic seizures, evaluation of sleep disorders, cerebrovascular disease and movement disorders [4]. The use of CP, particularly polyaniline and polypyrrole in smart textiles can have an important role in remote monitoring of chronically ill patients or those in rehabilitation. Garments with CPs with strain sensing capability offer continuous monitoring of body kinematics and vital signs. [5]

P-15 Study of surface phenomena in biomaterials: the influence of physical factors

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This study's purpose is pointing out the phenomenon that occurs at time of interaction between the tissue with implant. The materials used are Ti and its alloys. The oral tissue must be compatible with the materials used in surgical implant to human body. The bio materials surface behavior is influenced by physical characteristics. The methods we use show a number of bio-compatibility aspects. The success of an implant in a hard tissue depends not only on the initial attachment and the osteogenics cells consecutive proliferation, but also on their capacity to create a new bone.

P-16 The test of bio-compatibility for "in vivo" polymeric materials, optimized by physical methods

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We have made a study concerning the surface state of acrylic protectical bio-materials, both optimized and unoptimized ones. We have studied their compatibility on test animals and we studied the casuistry that stood up for the data base to process. The main characteristic for the saliva in the oral cavity is its capability to moisten the teeth and gums. Practically, the moisturizing of dental materials is fully characterized by the angle of contact between the drop of biological liquid and the surface. Small contact angles indicate a good moisturizing. A very important physical characteristic is the roughness of the surface of dental bio-materials, which offers interrelations between the mechanical work of adhesion and the absorption of liquid biological molecules.

TOPIC 10

Functional Materials. Processing and Characterization

PL-1 Fundamental parameters in solution growth

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The KDP (KH_2PO_4) crystal as a non-linear material has extremely important technological applications in the nuclear fusion program. Some other important applications of KDP and ADP ($NH_4H_2PO_4$) tetragonal crystals family in non-linear applications are also very important. Thus, crystal growth mechanism, kinetic and peculiar aspects are very important in growth and properties of crystals for applications. Solution-based crystal growth needs to answer some fundamental questions: (1) Which are the kinetic factors that control crystal growth rates - Surface diffusion or 2D nucleation? (2) How the influence of impurities can be limited? (3) The dominating center of dislocations remains active at higher supersaturations? If dislocations still appear at higher supersaturations, 2D-nucleation mechanism can be considered dominant? The most "aggressive" impurities in KDP family crystal growth are Cr^{3+} and Fe^{3+} $\theta^{*}\sim 10\theta$which have about 18 kcal/mol adsorption energy on the faces of the crystals, much higher than for crystal growth (~ 9 kcal/mol). The fractional recrystallization was used to improve the quality of the basic substance (H.V. Alexandru 2007). Three supersaturation zones were discerned were the kinetic mechanism of growth is different. At smaller supersaturations, at the limit of the "dead growth zone", the estimated critical coverage of impurities $^{-3}$ is much higher than 10^{-6} at higher supersaturations ($\sigma \geq 8\%$) were 2D nucleation kinetic is dominant. Dislocation growth which has some other unexpected characteristics is dominant in-between. The very large dispersion of the growth kinetic data at supersaturations of 1÷5 % fits a large number of distinct BCF curves, corresponding to several growth efficiencies. This non-univocal supersaturations dependence shall be discussed in relation with a puzzling effect of dislocation switching effect, found by micro-laser interferometry in the literature.

PL-2 Crystallographic processes and functional characterization of shape memory alloys

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Shape memory alloys exhibit a peculiar property called shape memory effect. These alloys return to a previously defined shape on heating after deformation in low temperature product phase region and take place in a class of functional materials due to this property. Shape memory effect is facilitated by martensitic transformation which is a solid state phase transformation and occurs in thermal manner in material on cooling from high temperature parent phase region. This transformation is governed by changes in the crystalline structure of the material. Martensitic transformations usually occur with the cooperative movement of atoms by means of lattice invariant shears on a {110} - type plane of parent austenite matrix. The ordered parent phase structures turn into twinned structures with this movement in crystallographic manner in thermal induced case. Therefore 24 martensite variants occur in self-accommodated manner on six planes of {110} – plane group. The twinned martensite structures turn into the detwinned or oriented martensite by stressing the material at low temperature martensitic phase condition. The detwinned martensite turns into the parent phase structure on first heating, first cycle, and parent phase structures turn into the twinned and detwinned structures respectively in irreversible and reversible memory cases. This result reveals that shape memory behaviour of these alloys is closely related to the twinning and detwinning processes as well as martensitic transformation. Copper based alloys exhibit this property in metastable beta phase region, which has bcc-based ordered structures at high temperature parent phase field, and these structures martensitically turn into layered complex structures Lattice invariant shears can be called as {110}<110> -type mode and gives rise to the formation of layered structures, like 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice, due to the non-uniform character of shear. In the present contribution, x-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based alloys which have the chemical compositions in weight; Cu-26.1%Zn 4%Al and Cu-11%Al-6%Mn.

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PL-3 Thermochromic coatings grown by chemical vapor deposition at atmospheric pressure

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Thermochromic materials, such as vanadium dioxide, have the ability to change from a semi-conductive to a metal state when their temperature reaches a specific value, which is called transition temperature (Tc). For the deposition of a thermochromic layer, many methods have been used such as magnetron sputtering, pulsed laser deposition, atomic layer deposition, sol-gel, spin coating etc. Nevertheless, a low cost method using non-toxic precursors and easily transferred to large scale is needed. The growth of thermochromic amorphous vanadium dioxide coatings by chemical vapor deposition at atmospheric pressure was performed using vanadyl (V) triisopropoxide as single-precursor. For the control of the samples' characteristics and their subsequent thermochromic performance, various growth conditions were employed, such as substrate type, N_2 flow rate through the vanadium bubbler, deposition period and growth temperature. The samples were characterized by X-ray diffraction, Raman spectroscopy, Scanning Electron Microscopy (SEM), UV-Vis-NIR spectroscopy measurements at temperatures below and above Tc as well as transmittance measurements as a function of temperature at an incident radiation of 1500 nm. As found out, only coatings grown on SnO_2-precoated glass substrates present thermochromic behavior, this being optimized for a growth temperature of 450 ^{o}C, a deposition time of 150 min and a N_2 flow rate of 0,5 $Lmin^{-1}$. The respective transition temperature was found to be in the range of 60-66 ^{o}C, which was reduced down to 44 ^{o}C after doping with W.

I-1 Periodically poled Lithium Niobate waveguides for co- and counter-propagating optical parametric interactions

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Optical parametric interactions are widely used for different applications: tunable amplifiers, tunable sources, all-optical signal processing, quantum communications… Periodically poled materials offer a versatile way to ensure that those interactions are efficient at any desirable wavelength. Furthermore optical waveguides allow to dramatically enhance the efficiency of the interaction. Lithium Niobate is nowadays the more advanced material that allow to combine both advantages of the periodically poling and of the waveguides. This contribution will first discuss the interest of Lithium Niobate for this domain of activity. It will then give an overview of its applications in the standard co-propagating regime. Finally it will discuss the challenges to move to the counter-propagating regime.

I-2 Elaboration of functional oxides thin films by Physical Vapour Deposition: nanostructure and related properties

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Insulating, conductive, magnetic oxides are commonly used in a wide variety of device applications. The scale reduction and the nanostructuration of these materials is one of the key points for the integration in new devices and a new way to enhance or obtain new properties (tuneable function). The control of the processing in thin films is still a challenge to establish the relationship between the structure and the nano and macroscopic properties. Thin films of oxides as rare earth oxide have been recently an active area of researches because of several physical properties particularly relevant for devices and optical applications (high k) or in the field of conductive oxide. The physical properties of these materials strongly depend on the elaboration conditions, two examples will be presented. 1) Y_2O_3 thin films were deposited by Ion Beam Sputtering (IBS) with different nonstoichiometric or defects concentration. It is shown that oxygen stoichiometry can be accommodated either by a local disorder or by extended defects (dislocation loops). Both types of defects, oxygen vacancy network disorder and dislocations, induce a high compressive stress in the films which lead to a possible explanation of non-equilibrium crystallographic phases stabilization. 2) ITO thin films are deposited by GLancing Angle Deposition (GLAD) using IBS. The morphology of the columns can be controlled by changing the substrate orientation in respect of the sputtered particles flow. This work is focused on the relationship between the nanostructuration, the optical and electrical properties. Temperature dependent Hall Effect measurements combined with FTIR measurements were performed. ITO thin films deposited with the highest glancing angles lead to surprising modification of optical properties and conductivity mechanisms with new functionalities (Metal-insulator-Transition is observed) The importance of the surface effect and the in-plan organization of the nanorods is discussed.

I-3 Rapidly quenched FeNiCoAlTaB ferromagnetic superelastic alloys

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Ferromagnetic shape memory alloys (SMAs) with high levels of superelasticity to be used where application of large levels of force or high damping are needed have been recently developed. The breakthrough into superelastic SMAs materialized in 2010 in the form of a FeNiCoAlTaB alloy, a close relative of the FeNiCoTi MSMA, which also uses the fcc–bct transformation was reported by Tanaka et al [1]. Tensile superelastic strains higher than 13% at room temperature in a <100> textured Fe40.95Ni28Co17Al11.5Ta2.5B0.05 polycrystal which reaches strengths of >1 GPa have been achieved, associated with γ/α' martensitic transformation and the precipitation of γ' - Ni3Al in the alloy. In the need for a superelastic material with better properties and easier processing we have designed these materials enabling lower dimensions, lower processing temperatures, lower mechanical reductions, and ideally enhanced response in a wide range of temperatures by using an alternative route, the rapid quenching from the melt technique, for their fabrication as ribbons and wire-shaped materials. Recent results concerned with the most favourable composition, cold-drawing, annealing, and tensile stress treatments for both enhanced superelastic and magnetic properties will be presented. The results on these novel, intelligent, high-performance shape memory materials which possess simultaneously high ductility, excellent magnetic characteristics and enhanced superelastic properties, prepared by using a cost effective technique, demonstrate the high sensitivity of the Fe-Ni-Co-Al-Ta-B microwires to mechanical, thermal and magnetic factors with potential applications such as mechanical damping and microsurgery. Acknowledgements – Work supported by the Romanian Ministry of National Education through the NUCLEU Programme (Theme PN 09-43 02 03).

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I-4 Novel approaches in designing smart coatings for materials protection

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The huge economic impact of the corrosion of metallic structures is a very important issue for all modern societies. Reports on the corrosion failures of bridges, buildings, aircrafts, automobiles, and gas and oil pipelines are not unusual. It is estimated that corrosion and its consequences cost developed nations between 3% and 5% of their gross domestic product. The process involving hexavalent chromates is the most effective and most widely used conversion coatings for corrosion protection for many metals and alloys. However, the carcinogenic effect and environmental waste due to chromates are well documented. The concept of 'self-healing', 'self-repairing' or 'smart' materials has in recent years been developed experimentally in new types of manufactured materials creating a new class of multifunctional materials of self-healing properties. Such properties add functionality to the materials to heal themselves automatically after mechanical, physical or chemical damages caused, for example, by scratch, impact, abrasion, erosion, friction, corrosion, wear, fire, ice, etc. The development of active corrosion protection systems for steels, Al and Mg substrates is an issue of prime importance in key industries, including petroleum, chemicals, transportation. This project will discuss new insights towards the development of new protective systems with self-healing functionality. The approach described herein can be used in many industrial applications where active corrosion protection of materials is required.

I-5 Gamma radiation: an alternative to sol-gel for the preparation of glasses and hybrid materials

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Glass is formed in nature through the melting of sand or rocks followed by fast cooling, as occurs when volcanoes spew lava or lightening strikes sand dunes. At least since 1500 B.C. man has been producing glass by melting together sand or stone pebbles and plant ashes. These latter contain soda and lime decreasing the melting point of silica (ca. 2000 °C). Glass is an amorphous material that has cooled rapidly without crystallizing. Improved properties are obtained when some metallic oxides are added such as ZrO_2 that confer high resistance to alkaline attack and improve optical properties. Such addition also increases the melting point of the glass and causes devitrification except when present in small contents. The sol-gel process is an alternative method to the oxides melting for the glass preparation. A binary SiO_2-ZrO_2 glass was first obtained by sol-gel in 1980. In this process an oxide network is formed by poly-condensation reactions of molecular precursors in a liquid solution or sol. The network growth process develops as reactions continue until a 3D continuous network, known as gel, is attained. The idea of the sol-gel synthesis is to disperse the molecules of the precursors in a liquid, mixing them at atomic level, and controlling the reactions to obtain a solid with tailored characteristics. As the gel encloses the liquid phase, drying is essential. When the gel is dried by evaporation, capillary forces cause shrinkage, the gel network collapses leading to an amorphous porous material known as xerogel. Gamma irradiation of the precursors mixture (no liquid added) is an alternative to the sol-gel process. Due to the absence of liquid at the preparation stage, drying of the gel leads to a reduced volume change and, hence, to a reduced porosity. Radiation produces reactive centres in the molecules from which condensation reactions proceed leading to a three-dimensional network that is structurally and mechanically stable. This work focus on the results of the investigation of glasses and hybrid materials prepared by gamma radiation and by sol-gel, starting from the same precursors and contents.

I-6 Synthesis, stucture and magnetic properties of $Pb(V_{1-x}Fe_x)O_3$ multiferroics compound

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Multiferroics perovskites are materials which contain both ferromagnetism and ferroelectricity in the same phase, used to obtain transducers, actuators, piezoelectric devices. $PbVO_3$ is isostructural with the known ferroelectric $PbTiO_3$ compound. V atom is oxidized 4+ so it carries a ½ spin therefore magnetism is expected. This compound can only be synthesized under high pressure – high temperature conditions, usually not a single phase and with a very weak magnetic signature (explained by 2D AFM model). Our objective is to test the effects of isovalent substitution of V with Fe. By solid state reaction under high pressure and high temperature conditions, single phase samples from the multiferroic oxide series $Pb(V_{1-x}Fe_x)O_3$ were successfully synthesized. The oxidation state of vanadium and the samples composition were characterised by X-ray absorption spectroscopy (XAS) and EDX, respectively.XAS data confirms that the oxidation state of V and that the Fe substitution is hererovalent. X-ray diffraction (XRD) and neutron powder diffraction (NPD) used in conjunction allowed to determine accurately the atom positions and the oxygen stoichiometry. The effect of the Fe content on the cell parameters, size domain, strain, atomic positions was studied. Raman spectroscopy was used as a local probe sensitive to even subtle changes of symmetry. The magnetic properties were studied from magnetic susceptibility and electron pramagnetic resonance (EPR) measurements function of temperature. The effect of partial substitution of V with Fe in $Pb(V_{1-x}Fe_x)O_3$ samples is the occurrence of both AFM and FM interactions. Spin glass and relaxor ferroelectric states were observed. EPR hyperfine structure of V^{4+} and the characteristic EPR signals for Fe^{3+} confirm the paramagnetic contribution evidenced in susceptibility measurements.

O-1 The corrosion behavior of the alloy based on Ti, Zr, Al and Fe

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In this work, we studied the corrosion behavior of the alloy based on titanium, zirconium, aluminum and stainless steel. Currently the contact of these metals is a fairly common cause of local corrosion fracture of steel structures. Relevance of the topic is that the vast majority of structures, machinery or appliances can not be constructed from a single metal. They include a large number of the contacting parts made of various metals, corrosion behavior which is not easy to predict. For a given pair of corrosion experiments conducted in a variety of corrosive environments: distilled water, 3% and 6% solution of NaCl. Contact corrosion can occur without direct contact of dissimilar metals, so experiments are made out of contact and contact. In this paper we calculate the mass and depth of the score for each sample in different solutions. Defined a group of resistance and resistance to corrosion point pairs in different environments. These data confirm that the value of the potential is strongly dependent on the nature of the corrosive environment. For example, in 6% NaCl solution potential of aluminum in 0.031V shifted in the negative direction, and a stainless steel 0,006V positive. At the 3% NaCl solution for aluminum 0.017V and 0.003V stainless steel in a similar way. Evans' diagrams were constructed for corrosive vapor in 3%, 6 % solution of NaCl. Determine the intersection point, which corresponds to the maximum current that can give a couple. Thus the results of the study will be used in the nuclear industry for the rational design of metal containers for storing water.

O-2 Comparison between ultraviolet light and plasma polymer treatments for improving biocompatible proprieties

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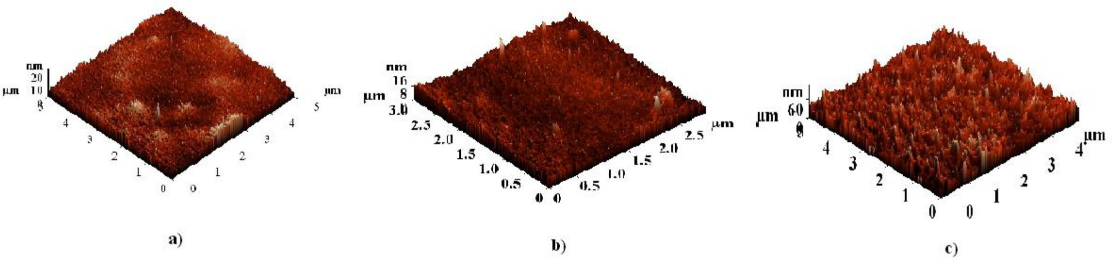
Polyethylene terephthalate (PET) is one kind of common polymer materials with excellent physical and mechanical properties, chemical stability, as well as high permeability of human body fluid, usually used to be artificial vessel, artificial heart ale closure, cardiac patches, artificial ligaments and surgical suture [1]. In the present work, PET films have been exposed to radio frequency helium plasma utra-violet light UV (256 nm) in order to induce the formation of free radicals in the polymeric chain and in this way to insert or interact certain function groups on the polymer surface which will enhance the surface properties of the polymeric films. In order to obtain a higher amount of new functional groups at the polymer surfaces, the plasma parameters (power and time) and the UV parameter (time of exposure) were varied. After the non-conventional treatments, the PET films were introduced in a collagen solution and the modified surfaces were characterized by x-ray photoelectron spectroscopy (XPS) analysis, contact angle measurements, atomic force microscopy (AFM) measurements, Fourier transform infrared spectroscopy attenuated total reflection (FTIR-ATR) measurements and small angle x-ray scattering method.



AFM measurements: a) untreated PET; b) UV treated PET; c) plasma treated PET

The cytocompatibility of the samples after collagen immobilization was investigate and all treated samples sustained adherence and proliferation of cells.

Acknowlegments The work has been funded by the Sectoral Operational Programme Human Resources Development 2007-2013 of the Ministry of European Funds through the Financial Agreement POSDRU/159/1.5/S/132395.

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O-3 Bioimmobilization of ZnO nanoparticles functionalized by surface-wave plasma processing

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Biomolecular imaging is an important field for understanding the biological processes and for facilitating the interactions with biological targets. Bioimaging with the use of nanostructures, enriched with different functional groups and even biomolecules, is an emerging technology in medical science having the great potential to revolutionize the way of diagnosis and treatment of diseases. Functionalization of zinc oxide through amine functional groups grafted on the surface by plasma processing is a novel approach to tailor the chemical, physical, and electronic properties of nanoparticles surfaces [1]. Plasma-surface modification is an effective and economical surface treatment technique for many materials and of growing interests in biomedical engineering. The unique advantage of plasma processing is that the surface properties and biocompatibility can be selectively enhanced, thus enhancing the performance of the nanomaterials. Functionalization efficiency of the ZnO is directly correlated with the mixture of ammonia and argon gas mixture used to excite the surface wave plasma for the generation of the species that are responsible for amination [2]. For this study the amine groups grafted on the surface of the zinc oxide are used as reactive sites for further connection with biomolecules, in this case sugar chains. These sugar chains can serve as spacing molecules, having the ability of further binding biomolecules, offering biocompatibility properties and higher stability. Dextran is a suitable candidate to connect with the amine groups from surface of the plasma processed ZnO. By fluorescence microscopy we have checked the possibility to connect labeled dextran and the result show good premises to use these biofunctionalized ZnO as support for detection and interaction with different biological systems. ZnO luminescence at room temperature is also taken into consideration and plays an important role when dealing with the detection of specific processes.

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O-4 Nanomechanical studies of ZnO nanowires by nanoindentation and scanning probe microscopy

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Recent breakthroughs in nanoscale research pave the way for the development of prototype nanoscale devices while taking advantage of size-effect characteristics of 1D ZnO nanostructures for possible electrical, photonic and electromechanical applications. Nanowire-based electromechanical devices, designed to have high-endurance during operation, have to be mechanically stable and highly-sensitive at variable load inputs. For this reason, a systematic assessment of structural and mechanical properties is of much importance, from the design perspective, in order to use ZnO nanowires for optimum device integration and applications. Thus, this study aims to synthesize ZnO nanowires with structural and mechanical properties suitable for piezoelectric applications. Vertically aligned and high-aspect ratio ZnO nanowires with high c-axis crystal growth orientation are deposited on ZnO-seeded Si substrate via low-pressure chemical vapor deposition technique. Vapor-liquid-solid self-catalytic process was observed based on the growth of tapered nanowires with spherical tips. Homogeneous nanowire growth is desired for unifom sensitivity of piezoelectric sensors. Morphology and structural characterization are done using SEM and XRD. Nanomechanical characterization is performed with a nanoindentation facility (with a Berkovich tip) that has the capability to measure buckling behavior of several nanowires mapped with scanning probe microscopy. Load-displacement curves are analyzed using Euler model to determine the critical buckling force and buckling energies for each applied force. Statistical data of nanowire density, length and diameter from SEM measurements are used to estimate the applied load, Young's modulus and critical stress. Radial component of the applied load due to nanowire misalignment from the indentation axis contributes to the deviation of Young's modulus estimates. Large hc/hmax ratio confirms the dominant plastic deformation of the nanowires predicted by Oliver-Pharr model.

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O-5 Coherent charge transport in dendritic nanostructures

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Dendritic nanostructures are promising candidates for a variety of applications, such as next-generation electrocatalysts [1], photovoltaic cells [2] or sensing devices [3]. Controllable growth of dendritic nanowire arrays has been achieved [4]. In the case of photovoltaic cells, the large surface area is essential for efficient carrier generation and, at the same time, the structures must ensure efficient charge transport. We investigate here the charge transport in the framework of coherent scattering formalism, based on the R-matrix method [5-7]. Our study is focused on the optimization of the dendritic interface. The transmission functions and charge distribution are evaluated for different tree shapes, ranging from regular interfaces to structures with different branching ratios and different lengths of the tree sub-branches. Besides prototypical tree models we also investigate the transport properties in the case of realistic tree structures generated by diffusion-limited growth.

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O-6 Characterization of recycled aggregate concrete by the means of non destructive test methods

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Aggregates are considered as essential constituents in the composition of the ordinary concrete or special concretes. The use of recycled aggregates is of great interest from the economic and environmental point of view. This study concerns the use of aggregates issued from the waste of crushing of the old concrete as a substitution for natural aggregates. An experimental program plan includes the study of the behavior of recycled aggregate concretes (RAC) at replacement ratio of 0 %, 30 %, 50 %, 70 % and 100 %, respectively. The objective of the present research work is to appreciate the effect of recycled aggregates substitution (RA) on the physical and mechanical characteristics of a local recycled concrete. The non-destructive test methods NDT (rebound hammer and ultrasonic velocity) were adopted to assess the mechanical respone. The correlation of these tests had been considered for the different properties of tests to see wether, they are reliaible to characterize a local recycled concretes, in this particular case of study. The results obtained showed that that there is a negative impact of replacement ratio of recycled aggregate on the physical and mechanical properties mainly, higher air content, lower density, greater adsorption and decrease in strength in comparison with reference crushed aggregate concrete (CAC). Further, low correlation coefficients were registered to predict the due compressive strength in this case regarding the effect of aggregate type.

O-7 Comparative electrochemical characterization of plasma sprayed zirconia and alumina coatings on titanium substrate

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Abstract Current ceramic solutions for applications in wear and thermal shock technology is now a necessity. The electrochemical characteristics of yttrium oxide stabilized zirconium oxide (YsZ) and alumina (Al_2O_3) coatings produced on titanium (Ti) targets were investigated in natural seawater. All coatings were produced by plasma spraying deposition. In order to study the electrochemical behaviour, the electrochemical impedance spectroscopy (EIS) and linear potentiodynamic polarization (LPP) performed. Equivalent circuit (EC) was used to modelling EIS data, in order to characterize YsZ and Al_2O_3 coated Ti surface. Scanning electron microscopy (SEM) observations were made before and after the LPP tests. It was found that both YsZ and Al_2O_3 coating showed a good corrosion resistance (polarization resistance and corrosion current density) after 1-day immersion in natural seawater. The Ti substrate was actually passive in these experimental conditions. resistance Keywords: zirconia, alumina, natural seawater, SEM, EIS, LPP

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O-8 Preparation and functional properties of Sm_2NiMnO_6 multiferroic ceramics

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In the last years, there is a great interest in developing new multiferroic materials having simultaneously in the same phase ferromagnetic and ferroelectric order. The multiferroic materials have attracted attention due to their future application in spintronics and magnetoelectric devices [1,2]. In the present work, it was reported for the first time the new synthesis of Sm_2NiMnO_6 double perovskite oxides by sol-gel auto-combustion method. The Rietveld analysis of the x-ray ceramics diffraction pattern recorded at room temperature for Sm_2NiMnO_6 ceramics sintered at 1000°C/5min from powders obtained at 700°C/7h confirm the formation of the double perovskite with a monoclinic structure and the space group $P2_1/n$. The magnetic transitions observed in the ZFC/FC cycle indicate a change in the spin ordering at low temperatures and a weak ferromagnetic/ferrimagnetic contribution that is attributed to the possible valence states in the magnetic ordering Ni^{2+}-O-Mn^{4+}. The complex impedance investigations indicate important contribution from at least two conductivity relaxation mechanisms (given by grains and grain boundaries). The non-linear dielectric character was checked for the first time in Sm_2NiMnO_6 double perovskite and the results reveals a strong nonlinearity and a small hysteretic behaviour. The non-linear field-dependence $\varepsilon(E)$ presents a tendency towards saturation for high fields (~ 30 kV/cm). In conclusion, the present structural, magnetic and dielectric data make the Sm_2NiMnO_6 double perovskite system for its multiferroic character a promising candidate to different applications.

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O-9 Influence of various impurities on the compensating defects in YbF_3 doped CaF_2 crystals

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Calcium fluoride (CaF_2) crystals doped with various rare-earth (RE) ions have attracted much interest in order to develop new laser materials. CaF_2 crystal is used as a host for applications in laser and opto-electronic devices due to its low refractive index limiting nonlinear effects, low phonon energy reducing non-radiative relaxation, wide range of solubility for RE ions, high transparency in a wide wavelength region varying from VUV to IR, high thermal conductivity and chemical stability and good mechanical properties. When YbF_3 is dissolved in CaF_2 the Yb ions are in trivalent state, consequently additional charge-compensating defects appear in crystals [1]. The local compensation, by pairing of Yb^{3+} ions with an interstitial / substitutional F^- or Na^+ ions, creates various crystal field symmetries of the Yb^{3+} ions (sites). The goal of this work is to study the influence of Pb^{2+} and Na^+ ions on the optical absorbtion and dielectric spectra of the YbF_3-doped CaF_2 crystals in order to obtain information about the impurity-defect formation. The influence of these ions on the emission spectra is also investigated in order to obtain information about the influence of the Pb^{2+} and Na^+ ions on the light emission intensity. Various concentrations of YbF_3 - doped CaF_2 and PbF_2 and NaF - codoped crystals were grown using the Bridgman method[2]. Room temperature optical absorption spectra have been recorded using a Shimadzu 1650PC spectrophotometer. Temperature and frequency dependence of the complex dielectric constant [3] gives information about the C_{4V} charge compensating defects.

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O-10 HiPIMS versus PLD depositions for metallo composites nanomaterials

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The effect of oxygen concentration and film thikness of ZnO and TiO2 thin films has been investigated on the films deposited by pulsed laser deposition (PLD) and high power impulse magnetron sputtering (HiPIMS). The aim is to observe the main advantages and disadvantages of the two depositon techniques in terms of deposition efficiency, films characteristics and ease of transfer to mass production. The structural and optical properties of the films were studied along with the effects of glass and silicon substrates. The results shows that the ionization efficiency of HiPIMS discharges tends to encompass all of the PLD strengths.

P-1 Creep Crack growth of CrMoV(Ti,B) Steel Using Electrical Potential Drop Technique

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Creep crack growth measurements, at 565°C and 25°C of 1Cr1Mo3/4V steel doped with Ti, are obtained using electrical potential drop technique .Tests are performed in air using creep machines under constant load conditions. The total crack length measurements are made using optical microscopy. A correlation between the potential reading and the crack length is made. Then a calibration curve is obtained. This later curve is used to deduce creep crack rate of the material under creep conditions. The aim is to measure the crack length as a function of time for low alloy steels under creep conditions. The present material shows that the incubation period is found to be dependent on the initial net section stress, while the crack growth rates are apparently unaffected by the increase of the initial net section stress.

P-2 The thermal treatment effect on dopants localization in thin films Si-LPCVD.

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We present the results of a comprehensive investigation concerning changes on the boron dopant profiles in polycrystalline-silicon films deposited by low pressure chemical vapor deposition and doped heavily after thermal oxidation treatments. The thermal-oxidation process is performed on sub-micron layers of 200 nm poly-Si/c-Si and 200 nm poly-Si/SiO2/c-Si deposited at two temperatures Td= 520°C and Td= 605°C and thermally-oxidized in dry oxygen ambient at 840°C and 945°C. The results show that the deposition temperature has a very important impact on the morphology structure of the films (the grains size), which affects the redistribution and localization of dopants. Also, the diffusion of dopants is strongly affected by the oxide thickness deposited between polysilicon layers and monocrystalline substrates.

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P-3 Adsorption of copper cations and sulphate anions from aqueous solutions on layered double hydroxides thin films deposited by PLD

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Mg-Al and Zn-Al layered double hydroxides (LDHs) -Al were deposited using pulsed laser deposition (PLD). Copper and sulphur are common pollutants in water from urban and industrial waste. We studied the ability of our as deposited films to detect copper cations and sulphate anions from aqueous solutions. The obtained films were characterized using X-Ray Diffraction, Atomic Force Microscopy, Scanning Electron Microscopy with energy dispersive X-ray analysis, Fourier Transform Infra-Red Spectroscopy and Secondary Ions Mass Spectrometry. The effects of various parameters such as the nature of the bivalent metal in the brucite-like layer, the Me2+/Al3+ atomic ratios, contact times were investigated. The results in this study indicate that LDHs thin films obtained by PLD have potential as an effective adsorbent for removing copper and sulphur from aqueous solutions.

P-4 Stearic acid/ layered double hydroxides (LDH) composite thin films deposited by laser techniques

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The aim of this work is to continue our previous experiments on producing thin films of layered double hydroxides (LDHs) and composite films of organo modified LDHs by laser techniques for hydrophobic surfaces. LDH based on Mg-Al and Zn-Al with Me^{2+}/Al^{3+} ratio of 2.5 were investigated and stearic acid was the tested fatty acid. Standard pulsed laser deposition (PLD) and matrix assisted pulsed laser evaporation (MAPLE) have been employed for the growth of the composite layers. Stearic acid was intercalated in co-precipitation step and subsequently the powders were used as guest materials for MAPLE or they were pressed and used as targets for PLD. The morphological, structural and chemical characterization of the films is presented; the type of the metal Me^{2+} (Mg or Zn) in the brucite like layer was found to strongly influence the film wettability.

P-5 Neural network modeling of the parameterized gold nanoparticles generation through photo-induced process

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Gold nanoparticles are studied at a large scale due to their excellent biocompatibility, large effective surface area, excellent conductivity and their metallic properties which vary with their dimension [1]. The control over the gold nanoparticles surface plasmon resonance peak and diameter is very important because most of the applications depend on their size [2]. Therefore various gold nanoparticles have been fabricated for applications in nonlinear optics, electronic devices, catalysis, material science and biosensing [3]. In this work we used a direct light writing (DLW) technique to generate gold nanoparticles through a dynamical photo-induced process. Its parameters have been tested using an automatically controlled set-up, in a stable and reproducible chemical system. Our aim was to build a neural network (NN) based on the experimental data obtained through the photo-chemical generation of gold nanoparticles (GNPs) and their characterization by spectroscopic and morphologic methods. The obtained data served as input and output parameters of our network. Based on parameters such as reactants ratio, velocity and fluence two neural network models that can predict the surface plasmon resonance peak and diameter of the particles were developed. Due to a less than 2% error the first model has an excellent prediction performance. The correlation factor for both models has values above 0.93 which means that these models have the potential to analyze the best conditions for preparing nanostructures with specific properties.

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P-6 Effective segregation coefficient of rare-earth ions in fluorite crystals

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Fluorite crystals (MeF_2: Me=Ca, Ba, Sr) are used as a host for applications in laser, opto-electronic devices and detectors due to its low refractive index limiting nonlinear effects, low phonon energy reducing non-radiative relaxation, wide range of solubility for RE ions, high transparency in a wide wavelength region varying from VUV to IR, high thermal conductivity and chemical stability and good mechanical properties. Calcium fluoride (CaF_2) crystals doped with various rare-earth (RE) ions have attracted much interest in order to develop new laser materials. BaF_2 is a scintillating crystal, having two fast emission components (195 and 220 nm) and a slow emission at 310 nm. Among the RE ions, the Er^{3+} and Yb^{3+} ions are more investigated in order to improve the laser efficiency, both of various alkaline-earth fluorides crystals and glasses. The homogeneous distribution of the impurity in laser crystals is important because this affects the

efficiency of the laser. The spectroscopic and laser properties of the ErF_3 and YbF_3 doped CaF_2 crystals are well studied [1-3]. Although these crystals are known as good laser host, surprising, the analysis of the Er^{3+} and Yb^{3+}/Yb^{2+} ions distribution along the CaF_2 and BaF2 crystal has been less investigated. The goal of this work is to determine the effective segregation coefficient of the Er^{3+}, Yb^{3+}, Yb^{2+} ions, in ErF_3 and YbF_3 doped CaF_2 and YbF_3 doped BaF_2 crystals using the optical absorption method [4]. ErF_3 and YbF_3 –doped CaF_2 crystals and YbF_3 doped BaF_2 were grown using the vertical Bridgman method. The optical absorption spectra reveal the characteristic peaks of the Er^{3+}, Yb^{3+}, Yb^{2+} ions. The dopant distribution along two crystals has been investigated using the optical absorption method. The effective segregation coefficient of the various ions has been calculated using the classical Scheil relationship between the impurity concentration and the crystal growth conditions. Our study shows that the effective segregation coefficient of the Er^{3+}, Yb^{3+}, Yb^{2+} ions in the CaF_2 and BaF_2 hosts depends on the doping concentration and on the host.

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P-7 Microstructure and Mechanical Properties of a Dissimilar GTA Weld between 2205 duplex stainless steel and API X-70 high strength low alloy steel (HSLA)

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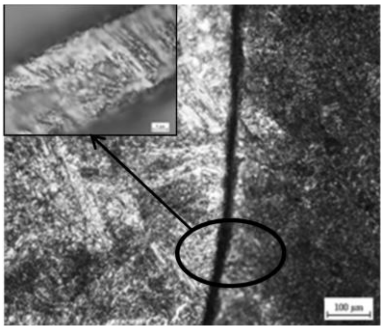
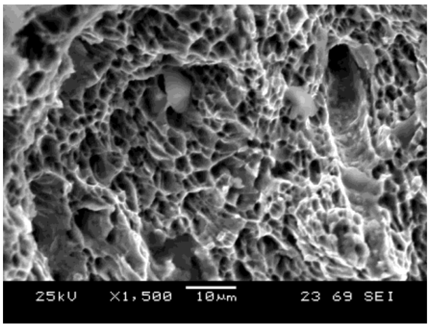
Duplex stainless steels and HSLA are finding increased application in oil and gas industries, transportation and for general engineering thanks to their properties. Dissimilar weldments have been widely used in the oil and gas industry because of economic benefits as well as the full advantage of outstanding performance of two different metals. however dissimilar welding with the highest possible quality is generally more challenging than welding of similar metals, due to the differences in the physical, mechanical, and metallurgical properties of the metals to be joined. The aim of the present study is to investigate the influence of the welding process parameters on the microstructure and mechanical properties of dissimilar weldement of 2205 duplex stainless steel /API X-70 high strength low alloy steel (HSLA) produced by GTA welding.



weld interface



Fractographs of tensile specimen

The microstructures of the welded joints were investigated by the optical microscopy (OM), the mechanical properties included hardness, impact and tensile strength was investigated, the fracture surfaces of the tensile specimen were examined by scanning electron microscopy (SEM). From this investigation, it is observed that, the microstructural characteristics and mechanical proprieties of the weld are influenced by the heat input.

Riad Badji et al, Phase transformation and mechanical behavior in annealed 2205 duplex stainless steel welds Materials Characterization 59 (2008) 447 – 453

P-8 Plasma-induced functionalization of the surface of sputtered ZnO films

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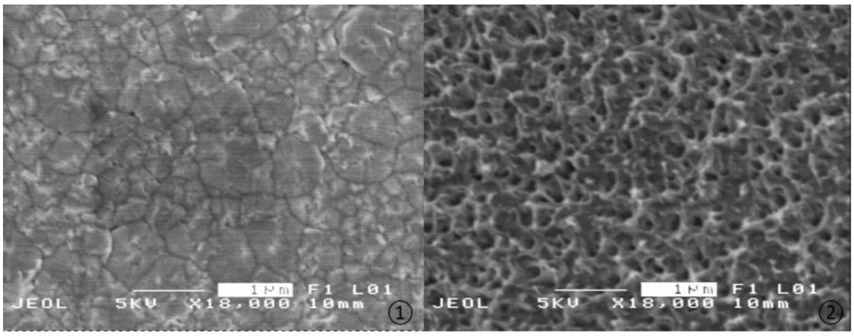
Zinc oxide is a II-VI semiconductor material that attracted much interest in the research community due to its interesting properties that promoted it as a suitable material for developing various applications, recently even bio-applications. For this purpose, zinc oxide needs to be prepared: first to decrease the size of the materials in order to fit the required dimensions with the ones in bio-applications, secondly to be bio-functionalized, i.e. provide them with a bio-suitable interface. We have shown recently [1,2] a new method for zinc oxide nanomaterial functionalization using plasma processing. Plasma-surface modification is an effective and economical surface treatment technique for many materials. By altering the surface functionality using plasma processing, optimal surface, chemical and physical properties can be attained. In our previous studies we focused our attention on amine groups functionalization of ZnO nano and micro-sized particles. We proved that amine groups successfully bind the surface of ZnO, then biomolecules can be bound to the amine functionalities. However, we could not establish the insights of the connection between amine groups and ZnO crystalline structure, or accurately quantify the outcome as a function of plasma conditions.



SEM images of magnetron sputtering ZnO thin film 1) before and 2) after ammonia plasma processing.

In this study we focus on ZnO films, where we assumed that it would be easier to study the mechanism of interaction between plasma species and ZnO. ZnO thin films were deposited by magnetron sputtering. After deposition, the films were exposed to ammonia surface wave plasma. Two aspects were of interest: the modification taking place in the lattice, and the activation of the surface by extra features given to the thin ZnO films. Scanning electron microscope (SEM) measurements in Fig.1 clearly show the modifications induced by plasma treatment in ZnO topography. A fluorescent dye that specifically connects with amine groups was used to detect whether the functionalization works for thin films as well. The fluorescence microscopy measurements indicate the successful connection of amine groups. More results about functionalization quantification and mechanism will be given in the conference presentation.

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P-9 Post-treatment recovery of atmospheric-pressure plasma treated polymers

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Many polymer properties rest on the surface chemical composition, material structure and surface orientation of specific chemical functionalities, all intrinsically related, and defining the material interaction with its environment. In this respect, the surface modification of polymers is a constant challenge. The knowledge on the processes by which a treated polymer surface tends to reorganize, as to achieve stability, the relation between the polymer surface characteristics and the surface dynamics, and the factors allowing to control the interaction, on a time-space scale, is most important for all polymers applications. Recognizing the above, this work provides an investigation on the surface modification processes of polymers treated by plasma and an assessment on the dynamics and stability of modified surfaces. Here polymers offering variety of structure, functionality, degree of oxidation, polarity, crystallinity are tested, in order to demonstrate the plasma capability for efficient modification by creating complex surface structure. The surface treatment is performed using atmospheric-pressure helium plasma, for variable exposure time. The surface of the polymers, before and after treatment, is analyzed by contact angle, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and solvent absorption. The dynamics of the surface is assessed monitoring the ageing of samples tested before and after immersion in water, to assess the loss of polarity and the mechanisms related to it. The relationship linking the surface polarity, the chemical structure and composition contribution in the surface modification mechanisms of plasma-exposed polymers is explored, establishing the limiting level of modification attainable and the factors controlling it, concluding on the role of crosslinking in restraining the ageing process, as a necessary condition for polymer operational stability.

P-10 Mechanism of Ni uptake on Mg, and Ni-Mg LDH thin films deposited via laser techniques

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Layered double hydroxides (LDHs) are a class of layered materials consisting of positively charged brucite-like layers and exchangeable interlayer anions, which have received increasing attention in the last years, due to their versatility and to their prospects in a wide range of technological applications such as catalysis, separation, sensor and environmental remediation.We have demonstrated the ability of Mg-Al thin films deposited using PLD to retain Ni and Co from aqueous solutions[1] In this work, the mechanism of Ni uptake from acqueous solutions were deeper analysed by a comparative study of Ni adsoprtion on Ni -containing thin films. Ni-Al, Ni,Mg-Al and, as reference, Mg-Al double hydroxidesthin films were obtained via pulsed laser deposition (PLD) technique. The thin films were deposited on Si and glass using a Nd:YAG laser (1064 nm) working at a repetition rate of 10 Hz. X-Ray Diffraction (XRD), Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), Fourier Transform Infra-Red Spectroscopy (FTIR), Secondary Ions Mass Spectrometry (SIMS), Impedance Analyzer and ellipsometry were the techniques used for the as deposited thin films investigation. The effect of the Ni amount as deposited and/or adsorbed on the structural, morphological, optical and electrical properties of the Ni based LDHs thin films are evidenced.

1.A. Vlad, R. Birjega, A. Matei, C. Luculescu, B.Mitu, M. Dinescu, R. Zavoianu, O. D. Pavel, Appl. Surf. Sci, 302, (2014), 99-104

P-11 Effects of tungsten substitution on the microstructure, electrical and magnetic properties of different ferrite materials

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The purpose of this study is to investigate the comparative effects of tungsten ions substitution on the microstructure, electrical and magnetic properties in different ferrite materials such as hexaferrites and spinel ferrites [1-5]. The ferrite materials are prepared in the same conditions following the sol-gel autocombustion technology. Hexaferrite and spinel powders resulting from autocombustion were heat treated for 30 minutes in air at temperatures between 850 ºC and 1200 ºC.

X-ray diffraction and scanning electron microscopy investigations have revealed the composition and the effects of tungsten on the crystallites shape and size. Also, the influence of tungsten ions on to electrical and magnetic properties are compared both spinel and hexaferrites, highlighting different applied characteristics from record industry to sensors.

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P-12 Nitrogen Containing Tungsten Coatings Obtained by HiPIMS as Plasma Facing Materials for Fusion Applications

Vasile Tiron[1], Ioana–Laura Velicu[1], Claudiu Costin[1], Gheorghe Popa[1], Corneliu Porosnicu[2], Mihai Straticiuc[3], Ion Burducea[3], Cristian Lungu[2]
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Tungsten-based materials are excellent candidates for plasma-facing component (PFC) for fusion applications. The main requirements for PFC materials are: good chemical and structural stabilities, high damage resistance against neutron radiation and high transient heat loads, low physical and chemical sputtering yields and low nuclear fuel retention. During the normal reactor operation of ITER, particles will impinge the divertor plates with energies close to few eV. As a consequence, when seeding gases are injected in the divertor zone during the transient events, a part of the seeding ions will reach the divertor with energies up to ~2.5 keV. The irradiation of the energetic seeding impurities as nitrogen (N) and argon (Ar) will lead to significant microstructural and chemical changes in the irradiated surfaces. These newly formed materials will influence both nuclear fuel retention and release behaviour. In this work, tungsten coatings having different N content were deposited on polished molybdenum and graphite substrates by reactive High Power Impulse Magnetron Sputtering (HiPIMS) technique. The N content in the deposited films was controlled by the nitrogen/argon mass flow ration, target potential, pulse duration and frequency. The chemical composition and corresponding structural changes in the obtained films were investigated by Rutherford back-scattering (RBS) and X-ray diffraction (XRD), respectively. Deuterium (D) implantation was performed using a deuterium plasma torch. Using a fluid model simulation, the D flux onto each substrate surface was calculated to be 2.5×10^{15} D/cm^{2}s. N content in the coatings and the films microstructure highly influences both D retention and release behaviour. These dependencies were studied by ion beam analysis (IBA) and thermal desorption spectroscopy (TDS). These experimental results provide information about the D amount retained, as well as about its temperature (de-trapping energy), in correlation with the film's composition and structural changes.

P-13 Influence of heat input on microstructure and mechanical properties of Ferritic Stainless Steel welds

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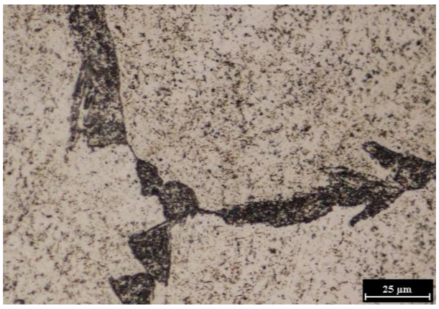
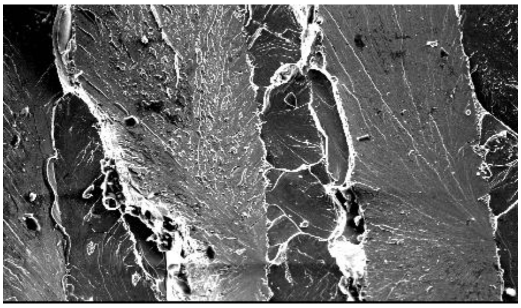
Ferritic stainless steels are classified as such because the predominant metallurgical phase present is ferrite. These steels are characterized by good resistance to stress corrosion cracking (SCC), pitting corrosion, crevice corrosion (particularly in chloride environments), higher thermal conductivity, low coefficient of heat dilation and lower cost, when compared to austenitic stainless steels. The combination of low cost and good properties has made ferritic stainless steel more and more attractive in various application fields, such as, heat exchangers, petroleum refining equipment, storage vessels, protection tubes, solar water heaters, and exhaust manifold applications. However, ferritic stainless steel steels are associated with many problems during the welding process.



Martensite formation in fusion zone



Fractograph of tensile specimen

These problems are the martensite formation and grain growth, causing a reduction of ductility and toughness. For these reasons, until recently, the application of this group steels is limited in welded structures. The aim of the work is, first to characterize the weld metal, as variable GTA welding process parameters and optimize the heat input. We focused on improving tensile strength of ferritic stainless steel. The results show that, the heat input has a great influence on microstructure and mechanical proprieties of of weld metal. The details of tensile tests, optical microscopic observations, microhardness, and Scanning electron microscopy (SEM) fractography, are discussed.

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P-14 Structure optimization and characterization of TCO/kapton thin films for CIGS solar cells

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In this paper we report on the CuIn1-xGaxSe2 (CIGS) solar cells realized by successive rf magnetron sputtering deposition of thin films (CIGS/CdS/Au) onto kapton substrate, and coated with a TCO layer. TCO/kapton thin films (ITO, SnO2, AZO (2%)) with thickness of 400 nm were deposited using individual targets and their structural morphology and optoelectronic properties were investigated. Structural properties of the deposited thin films (CIGS (1200 nm), CdS (60 nm)) and contact electrodes were investigated. Structural analysis shows that the microstructure (crystallite size, roughness, internal stress) depends on the power applied to the targets during deposition. AFM analysis showed that CIGS thin films have a high porosity. The CdS “reference sample” film directly deposited onto substrate is characterized by a low surface roughness (Rrms = 2 nm) while the CIGS solar cell has crystallites with a greater size (e.g. roughness is about 70 – 150 nm). XRD analysis indicates that the obtained TCO/kapton (ITO, SnO2, AZO (2%)) films have a polycrystalline structure. The surface topography of the samples was analyzed using scanning electron microscopy (SEM). Optical and electronic transport properties of the TCO/kapton films were investigated and then were correlated with their preparation conditions and the applied power to the target during deposition. Some specific parameters, such as energy barrier, concentration of impurities, or distribution state of the interface have been determined. Optical properties of the TCO/kapton films were investigated and it was observed that, in the visible domain, optical transmission varied between 85 and 95%.

P-15 Soft material printing by laser-induced forward transfer

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The use of lasers is so far reaching and widespread, making them appealing tools in the development of direct writing processes for micro-patterning applications. One of the most common approaches is laser induced forward transfer (LIFT). In LIFT, a laser beam is focused through a transparent plate onto the backside of a photodegradable triazene polymer (TP) thin film coated with the material to be transferred (donor film). The TP acts as a dynamic release layer and also protects the material to be transferred from direct laser irradiation. Each laser pulse promotes the transfer of the thin film material onto a receiver substrate that is placed parallel and facing the thin film. The donor-receiver system is placed on a xyz stage allowing the fabrication of well-defined 2D and 3D patterns. The objective of this work is the investigation of various experimental parameters determining the characteristics of the micrometric patterns (i.e. polymers and carbon nanotubes) deposited by LIFT. The underlying transfer mechanism, in the case of inorganic materials such as metals or oxides, consists in the vaporization of a fraction of the transferred material followed by a recondensation of the laser-generated vapour onto the receiving substrate. However, in the case of more complex materials i.e. polymers or carbon nanotubes the energetic laser pulses may damage these materials and result in the loss of functionality. Therefore, the dynamics of the transfer process of soft materials is investigated through time resolved imaging.

Alexandra Palla Papavlu was supported by the strategic grant POSDRU/159/1.5/S/137750, ”Project Doctoral and Postdoctoral programs support for increased competitiveness in Exact Sciences research” cofinanced by the European Social Found within the Sectorial Operational Program Human Resources Development 2007 – 2013.

P-16 Improving the behavior of austenitic stainless steels subjected to cryogenic temperatures by coating deposition

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Stainless steel shows a better mechanical behavior at low to cryogenic temperatures then normal steels. Usually the stainless steels used for low temperatures applications have an austenitic microstructure which enhances the mechanical behavior of the material. Austenite stainless steels have a microstructure composed of austenite grains and annealing twins which can suffer changes due to prolonged exposure to cryogenic temperatures. The changes that appeared consist of an increase of the number of twining planes inside grains and even phase changes due to the dissociation of alloying elements. The purpose of this paper is to analyses the possibility of improving the behavior of an austenitic stainless steel at cryogenic temperatures by coating deposition on the outer surface of the material. In the study two different materials were deposited on a AISI 304 stainless steel by atmospheric plasma spraying and electrochemical deposition. The two materials considered in the study were Al2O3 with 99,5% purity and TiO2. The samples were exposed to cryogenic temperatures by immersion in liquid air which has a temperature of -196 ºC. The influence of the cryogenic temperatures over the base material and coatings was highlighted using X-ray diffraction and SEM analyses.

P-17 Effect of heat treatments on mechanical properties of HSLA-X70 weld

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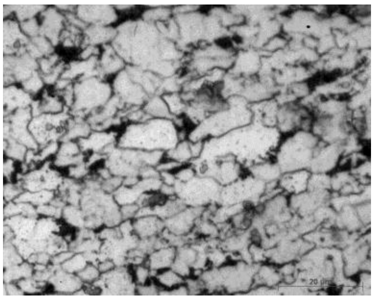
Pipelines welding assembly occupies an important place in Oil industry. Precisely HSLA-X70 steels are more usable because of their good weldability by SMAW processes. Accordingly, the temperature gradients created during welding cause inevitably the creation of residual stresses. The HSLA-70 steel, getting its name from its minimum yield strength of 70 ksi or 483 N/mm2, is a high-strength low-alloy (HSLA) steel or fine grained structural steel used in quenched and tempered condition, with a combined Pearlito-Ferritic microstructure. Its many attractive properties, like good formability, weldability, and acceptable corrosion resistance, have made this steel a good selection for applications in many engineering fabricating operations. Despite these useful properties, the welding of this steel, when not critically controlled, has often posed problems, particularly in the shop floor conditions.



optical microscope

According to their metallurgic characteristics, heat input of welding process significantly affects the heat affected zone (HAZ) mechanical properties. Our study comes to complete previous works. We focused on heat treatments, their consequences on mechanical and metallurgical proprieties of ferrito-perlitic steel after welding. We made an annealing for different temperatures followed by oven cooling. Rolled pipes samples of 12 mm thickness were used as the base material for preparing five passes butt welded joints. Tensile and impact properties, microhardness, and microstructures of the treated welded joints have been evaluated and the results are compared.

Zidelmel Sami, SahraouiTahar, Hadji Mohamed. Microstructure and Charpy impact properties of ferrite–martensite dual phase API X70 linepipe steel. Materials Science&EngineeringA598(2014)338–342

P-18 Luminescent properties of Ce(III) and Dy(III) complexes : Structural and spectral characterization of lanthanide complexes with 2-(1H-1,2,4-Triazol-3-yl)-pyridine

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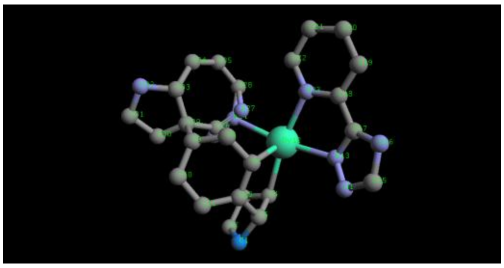
In this work , 2-(1H-1,2,4 –Triazol -3-yl)pyridine (denoted as L) was investigated as suitable ligand for preparation of new Ce3+, Dy3+, Ho3+ and Tm3+ complexes. All complexes were characterized in detail using elemental analysis, TG, FT-IR, P-XRD and fluorescence spectrometry. Data obtained through analysis revealed the formation of the Ce3+, Dy3+, Ho3+ and Tm3+ complexes with above mentioned ligand at 1:3, metal to ligand (M:L) molar ratio with the general [LnL3(H2O)3] formula. In case of Dy3+ the recorded photoluminescence spectra revealed metal centered specific narrow band emissions due to the f – f transitions within 4f orbitals while in case of Ce3+ complex the observed luminescence is most probably due the heavy ion influence over the excited states of the ligand.



structures

figures

From the practical point of view, the photoluminescent properties of the above mentioned complexes may be potential interesting for applications in optical devices or through embedding in various compatible media as luminescent probes for biological and medical investigations.

1. Koen Binnemans, Lanthanide-Based Luminescent Hybrid Materials, Chem. Rev.109 pp. 4283-4374, 2009. 2. N. Sabbatini, Massimo Guardigli, Ilse Manet, R. Ungaro, A. Casnati, Raymond Ziessel, G. Ulrich, Z. Asfari and J.-M. Lehn.

P-19 Influence of thermal treatment on structure and mechanical properties of zirconia layers coating some stainless steels

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Zirconium oxide (ZrO_2), also called zirconia, is an important versatile ceramic material due its novel physical-chemical properties. Zirconia based ceramics are most commonly used as material of thermal barrier coatings. As it has been well established, yttria-stabilized zirconia (YSZ) ceramics are considered a desired thermal barrier coating (TBC) materials because of its low thermal conductivity, refractory, chemical inertness, good erosion and wear resistance, and compatible thermal expansion coefficient with metallic bond coating substrate. TBC is used as thermal protective layer dedicated to metallic components in high-temperature regions or engines and gas turbines, and it can enhance component reliability and increase the operating temperature resulting in higher efficiency and better environmental benefits. The use of YSZ ceramics coating on austenitic stainless steel was also proposed for generation IV of nuclear energy reactors. Morphology of the YSZ TBC’s is closely related to the mechanical and thermal performances. Laminar structures YSZ TBCs are typically porous and lack of periodicity, which tends to crack within the layer when exposed to mechanical and thermal stresses. Fully-dense or porous free YSZ TBC are reported to have lower ohmic resistance and has better thermal resistance than laminar structures and zigzag porous structures and highly porous TBC’s are tend to have much lower thermal conductivity. Our aim was to obtain some preliminary information concerning the methodology necessary to obtain a stable zirconia layer on austenitic steel and to investigate its structure and mechanical properties. We have chosen a stainless steel used for nuclear reactors (316L) and have performed some zirconia coating in various conditions. The layer and substrate structure were investigated by means of XRD. The microhardness was also determined vs coating chemical composition and treatment condition.

P-20 Structural and functional properties of LPMO thin films deposited by RF magnetron sputtering

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Lanthanum perovskite La0.6Pb0.4MnO3 (LPMO) is a semi-conducting oxide and has been extensively studied with reference to several potential applications, such as magnetic sensors, catalysts and gas sensors. We have studied in this work the structural and gas sensing properties of some thin films obtained through RF magnetron sputtering using as target the $La_{0.6}Pb_{0.4}MnO_3$ perovskite. We have investigated the effects of the substrate and its temperature during deposition, of plasma composition (Ar/O_2 ratio) and of subsequent thermal treatments. The microstructure of the thin films was characterized by XRD, SEM, EDX and AFM analyses. Also, the films sensitivity was investigated to different gasses, at various operating temperatures.

P-21 Obtaining surfaces with taylor cone shaped asperities of micro- and nano-scale dimensions using the edi method

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The present paper is devoted to experimental investigations concerning the treatment of conductive surfaces by applying electric discharges in impulse (EDI). We have particularly focused on the modifications of metal surface micro-geometry leading to the formation of Taylor cone shaped asperities. We have established and presented the best energetic regimes of extracting the latter from cylindrical and flat pieces made of W+10%Re using EDI. The modern stage of scientific and technical progress is characterized by a transit from macro- to micro- and nano-organization of matter. Having studied the samples of the surfaces treated via the method of EDI using the method of optic microscopy with the optical microscope XIM600 and the SEM with electronic microscopes Vega TESCAN 5130 and QUANTA 200 (FEI Fillips), we can observe that Taylor cones are formed not only in the centre of the crater but also at its peripheries due to the development of electro-hydrodynamic instability on the melted tungsten surface as a reaction of the plasma channels and the substance interaction (Fig.1). Varying the interstice size, it is possible to obtain almost any degree of intensification of the working surfaces with the emission of energy on the surfaces subjected to treatment or in the interstice. Increasing the interstice size, we may obtain such states when the heating of the volume of the treated material is not essential and the geometry of the sample surfaces does not change. This possibility may be applied in the development of new surface treating technologies by applying electric discharges in impulse.

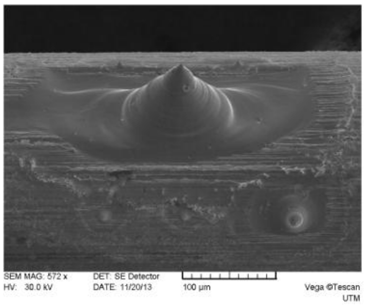

Fig. 1 Scanning electron microscope (SEM) image of a conic asperity surrounded by smaller ones, extracted on the surface of the piece material at a solitary discharge

Conclusions - The extraction of conic asperities in the process of treatment with EDI is more favorable if the piece is connected as anode. However the successful extraction of asperities from the cathode in conformity with the theory of developing capillary waves is not excluded; - The use of the EDI method to modify the micro-geometry of metal surfaces permits the increase of its active area by several times.

P-22 Nanostructured composite layers for electromagnetic shielding in the GHz frequency range

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Today, various electronic devices that have been developed and used in wireless communication systems result in an increased electromagnetic radiation background. This radiation differs from natural electromagnetic background and introduces complex influence on biological systems as well as in the operation of electronic devices. This is known as electromagnetic interference (or EMI), an effect that can cause malfunction of sensitive medical devices, robotic systems or even become harmful to life. In order to address the electromagnetic interference problems, it is necessary to develop materials that can absorb or reflect the electromagnetic radiation of a particular frequency, since then, these materials can offer electromagnetic shielding. Since the shielding materials must possess good electrical conductivity, metals such as aluminum, copper and steel are today among the most common and active materials used for electromagnetic shielding. There are several limitations in the applicability of metal in shielding applications since they are heavy, not easily handled/applied and they suffer from corrosion. As a result, the scientific community is trying to develop new shielding materials, a trial that has been significantly promoted by the advances in materials science and nanotechnology. In our work we investigate the applicability of nanostructured composite layers in electromagnetic shielding for the frequency range of 2-30 GHz. Various combinations of commercial products with novel nanomaterials have been employed including PEDOT:PSS, polyaniline, graphene platelets, carbon nanotubes and metal particles.

Acknowledgements: This project is implemented through the Operational Program "Education and Lifelong Learning" action Archimedes III and is co-financed by the European Union (European Social Fund) and Greek national funds (National Strategic Reference Framework 2007-2013). Part of the work was partially supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-RU-TE-2012-3-0202 and by the strategic grant POSDRU/159/1.5/S/133652, co-financed by the European Social Fund within the Sectorial Operational Program Human Resources Development 2007–2013.

TOPIC 11

Trends in Condensed Matter and Field Theory

O-1 Temperature Dependent Surface Properties of Liquid Bi, Sn, Pb and Sb

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Liquid metals are in common use in modern industries/areas such as casting, metallurgy, welding, glass forming, the nuclear industry and crystal growth. In addition, how the physical, structures, surface properties change with temperature, concentration and pressure is also of interest to researchers in physics. The surface properties of liquids have attracted much more interest both physicist and metallurgists from the long past to the present day because of either scientific or technological importance. During the soldering, brazing, sintering and dying, the knowledge of surface properties of the liquid state is required. Although there are a large number of methods to determine the surface properties of liquids such as surface tension, those suitable for liquid metals are limited by their chemical reactivity and high melting points. On the other hand, it is not fully understood how the surface properties depend on the structure and the thermodynamics of the liquids as well. Present study deals with theoretical investigation of temperature dependent surface properties like surface tension (γ) and surface entropy (SV) of liquid Bi, Sn, Pb and Sb are studied in the present paper. Our newly constructed parameter free model potential is used to describe the electron-ion interaction. To see the influence of local field correction function on surface properties of liquid Bi, Sn, Pb and Sb, we have used Sarkar et al local field correction function. The present results are found in good agreement with available experimental data as well as other theoretical data. Lastly we conclude that our model potential is capable to explain surface properties of liquid Bi, Sn, Pb and Sb.

O-2 First-principles study of the Optical properties of Gd_2O_3 nanoparticles

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The optical properties of Gd_2O_3 in the hexagonal phases have been studied using the all-electron full potential linearized augmented plane wave (FLAPW) method within the local density approximation (LDA) for both bulk and nanoparticels. The theoretically calculated optical properties yield static refractive index of nanoparticels are three orders of magnitude higher than bulk. The results also show an indirect band gap at K– Γ points in the Brillouin zone.

P-1 The study of the optical properties S changes due to temperature by using neural networks. Case study for bismuth trioxide

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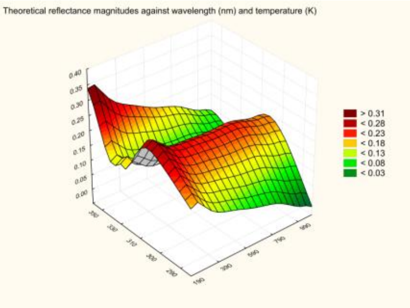
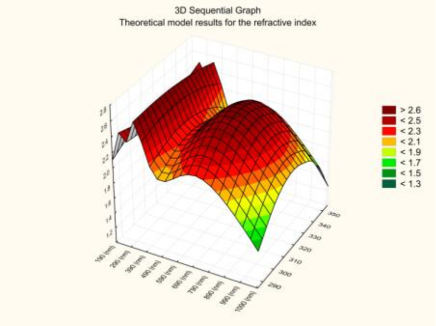
The study is implemented for Bi_2O_3 films deposited by thermal vacuum evaporation at different temperatures of the glass substrates. The optical reflectance was measured for different five samples. Two different neural network models were considered in order to succeed in evaluating the best method for a global representation of the optical proprieties changes due to temperature of the reflectance and refractive index.



Global reflctance model



Theoretical results for refractive index

The novelty of the present study is due to the implementation of a MAPLE software approach to the complex computations implied by this assessment. The neural network obtained results was preceded by a careful selection of the considered models. For each sample were considered 20 different models and were selected the best ten of then.

Gabriel Murariu, Simona Condurache-Bota, and Nicolae Tigau, INT. J. MOD. PHYS. B 26, 1250049 (2012) DOI: 10.1142/S021797921250049X Gabriel Murariu, Simona Condurache-Bota, and Nicolae Tigau, INT. J. MOD. PHYS. B 26, 1250049 (2012)

P-2 Temperature dependence of the optical properties of Bi_2O_3. Comparison between two polynomial mixed models

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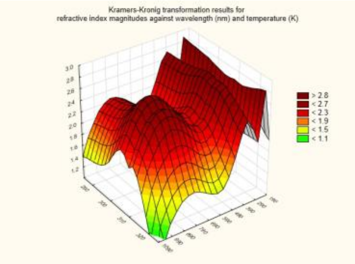
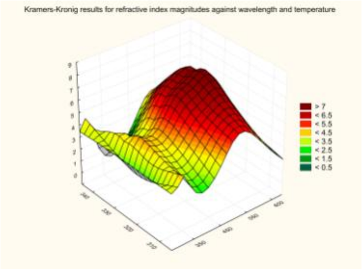
The present study is implemented for Bi_2O_3 thin films deposited by thermal vacuum evaporation at different temperatures of the glass substrates. Since the extraordinary properties of this fabric allow us to consider particular analytical approach as it was previously shown, the reflectance properties of Bi2O3 as a function of temperature could be studied. The novelty of this article is the studying of a global effective analytical representation, based on polynomial functions.



Kramers Kronig transformation for first model



KK transformation results for the second model

In the mathematical expressions, were included mix combined term in order to avoid the effects of Runge phenomenon and for the other one approach were considered independent temperature function coefficients. The obtained results allow to select the best method for this approach. As a case study was chosen Bi_2O_3 — a substance less studied in literature.

Gabriel Murariu, Simona Condurache-Bota, and Nicolae Tigau, INT. J. MOD. PHYS. B 26, 1250049 (2012) DOI: 10.1142/S021797921250049X Gabriel Murariu, Simona Condurache-Bota , Temperature dependence of the optical properties of Bi_2.

TOPIC 12

Self-assembly and Patterning

PL-1 Bio-inspired composite materials obtained by magnetically-driven nanoparticles self-assembly

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Naturally occurring materials have been always inspired scientists, who tried to either replicate or mimic their structural features. Examples include gutta-percha, wood, opals, bones and nacre. Wood has been the construction material of choice for centuries. Its porous anisotropic fibrous microsctructure is mainly responsible for its properties. Nacre, on the other hand has gained considerable interest in the last few years. In this work we demonstrate how ceramic-polymer composite materials bio-inspired by the structure of wood and nacre can be prepared by means of magnetically drive self-assembly of magnetic nanocolloids. The preparation of such materials consists of two steps. First a monolithic skeleton of silica is created, with the desired microstructure, and subsequently reinforced by butyl acrylate-based polymer. The silica skeleton is produced via a modification of the magnetically controlled phase separation in sol-gel systems previously developed in our laboratory [1]. In this process polymer-magnetite nanoparticles produced via miniemulsion polymerization are dispersed in an acidic solution where a silicon precursor has been previously hydrolysed. The obtained solution was then transferred to a mould and placed between the poles of an electromagnet. The application of a static magnetic field during the silica sol-gel transition leads to the formation of a silica monolith composed of elongated fibre-like structures, similar to the hard skeleton of wood. Instead, the application of a rotating magnetic field leads to the formation of two dimensional sheetlike structures, resembling the inorganic microstructure of nacre. Afterwards, the monoliths have been first functionalized with 3-methacryloxypropyltrimethoxysilane, and then impregnated with a solution of butyl acrylate and an initiator, before being polymerized. The functionalization of the silica monoliths allows the polymer to covalently bind the silica surface during the free-radical polymerization. The obtained structures have been analysed with SEM microscopy and mechanical compression test before and after the polymer impregnation step.

[1]Furlan M. and Lattuada M., 2012, “Fabrication of Anisotropic Porous Silica Monoliths by means of Magnetically-Controlled Phase Separation in "Sol-Gel processes” Langmuir, 28(34), 12655–12662.

PL-2 Self-Assembly Of Functionalized Organic Molecules On Metal Substrates: Intermolecular Vs. Molecule-Substrate Interactions

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Molecular self-assembly is one of the most promising routes to realize highly ordered molecular structures on surfaces. These structures are interesting from a fundamental point of view as well as for possible applications in organic electronic devices like organic field effect transistor or photovoltaic or as molecular sensors. Usually weak non-covalent intermolecular interactions like hydrogen bonding, dipolar coupling, π-π stacking or metal coordination are employed. Besides the intermolecular interactions, which can be controlled via specific functional groups, also the molecule-substrate interactions play an important role, which are influenced by the corrugation of the adsorption potential, the reactivity of the substrate and its crystal structure. In this talk, I will discuss different examples of the self-assembly of functionalized molecular building blocks on metal substrates. [1] We use scanning tunnelling microscopy and spectroscopy, photoelectron spectroscopy, low-energy electron diffraction and density functional theory calculations to investigate the electronic and structural properties of the self-assembled patterns. In particular, emphasis is placed on the influence of the substrate, which can lead to metal-coordination bonds and to different molecular orientations due to the surface corrugation. Furthermore, I will focus on electronic and structural properties of mixed molecular layers consisting of two complementary molecular building blocks.

[1] S. Gottardi, K. Müller, J. C. Moreno-López, H. Yildirim ,U. Meinhardt, M. Kivala, A. Kara, M. Stöhr, Adv. Mater. Interfaces 2014, 1, 1300025

I-1 Nanoarchitectonics of Au/LDHs self-assemblies: fabrication, properties and specific applications

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Nanosized gold has size-dependent optical and phototermal properties that are of high interest for applications in targeted cancer detection and thermo-therapy. The stability and controlled delivery of gold nanoparticles are key-variables in tailoring nanogold for biomedical applications. We present here nanoparticles of gold-layered double hydroxides (Au/LDHs) as new nanoarchitectures able to incorporate, storage and controlled release nanoparticles of gold. Layered double hydroxides (LDHs) are a class of anionic clays. They have attracted great attention in many technological important fields, such as nanomedicine and nanotechnology, due to their interesting properties in anion exchangeability, adsorption flexibility and biocompatibility [1]. The fabrication of Au/LDHs as self-assemblies is simple and cost effective [2, 3]; it is based on the formation of nanoparticles of Au on the surface of the anionic clay during the structural reconstruction process of the layered clay matrix. Powder X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), high resolution transmission electron microscopy (TEM) and UV-Vis spectrometry (UV-Vis) measurements were used to investigate the structure, morphology and size-dependent optical features of the gold-clay assemblies. Results show that the release profiles of the gold nanoparticles from the clay matrices is influenced by the anionic clay composition. The antimicrobial properties of Au/MgAlLDH and Au/ZnAlLDH against gram-positive bacteria and gram-negative bacteria are also studied.

Acknowledgment: The authors gratefully acknowledge the financial support from the Romanian National Authority for Scientific Research, CNCS-UEFISCDI; project number PN-II-IDPCE 75/2013.

I-2 Growth of strained quantum dots on a patterned substrate

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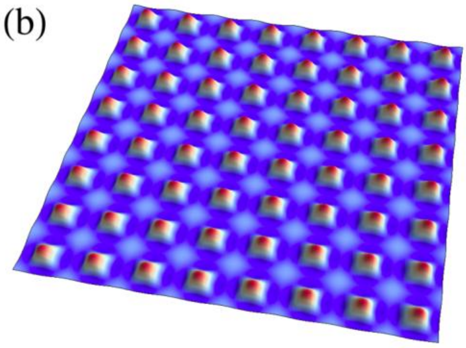
We will present a dynamical modelization of the growth of strained islands on a pattern. We study the morphological instability of a strained film, called the Asaro-Tiller-Grinfeld instability, which occurs on a patterned substrate. The instability, which develops with a characteristic wavelength, is thence influenced by the presence of an external forcing due to the underlying patterned substrate with another wavelength. We find in some conditions that the islands can form in well-organized arrays located either on the peaks or valleys of the pattern depending on the film thickness and ratio of the two characteristic wavelengths.



Quantum dots grown on a pattern

These results are rationalized by a kinetic phase diagram and correlated with the morphology when the islands and the wetting layer grow. We find that the islands may be ordered and homogeneous when their coarsening is significantly slowed down in agreement with experimental observations reported in the literature.

O-1 Investigation of surfaces of drying evaporating microdroplet containing silica and SDS admixtures

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[1]*ON2.2. Group of Laser Spectroscopy, Institute of Physics of Polish Academy of Sciences, Al. Lotnikow 32/46, Warsaw, Poland*

We analyze the intensities of the copolarized and cross-polarized scattered light from an evaporating single levitated glycol microdroplet containing 450 nm diameter SiO2 nanoparticles and SDS (Sodium dodecyl sulfate) admixtures. In particular, we focus on the temporal changes of the interaction of elastically scattered light with the surface of an evaporating microdroplet of suspension undergoing nano-spherical aggregate formation. As the liquid evaporates, we observe successive stages of drying processes manifested in the light scattering properties [1] : from light scattering on clean liquid droplet surface (evidenced by whispering gallery modes) to a rapid increase of scattered light accompanied by light depolarization (speckles) on the spherical aggregate. The nanoparticles ordering process on the surface of the evaporating microdroplet can be described as a first-order phase transition like the analogous transition of the atoms or molecules from the gas phase to a liquid or the solid. We present the analysis of the surface phase transitions using the intensities of the copolarized and cross-polarized scattered light via surface pressure isotherms and the temporal evolution of the droplet radius.

[1] G. Derkachov, K. Kolwas, D. Jakubczyk, M. Zientara and M. Kolwas, "Drying of a Microdroplet of Water Suspension of Nanoparticles: from Surface Aggregates to Microcrystal". J Phys Chem C 2008; 112:16919–23

O-2 Janus nanoparticles and nanobowls synthesis

Florian Guignard[1], Marco Lattuada[1]
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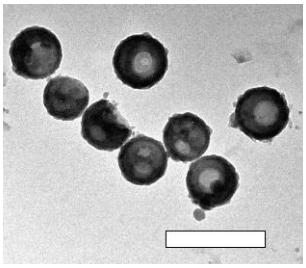
Over the last year, researchers dedicated many efforts to synthesize anisotropic materials. In the field of nanoscience, Janus nanoparticles are a topic of choice, as these nanoparticles possess properties which strongly differ from their isotropic counterparts. Here, we report the synthesis of shape-anisotropic, asymmetrically functionalized polymer nanoparticles. These dumbbells have been synthesized via a multistep synthesis [1]. Monodispersed seeds polystyrene nanoparticles are first coated with a hydrophilic layer, which contains silane moieties coming from 3-trimethoxysilylpropylmethacrylate (MPS). Upon a second swelling step followed by polymerization, the newly formed polymer chains bulge out and give birth to a second hemisphere. The resulting dumbbells are not only shape anisotropic, but have also a different surface chemistry on the two lobes, as just the first one contains silane groups. This particular feature is of great importance, as it permits to perform selective reaction on one hemisphere only. [2] One possible option is to use this asymmetrically functionalized dumbbels as template for silica nanobowls.



Transmission electron microscope image of silica nanobowls obtained
by dissolution of the polymer template. Scale bar is 500 nm

In stöber-like conditions, a silica precursor like tetraethylorthosilicate (TEOS) can be hydrolyzed and condensed on the first hemispheres only. The polymeric template can be removed, giving birth to silica nanobowls bearing a clear defined hole. This is a consequence of the TEOS being only condensed on one hemisphere, and having the junction between the two lobes as the precursor for the nanobowls hole. Moreover, the composition of the inner wall of the nanobowls can be made different, depending on how the polymeric template is removed. By calcination at 550°C, all the polymer chains are burned, and the resulting nanobowls are made of pure silica. By dissolving the silica-coated dumbbells in tetrahydrofuran (THF), the polymer chains which are covalently bounded to the silica via the MPS molecule will remains, and a small hydrophobic polymer layer is therefore present on the inner wall of the nanobowls. The difference between the two type of nanobowls prepared has been analyzed by elemental analysis, thermogravimetry and spectroscopy techniques

[1] Dufresne et.al, J. Am. Chem. Soc., 2010, 132, 5960-5961
[2] F. Guignard, M. Lattuada, Chimia (Polymer and Colloid Highlights), 67, 829, 2013.

O-3 Influence of the potential barrier on the breakage of colloidal aggregates under external shears

Zhiqiang Ren[1], Marco Lattuada[1]
[1]*University of Fribourg, Adolphe Merkle Institute, Marly, Switzerland*

In this work the effect of interactions between particle-particle and particle-fluid on the breakage of colloidal clusters was investigated. The understanding of these phenomena is of crucial importance to better design nanoparticles redispersion and coagulation processes. The colloidal aggregates under simple shear and extensional flows were analyzed by means of Stokesian Dynamics simulation. A library of clusters made of identical spherical particles covering a broad range of masses and fractal dimension values (from 1.8 to 3) have been generated by means of a combination of several Monte-Carlo methods. The hydrodynamic interactions among the particles have been accounted for by Stokesian Dynamics. DLVO theory has been used to describe the interparticle interactions, while contact forces, described by means of discrete element method, have been included to provide the clusters with realistic structural rigidity. The aggregates breakage process was investigated by exposing them into a well-defined simple shear and extensional flow fields. To investigate the evolution of aggregate size and morphology, respectively, the mean radius of gyration and the cluster fractal dimension were monitored during the breakup process. Considerable attention has been given to understand the effect of electrostatic repulsive interactions on both the breakage rate and cluster fragment mass distribution. The breakage rate of clusters was found to be controlled by the potential barrier between particles that was dominated by DLVO theory. Finally, a semiempirical exponential equation that related to potential barrier and the breakage rate has been proposed.

O-4 Ultrafine patterning of functional groups on polymeric surfaces using nano-capillary atmospheric pressure plasma jet

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[2]*Science Department, University of Agricultural Science and Veterinary Medicine , Iasi, Romania*
[3]*Graduate School of Science and Technology, Shizuoka University, Hamamatsu, Japan*

The advantages of plasma processing for surface functionalization are numerous, including the ability of treating various materials of different sizes and shapes, bulk properties and for different purposes, with a friendly environmental and low cost aspect when using low temperature atmospheric pressure plasmas. In this work we present results of amine groups functionalization of patterned micro sized dots. The functionalization is realized through plasma reactive species. Dotted or line patterns are produced using a 3D automatically controlled stage. Two step process was applied: in the first step the polymer surface is activated by applying a helium discharge and bias on the substrate under the polymeric sample and in the second step the treatment using a mixture of helium and ammonia and has the role to functionalize the polymeric surface by introduction of amino groups.

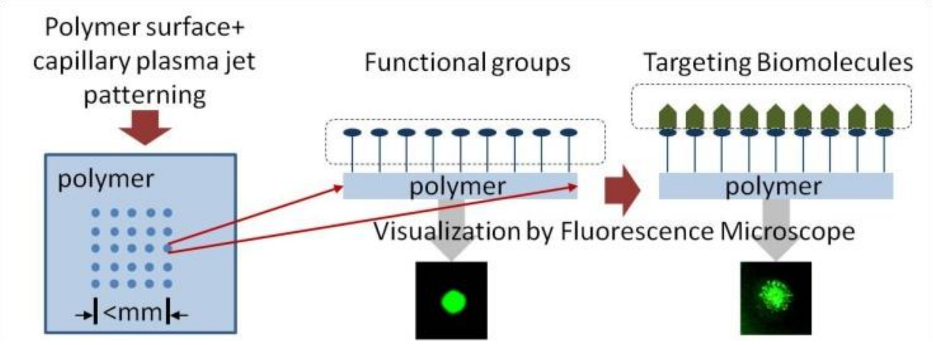

Figure 1 Schematic of patterned functionalization.

After producing the functional patterns on polyurethane sheet, the samples are analyzed by chemical derivatization and fluorescence microscopy to determine the number of the functionalities per processed area (Fig.1). We show that the density of reactive amine functionalities introduced on the surface can be controlled by adjusting the pretreatment time and monomers produced in the discharge. The size of the patterns can be controlled by adjusting treatment parameters. After functionalization, the possibility of using the patterns as biosensors is successfully proven by fluorescent dye labeled sugar chain connection to the patterns.

P-1 ZnO hollow microspheres using electric discharge plasma

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[1]*Physics, Alecu Russo State University, Balti, Moldova*

The paper describes some original experimental results obtained by applying the method of synthesis of zinc oxide structures in plasma. Crystal structures of ZnO in the shape of hollow microspheres with sizes 50-200 μm with transparent walls are presented for the first time. The device construction and technology through which the synthesis was performed were described. Photoluminescence spectra study results, surface morphology and crystalline structure of the obtained microspheres are presented.

1. Aurangzeb Khan, Wojciech M. Jadwisienczak, Martin E. Kordesch, Physica E, v.33, 2. 2. O. Lupan, L. Chow, G. Chai, A. Schulte, S. Park, O.Lopatiuk-Tirpak, L.Chernyak, H.Heinrich, Superlattices and Microstructures, v.43,2008.

TOPIC 13

Art, Science and Technology

PL-1 NANO Culture - Subculture NanoArt

Cris Orfescu[1]
[1]*Art / Science / Technology, Nanoart 21, Los Angeles, California,*

This attempt to introduce NanoArt goes back in time to the first uses of nanomaterials and nanotechnologies to create art and continues with the beginnings of NanoArt. Then, it follows a status on this new artistic-scientific discipline and the movement that evolved from recent technological developments in the multidisciplinary area known as nanotechnology. “NANO Culture - Subculture NanoArt” defines the scope of NanoArt and the ways nanoartists incorporate modern science into their art. The presentation informs about the international juried NanoArt competitions, introduces NanoArt 21, an emerging art group founded in 2004 and dedicated to art and science collaborations worldwide, displays select NanoArt works, and finally presents a few thoughts of several nanoartists and art people.

PL-2 Art Science

Michaela Pelusio[1]
[1]*Residence SEA, Crete Greece*

The separation of art and science initiated on the Renaissance it's redundant!

We are living an interdisciplinary century where sometimes it is difficult to distinguish between techno-scientific research and art.

How artists and researchers inform each other and collaborate?

The recent advances in science such as neuroscience, nano engineering and the philosophical implications of Quantum mechanics, Synthetic Biology and so on may spur new artistic methods and visions. For science, art plays an important role in allowing citizens to understand new scientific discoveries; Art can visualize bizarre scientific models and theories. On the other hand, scientific discoveries promise new artistic expressions and experiences.

In this talk Michela Pelusio will show her own work *SpaceTime Helix*, a kinetic sculpture developed as a sonic and visual instrument. SpaceTime Helix is a spinning standing wave in a white string, forming a large helicoid up to the roof. The helix surface is bright transparent, with waves running over it, disappearing into the past. More and more distant in space-time.

Standing waves are common in modern physics, like string theory and quantum mechanics. In quantum mechanics the energy levels of a particle are standing (quantum mechanical) waves. In string theory particles themselves are strings in many space-time dimensions and the different types of particles are the different standing waves. With String theory they try to understand the origin of the universe. Why do we have particles, why do we have space time? String theory is really complex mathematics and hard to understand, and unfinished work. In string theory every type of particle is another type of standing wave.

I-1 ARS analogon rationis: the confutation of a dichotomy

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[2]*Aesthetics, Brera School of Fine Arts, Milan, Italy*
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Deeply rooted within the realms of time and necessity the human existence has always fathomed different possibilities to tackle the difficulties of life and quell the anguished related to the hardships of living. Since the appearence of the accomplished human creature, Art and Science have been two of the priviledged fields for the human to extend his most creative performances, aiming at a better life in all of its aspects. These two tenets in a lifelong period actually accompany both the acts and the thinking of the human, are present not only in a practical way, but also as a speculative possibility in everyone. Nevertheless, since many centuries, and in circumstances alien to the nature and substance of their deep connection, these two disciplines are aways seen as expressions of two radically opposit realms of the human social and intellectual existenceOne of the arguments raised to underline the “technical” differentiation between Art and

Science throughout the centuries is that whereas the scientific research is a sensible and organized procedure for the verification of facts, the artistic work implies mostly emotions; that is to say volatile situations based on the circumstantial and disorderly influence of the sensorial and mental faculties of Man, which provide only affections but no knowledge at all. Nevertheless, both the scientific disciplines—as neurophysiology etc—and the modern tendencies in psychology have proven that the emotions are nothing else than “the connection of the sensation with the belief and the evaluation” (according to the fortunate assertion of R.Nozick). And it suffices to ponder on the way this relation functions and which cognitive procedures implies: true beliefs are built on right emotions, and good evaluations are formed on the basis of good beliefs, and evaluating a belief depends on the rightful emotions, etc. If we are allowed to expand the thought of Wittgenstein, who in his lessons about Aesthetics has advanced the idea that Art is an “open concept”, we could say that what characterizes radically the nature of both disciplines is this "openness" for the (re)construction of the World.

Key words: Art, Science, Cognition, World Construction, Method

I-2 Art in Crystallography: buildings at nano-level

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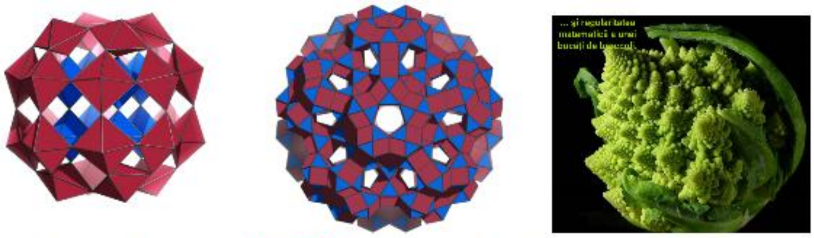
World around is three-dimensional…why we remain on the file of paper, drawing polygons?... since not all regular polyhedra pack to fill the Euclidean space, slight deviations from strict regularity will allow tilings of 3D Euclidean space [1,2]. In minerals, the atoms lie in ‘almost regular’ polyhedra (or their tranforms), what we can name „topological approximants”. Operations on maps allow to draw a huge variety of multi-shell structures, tiled with 3D-polyhedral approximants, instead of polygons.



Oct@Oct$_3$)$_8$_96 Ico@ID@CO$_{20}$@CO$_{50}$@CO$_{60}$_780 Broccoli

Figure. 3D-covering…inspired from Nature

The procedure is inspired fron Nature (see figure) and it ressembes the „lego” play of children...Many of the crystal and quasicrystal structures could inspire the architecture of XXI century...The design of nanostructures was performed by original software packages.

1. M. V. Diudea and C. L. Nagy, eds., Diamond and Related Nanostructures, Springer, Dordrecht, 2013. 2. Bergman, G., Waugh, J. L. T. & Pauling, L., Nature 169 (1952) 1057-1058.

O-1 Visible and invisible structures in the painting „The Creation of the World and the Expulsion from Paradise” (1445) by Giovanni di Paolo

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[1] *, Newcastle University UK and Romanian Academy Iasi branch, , Romania*

[2]*Faculty of Visual Arts and Design, George Enescu University of Arts, Iasi, Romania*

The rediscovery of the canons and constructive techniques used by the masters of the old traditional periods in painting history could offer successful alternatives to the identity crisis of the contemporary art. We analyse the Renaissance painting of the 15th century known under the name of „The Creation of the World and the Expulsion from Paradise”; this composition displays not only the artistic qualities specific to its style, but also the symbolic meaning of the image. The aim of our study is to reveal the internal geometric structure used by the Italian master when painting this pannel, a symbolic procedure that is based on a scheme developed around the three circles emphasized by the round halos of the Creator and of the Angel but also by the concentric circular universe depicted in the left half of the composition. A precise numerical ratio obtained through the expansion of these three circles reveals both the significance and location for all the elements distinguished in this wonderful piece of art.

https://www.youtube.com/watch?v=mYqlJBttHWY

O-2

Art in Transmission Electron Microscopy

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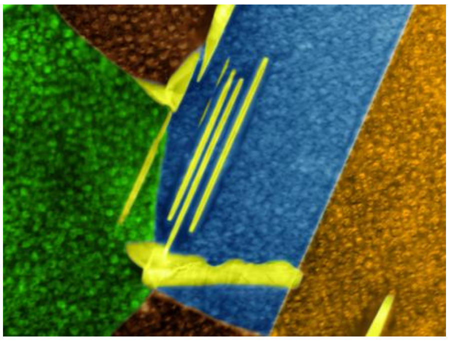
It is said that a picture is worth a thousand words. In science, this means that we can learn a great deal from an image. The image, however, needs to be carefully obtained in order to optimize its relevance and information content, so that it might be truly useful. With the development of advanced scientific imaging and data acquisition equipment, and powerful image-editing software, the new field of scientific art has appeared. In this presentation, we explain how to obtain quality images in transmission electron microscopy (TEM), and show how to optimize images for artistic content whilst retaining scientific content. We start with an overview of how imaging technology can open up our perception of the physical universe, from astronomic to atomic and subatomic scales. We then introduce the electron microscope, and give a basic outline of its design and operation. TEM is used to study the microstructure of materials, and with appropriate specimen-preparation procedures we can investigate solid samples such as metals, alloys, powders, thin films, semiconductors, carbon-based meta-materials, and organic structures such as cells and proteins.



Colourised image of grains and precipitates in the nickel-based superalloy ATI 718Plus

Information obtained from TEM tells us about crystallinity in the sample, the type of crystal structure and its symmetry, the size of crystal grains, atomic spacing, atomic species, the purity of the crystal, precipitates and defects such as dislocations and interstitial atoms. Traditionally, TEM was limited to 2D imaging, but new technology enables 3D tomographic imaging as well. We show micrographs that demonstrate the capability of TEM for obtaining aesthetically beautiful images that also tell us much about the sample material. And we show how post-processing, using graphical software such as Adobe Photoshop, can be used to bring out hidden details in images, and to colourise images to enhance meaning and to add artistic effects.