Sociedad Mexicana de Ciencia y Tecnología
de Superficies y Materiales A.C.

XI
International Conference on
Surfaces, Materials and Vacuum

September 24 - 28 2018, Playa del Carmen, Quintana Roo, México

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Sociedad Mexicana de Ciencia y Tecnología de Superficies y Materiales A.C.
XI International Conference in Surfaces, Materials and Vacuum
September 24th-28th , Playa del Carmen, Quintana Roo, México

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Dear Colleagues,

From the very beginning the Annual Conference of the Sociedad Mexicana de Ciencia y Tecnología de Superficies y Materiales (SMCTSM, Mexican Society of Science and Technology of Surfaces and Materials) has been an important forum used by the Mexican scientific community for the discussion of scientific and technological topics related to research in the areas of surface and materials science.

In these ocation we are pleased to welcome you to participate in the XI International Conference on Surface, Materials and Vacuum (ICSMV) which will held in Playa del Carmen, Quintana Roo 24th to the 28th of September 2018.

The scientific program of the Conference is divided into plenary conferences, short courses and the different symposia with oral and poster contributions. For the XI edition the symposium of Tribology has returned to the program and we have two invited symposia the Atomic Layer Deposition and Luminescence Phenomena: Materials and Applicationsan effort to bring together experiences for people who have successful constructed a relationship with the productive sector. The SMCTSM is also pleased to o joining the celebration of the IUVSTA 60th anniversay by having a series of talks than will empashise both the diverstiy of the research and also the ever growing importance of women in material science. Additionally, to the scientific program, there is a symposium of Science Divulgation which is a traditional forum for the bringing together of students and the general public with the work undertaken and developed within our Society.

We hope that the efforts of the organizing committee, sponsors and colleagues will result in an interesting friendly meeting, providing the opportunity for closer and new interactions between researchers coming from the diverse institutions.

The SMCTM acknowledge the financial support of Consejo Nacional de Ciencias y Tecnologia (CONACYT) for the realization of XI ICSMV.

The XI ICSMV
Organizing Committee SMCTSM
September 2018, Playa del Carmen, Quintana Roo, México.

XI INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM

PLENARY LECTURES

OPENING TALK

Structural stability, electronic and magnetic properties of bimetallic nanostructures

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I pretend to give an overview of the structural stability, electronic and magnetic structure of magnetic bimetallic nanostructures from the experimental and theoretical point of view. In particular I present an exhaustive study of the structural and magnetic properties of $Fe_{7-n}Pt_n$ bimetallic clusters with n=1, 2,... 7. Based on ab initio density functional theory that includes spin-orbit coupling and graph theory, the ground state geometry, local chemical order and spin and orbital magnetic moments are calculated. We show how the system geometry evolves gradually from 3-d Fe to quasi-planar Pt clusters as a function of n. These calculations show also that SOC is necessary to describe correctly the composition dependence of the binding energy of these nanoalloys. We observe that the ground state geometries on the Fe rich side resemble the *fcc* structure adopted by bulk samples. Furthermore, we observed how the spin and orbital magnetic moments depend on the chemical concentration and order.

PLENARY LECTURE I

Characterization of Defects in Chalcogenide Semiconductors for Photovoltaic Applications

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Chalcogenide semiconductors work surprisingly well as polycrystalline materials in optoelectronic devices, notably solar cells. There has been dramatic progress lately in performance of these devices based on Cu(In,Ga)Se$_2$ ["CIGS"] and CdTe. However, the physical properties of the materials suggest that further progress can be made, especially if they are produced as multijunction devices. This talk reviews some of the recent progress made in understanding the nature of the defects that control performance including point defects and grain boundaries. The talk also illustrates the use of a number of techniques to demonstrate these behaviors, primarily by capacitance and scanning probe methods. However, as time permits a brief discussion will be included on the use of solid state nuclear magnetic resonance for study of defects in Cu$_2$ZnSnS$_4$ ["CZTS"]. The results show a wide spectrum of variations in defect behavior on the atomic scale due to the variety of point defect configurations in CIGS. Replacing some Cu with Ag in CIGS also dramatically changes the behavior, especially in grain boundaries. CdTe is shown to exhibit significant depletion of carriers around grain boundaries when properly treated, resulting in carrier collection into the boundaries. NMR analysis of CZTS shows the presence of multiple phases and point defect structures that can limit device performance. Several relatively well-defined defect states appear in the energy gap of CIGS including a hole trap ~250 meV above the valence band edge, a deep trap near mid-gap, and an electron trap near the conduction band edge. The latter is reduced by alkali halide post-deposition treatment while the mid-gap state is not. The mid-gap state is shown to be localized near the grain boundaries and may be due to dangling bonds.

PLENARY LECTURE II

High-K Dielectrics: A Perspective on Applications from Silicon To 2D Materials

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In the 1990's, research accelerated on addressing the limits of the industry standard gate dielectric: SiO2. With the most aggressive integrated circuit scaling, it became clear that standby power for MOSFETs required the insertion of a gate dielectric material that reduced tunneling leakage while enabling performance expectations. Leveraging prior dielectric research and after exploring several dielectric material candidates, [1,2] Hf-based dielectrics became the dominant choice and were established in commercial Si technology fabrication processes in 2007 after at least a decade of research. [3] Although perhaps forgotten among today's 3D FET technologies, the introduction of a new gate dielectric, simultaneously with metal gate materials, was considered quite revolutionary in its day, and this development, in conjunction with other device engineering aspects like strain, enabled the continued march of the industry along Moore's original predictions. Since that time, the research on incorporating high-k dielectrics has expanded to address alternative channel materials including Ge, III-V, wide band gap semiconductors, and, most recently, perhaps the ultimate limit in channel scaling – atomically thin 2D materials. [4] This talk, from the author's perspective, will review some of these developments and provide some context on the resilience of the materials research as well as the challenges and opportunities that lie ahead. [5]

This work is supported in part by a ConTEX grant from the University of Texas System and the Consejo Nacional de Ciencia y Tecnología de México (CONACYT), US/Ireland R&D Partnership (UNITE) under the NSF award ECCS-1407765, and the Erik Jonsson Distinguished Chair in the Erik Jonson School of Engineering and Computer Science at the University of Texas at Dallas.

[1] J. Robertson and R.M.Wallace, *Materials Science and Engineering* R, **88**, 1-41 (2015)
[2] G.D.Wilk, R.M.Wallace, and J.M.Anthony, *Journal of Applied Physics* **89** 5243 (2001)
[3] M.T. Bohr, R.S. Chau, T. Ghani, K. Mistry, *IEEE Spectrum*. **44** (29) (2007).
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PLENARY LECTURE III

"Brilliant Nanodiamonds"

G.E. McGuire and Olga Shenderova

Nanodiamonds (ND) have a unique combination of chemical and physical properties making it a true platform material for a wide range of applications. Produced in large volume by a number of techniques including high-pressure high-temperature (HPHT) and detonation (DND) synthesis, they are readily available from a number of sources at prices which are comparable to that of other carbon-based nanomaterials. Although considered an inert material, ND surfaces are easily functionalized with a variety of groups allowing them to enter into chemical reactions or serve as carriers of chemical agents such as catalysts, drugs and pharmaceuticals. Crystallographic defects based on dopant atoms generated in the core of the particles lead to the formation of color centers with unique fluorescent and spin properties allowing their use in applications that include background-free and long-term cell imaging, super-resolution imaging, correlative microscopy, and magnetic sensors. While micron-sized diamond particles are widely used as abrasives, ND is now accepted as an additive to lubricants and greases as a means of reducing the coefficient of friction and the associated heat build-up and eventually leading to substantial fuel economy improvement. The basis for these applications will be elaborated and examples given

PLENARY LECTURE IV

Shapes (of) Matter

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The properties of crystalline materials continue to be exploited for a very large range of applications. In many cases, it is the bulk properties that are of interest. In the thermodynamic limit, i.e., for sufficiently large systems, these properties are either intensive or extensive depending upon whether they are independent of the system size or proportional to it. In either case, since the boundary regions make up a very small part of the complete system, it may be suggested that the boundary regions are of no importance. On the other hand, the properties of the boundaries themselves can also be of interest for applications. An example is heterogeneous catalysis, in which case the bulk part of the sample is often irrelevant.

These considerations suggest that bulk properties and surface properties are essentially independent of each other and can be treated separately. Theoretical studies of the properties of crystals often utilize this approach. For bulk properties, one typically treats the system as being infinite and periodic, thus completely ignoring the boundary regions. For the study of surface properties, one often constructs a simple model system that contains the surface of interest while ignoring other surfaces as well as the bulk region.

We demonstrate that there is a close connection between surfaces, shapes, and bulk properties of macroscopic, crystalline materials. Thus, the requirement that no atom in the bulk shall experience a force from charges associated with the surface, a requirement we formulate in terms of a generalized Tasker condition, leads to an interplay between the charge densities of different surfaces for a given sample. Thereby, we also demonstrate that so-called polar surfaces that often are considered as unstable essentially always can be stabilized, although the details of this stabilization then depend on all surfaces of the sample, i.e., on the shape of the material. The consequences of this interplay are studied through one property that usually is considered a bulk property, i.e., the polarization / dipole moment per volume, and one property that usually is related to surfaces, i.e., the activity of a surface in heterogenous catalysis. Our theoretical findings are illustrated through results of model calculations that are demonstrated to provide useful information.

Preliminary results have been published in:

M. Molayem, M. Springborg, and B. Kirtman: *Surface effects on converse piezoelectricity of crystals,* Phys. Chem. Chem. Phys. **19** (2017) 24724-24734.

M. Springborg, M. Zhou, M. Molayem, and B. Kirtman: *Surfaces, shapes and bulk properties of crystals.* J. Phys. Chem. C **122** (2018) 11926-11932.

PLENARY LECTURE V

Progress in understanding of plasmas in solids upon ultrashort laser action on transparent materials

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When powerful ultrashort laser pulses couple with the surface or bulk of dielectric substances, they create very dense but relatively cold free-electron plasma, a forerunner of laser-induced structural modification of materials. Nowadays the techniques employing laser-induced structural modification of materials experience tremendous development with applications in various fields ranging from electronics, photonics, and information storage to microfluidics and biomedicine. However, still direct laser writing is mainly based on intuitive experience and experimental explorations. Due to the extreme complexity of free-electron plasma development, its evolution during irradiation and post-irradiation relaxation followed by material matrix structural transformations, many physical phenomena observed upon ultrashort laser action on bandgap materials are poorly understood or even misinterpreted. In view of the absence of experimental diagnostics for monitoring these phenomena with femtosecond temporal resolution and, simultaneously, sub-micrometer spatial resolution, adequate theoretical models, which would enable to simulate laser-induced processes in optical glasses and crystals and even in water for the aims of laser surgery, are of high demand.

In this talk, one of the most advanced approaches for simulations of laser energy coupling into transparent material under the regimes of direct laser writing of 3D photonic structures will be presented with various examples of its applications to real experimental conditions. The main emphasis will be done on the possibility to localize and control laser energy absorption by matter for production desired structural changes. The whole chain of the processes which are triggered by laser pulse and continuing until the final imprinting of a modified structure into material matrix will be analysed in details that will be started from analysis of production of highly non-equilibrium dense plasmas in the regimes of warm dense matter. Kinetic pathways of plasma generation and evolution will be critically reviewed for single and multi-pulse irradiation regimes used in the experiments. Recent advances in understanding of several unexplained phenomena will be reported with underlying the dominating role of dense non-equilibrium plasma conditions. Finally, questions which remain unaddressed in this field will be discussed.

PLENARY LECTURE VI

Fundamental Properties of TM Nitrides:
Materials Design Strategies For Extreme Properties

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Physics Department, Linköping University, Linköping, Sweden
Mat. Sci. Dept, National Taiwan University of Science & Technology, Taipei, Taiwan

Transition-metal (TM) nitrides exhibit an enormous range of properties and offer a smorgasbord of opportunities for materials scientists. Cubic TM nitrides have wide single-phase compound fields that can be exploited. We show results for vacancy hardening in 3d Group-IV $TiN_x(001)$ and Group-V $VN_x(001)$; the hardness H (and resistivity ρ) of epitaxial layers increases, while the elastic modulus E and the relaxed lattice constant decreases linearly, as x is decreased from 1.0 to 0.67 and 0.80, respectively. In contrast, H(x), E(x), and $\rho(x)$ for 5d Group-V $TaN_x(001)$ remain constant due primarily to the presence of isoelectronic antisites.

All Group-IV TM nitrides, TiN, ZrN, and HfN, are very good metallic conductors with room-temperature resistivities of 12-14 $\mu\Omega$-cm. 3d Group-III ScN(001) is a transparent semiconductor with an indirect Γ-X gap of 1.3 eV. Reflectivity measurements from $Sc_{1-x}Ti_xN(001)$ layers show TiN is strongly reflecting up to the reflectance edge at $\hbar\omega_e = 2.3$ eV, while ScN is transparent, and $\omega_e \propto x^{0.5}$ for the alloy. ZrN is intermediate with $\hbar\omega_e = 3.04$ eV. Thus, hard decorative coatings can be obtained with a wide palette of colors.

Superconducting transitions T_c for the Group-IV TM nitrides range from 10.4 K for ZrN to 9.18 K for HfN to 5.35 K for TiN. For comparison, superconductivity is not observed for the Group-IV rare-earth (RE) nitride CeN. These results are consistent with electron/phonon coupling parameters of 1.11 (ZrN), 0.82 (HfN), 0.73 (TiN), and 0.44 (CeN). The acoustic phonon modes soften monotonically with increasing cation mass; optical mode energies remain approximately constant for the TM nitrides, but are significantly lower for the RE nitride due a lower interatomic force constant.

The extreme range of materials properties available in TM nitrides and related systems can be enhanced through the formation of self-organized superhard nanostructures consisting of commensurate nanolamellae, nanocolumns, nanospheres, and nanopipes.

An issue with hard ceramic films, however, is that they are typically brittle, leading to failure by crack formation and propagation. We show several approaches to obtaining TM nitride layers that are both hard *and* ductile (i.e., tough). IV-VI and V-VI alloys, e.g. $Ti_{1-x}W_xN$ and $V_{1-x}Mo_xN$, exhibit dramatic delocalization of electron density leading to a more ductile response to shear stress while exhibiting increased hardness under tensile and compressive loading. Vacancy-induced toughening is also observed in under-stoichiometric $(V,Mo)N_x$ alloys.

PLENARY LECTURE VII

Non-hydrolytic sol-gel chemistry to functional hybrid materials

Nicola Pinna
Humboldt University of Berlin, Germany

The current trend in various energy applications, ranging from lighting to batteries and electrolizers, lays in the control of structural, physicochemical and morphological properties of materials and their interfaces.

During this presentation, recent strategies for metal oxide and metal fluorides synthesis and nanostructuring targeting energy and environmental applications will be discussed. Especially, we will focus on one-pot strategies for the fabrication of hybrid materials by non-hydrolytic sol-gel chemistry focusing on the importance of the organic-inorganic and inorganic-inorganic interfaces.

Among the examples presented we will discuss the synthesis of downconverting white emitting phosphors based on photoactive boehmite nanoplatelets coated with an organic conjugated moiety acting as the sensitizer and the fabrication of complex metal fluorides nanostructures for applications in energy storage and conversion.

We will see that nowadays the non-hydrolytic sol-gel chemistry allows a control in terms of composition, crystalline structure, morphology and nanostructuration that would have been unimaginable just few years ago.

PLENARY LECTURE VIII

Interface design of metallic alloys for harsh environments

Tomas Polcar
Materials Science and Tribology at Engineering and the Environment
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Interface design of alloys opens new possibilities and promises materials with unrivalled properties, such as strength, toughness, or thermal stability. High density of interfaces is often beneficial, which led to development of nanograin alloys and nanolaminated materials.

Here we present two approaches to develop alloys for challenging working conditions. The first is nanolayered metallic alloy, which is tolerant to radiation damage and, in particular, designed to withstand high level of He implantation. The alloy was produced by magnetron sputtering in the form of Zr/Nb multilayer with a periodicity in the range 6 – 167 nm. Combination of transmission electron microscopy and nanoindentation indicated need to improve standard models (e.g. confined layer slip) due to crystallographic change in thinnest multilayers. The actual strength at these smaller length scales was effectively quantified by taking these structural aspects into account in the interface barrier strength model; further insight was gathered from molecular dynamics simulations of indentation. The alloys were then subject to irradiation (gamma, protons) and high energy implantation (He, C, Si, Cu) and the effects of radiation damage on mechanical properties are discussed in detail. The real interfaces obtained from experiments were used as an input for ab initio simulations to explore He mobility in the vicinity of Zr/Nb interface.

The second approach addresses unwanted grain coarsening of nanograin alloys at higher temperatures. By selective alloying and grain size control of binary metallic alloys, theoretical predictions promise existence of thermodynamically stable nanocrystalline alloy. We will critically discuss the prediction ability of such models and, in particular, investigate high temperature properties of some promising alloy candidates.

PLENARY LECTURE IX

Nanoscale pattern formation: an interplay between hard and soft condensed matter physics

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The study of pattern formation —namely, the emergence of a regular structure from a homogeneous medium which is perturbed by an external agent driving it out of equilibrium— has its roots in (macroscopic) contexts traditionally regarded as instances of soft condensed matter, such as fluids, chemical reactions, and even biological systems. However, the advent of high-resolution analytical and observation techniques has allowed to elucidate the occurrence of quite similar phenomena also in the context of traditional hard (solid state, microscopic) condensed matter systems. This fact has basic implications in terms of the relative economy of principles that governs the self-organization of matter. Within Nanoscience and Nanotechnology, it also has potential for the production of materials with new or enhanced properties, or through more efficient techniques.

This talk will attempt an overview [1] on the interplay between hard and soft condensed matter physics with respect to the formation of nanoscale-sized patterns. Given their relevance at microscopic scales, we will specifically address the nanopatterning of solid surfaces, through techniques like ion-beam sputtering [2] or other. By considering specific examples from seemingly disparate systems like colloidal mixtures, thin fluid films, or granular media, we will illustrate the experimental occurrence within the realm of hard condensed matter, of behaviors which are usually expected in e.g. soft matter, and vice versa. Consequently, a fruitful exchange of concepts and ideas between these two domains of condensed matter physics can be pursued that helps advance our general understanding of pattern formation at large, and potentially enlarge the variety and usefulness of surface nanopatterns that can be achieved in practice.

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2. J. Muñoz-García, L. Vázquez, M. Castro, R. Gago, A. Redondo-Cubero, A. Moreno-Barrado, R. Cuerno, Materials Science and Engineering R: Reports, 46 (2014), 1.

PLENARY LECTURE X

Biomedical Surface Analysis: Recent Developments and Future Opportunities

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Surface analysts have benefited from the significant and numerous advances that have occurred in the past 40 years in terms of improved instrumentation, introduction of new techniques and development of sophisticated data analysis methods, which has allowed us to perform detailed analysis of increasing complex samples. For example, comprehensive analysis of surfaces and surface immobilized molecules with modern surface analysis instrumentation provides an unprecedented level of detail about the immobilization process and the structure of the immobilized molecules. Results from x-ray photoelectron spectroscopy (XPS), time-of-flight secondary ion mass spectrometry (ToF-SIMS), near edge x-ray absorption fine structure (NEXAFS), surface plasmon resonance (SPR) and quartz-crystal microbalance with dissipation (QCM-D) biosensing, atomic force microscopy, and sum frequency generation (SFG) vibrational spectroscopy combined with computation methods such as molecular dynamic (MD) and Monte Carlo (MC) simulations provide important information about surface chemistry and structure. However, even with the advances that have been achieved with these powerful surface science techniques, there still remain many significant challenges for surface analyst. These include characterizing the surface chemistry and structure of nanoparticles, determining the atomic level structure of complex molecules bound to surfaces, 3D imaging of samples, and improved sample preparation methods that maintain materials in a relevant state when using ultra-high vacuum based analysis techniques.

This talk will focus on biomedical surface analysis and how it is has benefited from the multidisciplinary nature of surface analysis. The typical surface analyst is an expert in multiple techniques, surface modification, sample preparation/handling and instrumentation, all of which has us well positioned for addressing future challenges in the biomedical field.

PLENARY LECTURE XI

How to Have Your Cake and Eat it Too: Increased Rate and Ionization in High Powered Impulse Magnetron Sputtering (HiPIMS)

David N. Ruzic, Ian Haehnlein, Jake McLain, Ivan Shchelkanov, Priya Raman.
Center for Plasma Material Interactions, Department of Nuclear, Plasma and Radiological Engineering, University of Illinois at Urbana-Champaign, Urbana IL USA

High Power Impulse Magnetron Sputtering (HiPIMS) has been proven as an ionized physical vapor deposition (iPVD) technique to provide superior film quality and adhesion. The ionization of the target material is done without the use of additional plasma generators through high power densities at the target surface, ultimately increasing the ion flux to the substrate. The incident ions allow for controlled ion bombardment energy leading to superior quality films over that of direct current magnetron sputtering (DCMS). One limiting factor of implementation of HiPIMS in industrial settings is the decreased deposition rates as compared to conventional DCMS. The reduction in deposition rate is believed to be mainly due to the return of ionized target material back to the target surface. The Center for Plasma-Material Interactions has created a patented magnetic field configuration which allows for more ions and plasma to escape the target region, leading to a denser plasma drifting to the substrate. This plasma ionizes more of the sputtered material en route. In addition, when coupled to a new bipolar HiPIMS power supply, the deposition rates and ionization fraction of the flux onto the substrate increase even further. The bipolar supply allows for control, both potential and timing, of a positive polarity pulse following the negative polarity main pulse. The controlled positive polarity pulse expels more plasma and raises the plasma potential. In this way the ions which reach the substrate are given energy equal to that plamsa potential rise. This allows film densification and stress reduction even on insulating substrates, since no bias is needed. This talk will review the work done to date, and show the latest results both for circular and linear magnetron arrangements.

PLENARY LECTURE XII

How sputtering can be used as a nanotechnology for producing nanomaterials

Albano Cavaleiro
University of Coimbra
Coimbra, Portugal

Our idea of nanotechnology is a manufacturing procedure able to fabricate components and parts with nanoscale dimensions. On the other hand, nanomaterials are materials with structural features with nanometric dimensions. In this talk, we would like to discuss our concept of nanotechnology adapted to the coatings deposition using sputtering techniques. We will present several examples showing how we think it is possible to build a coating, possessing some sort of nanostructural arrangement, with specific functionalities by tailoring its structure and microstructure at nanoscale level. The co-existence of different phases with specific properties and shapes in the microstructure of a sputtered coating will allow that during a particular application each phase can give rise to a required functionality. Examples inspired on nature, as well as on very old practices, will serve to explain how sputtering can be used for achieving the specific optical and/or mechanical properties characteristics of those selected cases. The beautiful colors of butterflies, the outstanding mechanical resistance of mussels clams or the diversified colors of Middle Age cathedral windows were the basis of inspiration for our developments of coatings for optical and/or mechanical applications, as decorative or cutting tools fields are good examples.

PLENARY LECTURE XIII

Ultrafast laser-induced phase-change structures in silicon

Yasser Fuentes-Edfuf[1], Mario Garcia-Lechuga[1], Daniel Puerto[1], Camilo Florian[1], Adianez Garcia-Leis[2], Santiago Sanchez-Cortes[2], Javier Solis[1] and ***Jan Siegel***[1]

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Silicon can be considered as one of the pillars the electronics industry has been built on. It owes this position in part to the existence of two structurally different solid phases, having very different physical properties. Upon pulsed laser irradiation, silicon can re-solidify either in the crystalline or amorphous phase, depending on the local supercooling achieved. While this potential has been identified decades ago, it has been mostly employed in applications requiring the transformation of large areas, for instance for the fabrication of solar cells or organic light emitting diode displays. Little work has been done to imprint small phase-change structures.

In this talk, we will provide an overview of our work on amorphous-crystalline micro- and nanostructures written by ultrashort laser pulses. To this end we employ two different strategies. The first one is based on a laser-induced self-organization mechanism that leads to the formation of so-called Laser Induced Periodic Surface Structures (LIPSS). LIPSS are a universal phenomenon observed in metals, semiconductors and dielectrics upon irradiation with multiple short and ultrashort laser pulses. They manifest as self-assembled sub-wavelength periodic surface structures with different symmetries that depend on the processing parameters and are typically formed via ablation. In our case, we are able to prevent ablation and fabricate periodic phase-change structures whose lateral dimensions and thickness can be controlled at will. The second strategy consists in the fabrication of surface – depressed annular amorphous rings with a central crystalline disk. We show that these rings can be scaled in size and stitched together to form arrays with different symmetries, with their unit cells not being confined to circular symmetry. For both fabrication approaches we have studied the dynamics of the phase transformation using femtosecond-resolved microscopy, which enables the identification and duration of the different processes involved, including free electron generation, thermal and non-thermal melting, liquid phase overheating and rapid solidification into the amorphous phase. The applicability of the writing strategy and the monitoring technique to other materials is discussed, together with potential applications.

XI INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM

SHORT CURSES

SHORT CURSE A

QUASES Analysis

Sven Tougaard, University of Southern Denmark,

SHORT CURSE B

Plasma effects in short- and ultrashort-pulse laser processing of materials and in film deposition

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In spite of the fact that more than five decades have passed since the invention of laser, some topics of laser-matter interaction still remain incompletely studied. One of such topics is plasma impact on the overall phenomenon of the interaction and its particular features, including influence of the laser-excited plasma re-radiation, back flux of energetic plasma species, plasma shielding aspects, and massive material redeposition, on the processed surface and deposited films quality.

In this lecture, different plasma aspects will be analysed with comparing laser-induced plasma development in vacuum and ambient gases under short and ultrashort irradiation conditions. The following effects will be considered in detail: dynamics of laser-induced plume expansion with discussion of non-equilibrium plasma kinetics; ion acceleration in the dynamic double layer upon plasma expansion in vacuum or a low pressure ambient gas under film deposition conditions; ambient gas ionization above the target upon material processing with formation of a “plasma pipe”; back heating of the target by both laser-driven ambient and ablation plasmas through conductive and radiative heat transfer; plasma chemical effects on surface processing including microstructure growth on liquid metals; complicated dynamics of the ablation plasma flow interacting with an ambient gas that can result in substantial redeposition of material around the ablation spot. Together with a review summarizing the main to-date achievements in the control over laser-plasma-induced processes, required research directions will be outlined.

SHORT CURSE C

Raman spectroscopy Workshop for chemical and material identification in matrials research.

Richard W. Bormett
Renishaw Incorporated

This workshop will provide a review of the theory and the application of Raman spectroscopy techniques useful to the scientific community. Raman spectroscopy has been proven to be capable of providing material and chemical analyses of samples that may vary in size from the very large to the sub-micron, and that maybe in sealed containers (under glass or plastic). New advances in technology now allow Raman microscopy to be extended from the optical microscopes to AFM and SEM microscopes. Raman imaging supports a number of “fast” chemical and topographical contrast methods that can greatly simplify area composition distribution analysis. There will be emphasis on Raman microscopy, with imaging techniques that reveal layers and material distributions, for example in cells, and advanced materials including composites. A live demonstration of Raman microscopy with 785 nm and 532 nm excitation and the imaging processing and acquisition capabilities of dispersive multi-wavelength Raman system will be available so attendees are encouraged to bring microscope compatible samples.

Richard Bormett has been with Renishaw Inc, Hoffman Estates IL., since 1996 and the Renishaw Business Manager for Raman products since 2000. Richard;s experience with Raman spectroscopy extends to his time at the University of Pittsburgh working with Professor Sanford Asher on new instrument technology for deep UV Raman spectroscopy and vibrational circular dichroism. Richard's interest in vibrational spectroscopy developed during his brief time at UW-Madison's Synchrotron Radiation Center studying the chemistry of photoresists for the Center for x-ray Lithography.

SHORT CURSE D

Introduction to Tribology and Tribotesting

Giovanni Ramirez
Bruker

Tribology is the field that studies wear, friction and lubrication of moving mechanical surfaces that are in contact. To improve the performance of materials and/or lubricants, and also elucidate the mechanisms behind their tribological behavior, different kind of test rigs are actually employed. The challenging part of simulating real world applications is that wear and friction are not intrinsic properties of the materials, but they are system properties. A realistic benchtop tribological test requires the identification of the main factors that are involved in the mechanical system behavior. Here, we are presenting the critical elements of a tribological system, and examples of how to determine those, and in what way to design the finest Tribo-tests. Specifically, we will present and described in detail the different geometries in use to simulate materials under lubricated and unlubricated situations. Additionally, we will show different examples of real applications being simulated at the bench-top scale using UMT-TI.

XI INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM

TECHNICAL TALKS

TECHNICAL TALK I

Atomic Foce Microscopy (AFM) Present a Future Applications in Research

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Atomic Force Microscopy (AFM) is one of the major enabling technology paving the way to today's understanding of surfaces science at the nanoscale.

While a sharp tip with typically less than 10 nm radius is scanned across the sample surface, the interaction forces in the Nanonewton range give insight into surface morphology, surface potentials, incorporated charges or magnetic domains and more.

The first and most direct information AFM gives is the topography. Due to the small involved forces this can be obtained from soft or rigid materials, conducting or insulating surfaces both in air and liquid. Thus AFM can monitor growth processes during electrochemical reaction and reveal structure sizes of soft biological materials under physiological conditions.

In addition to nanoscale imaging, the high sensitivity of the AFM down to the low Pico Newton range allows to measure the tiny forces of molecular interactions of cells and extracellular matrices (force spectroscopy) [1].

Advancements of technology over the last three years allowed to merge microfluidics with the precision of the AFM in the way that a hollow cantilever filled with liquid can be controlled with nm precision to eject or intake liquids in femto liter amounts and all this under full force control. This has expanded the range of AFM as a new tool for deposition or spotting of material as well as single-cell micromanipulation [2-6].

During my presentation examples of contact, dynamic mode, phase-imaging, and force spectroscopy for different materials will be addressed. A live demonstration of FlexAFM will follow where participants can discuss AFM practical hints and measure their own samples. In situ electrochemical AFM on the whole substrat or local deposition through the tip will also be addressed.

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TECHNICAL TALK II

Nuevos desarrollos en XPS en Condiciones de Presión Cercanas a la Ambiental (NAP-XPS)

Alex Marco
SPECS Surface Nano Analysis GmbH

En los últimos 15 años, el XPS a Presiones cercanas al ambiente (NAP-XPS) ha demostrado su prometedor potencial en un amplio abanico de aplicaciones. Partiendo de la catálisis, el foco se ha ido desplazando hacia interfaces solido-liquido, jets de líquidos y procesos electroquímicos in-situ. Inicialmente, los experimentos tenían que llevarse a cabo mediante el uso de avanzadas fuentes sincrotron para alcanzar un numero de cuentas razonable. Pero desde hace un tiempo, el analizador SPECS PHOIBOS 150 NAP ofrece una transmisión optimizada para los electrones, incluso a presiones de hasta y por encima de 100mbar, por lo que los investigadores pueden utilizarlo ahora con fuentes de rayos X y de UV convencionales en sus propios laboratorios. Debido a la ampliación de los ámbitos de aplicación, se pueden obtener ahora medidas de XPS estándares con fuentes de rayos X monocromáticas que ofrecen un funcionamiento estable, spots pequeños de excitación, y densidades de flujo de fotones elevadas, incluso en condiciones de Presión Cercanas a la Ambiental (NAP). La presentación demostrara el uso de sistemas NAP-XPS para medidas XPS automatizadas , así como una amplia variedad de aplicaciones.

XI INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM

SYMPOSIA

ADVANCED AND MULTIFUNCTIONAL CERAMICS (AMC)

Chairmen: Jesus Heiras Aguirre (CNYN-UNAM)

José Trinidad Elizalde Galindo (UACJ)

ADVANCED AND MULTIFUNCTIONAL CERAMICS (AMC)
ORAL SESSIONS

[AMC-2] Processing and characterization of ceramic-based dual-phase membranes for CO2 separation and hydrogen production

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The fabrication and subsequent evaluation of a series of ceramic-carbonate dual-phase membranes for potential application on CO_2 separation is reported. Membranes are made of different ceramic ionic conductor phases such as samarium and copper co-doped cerium oxide-based materials ($Ce_{0.8}Sm_{0.19}Cu_{0.01}O_{2-d}$) and the fluorite-perovskite composite with chemical formula $Ce_{0.9}Pr_{0.1}O_{2-d}/Pr_{0.6}Sr_{0.4}Fe_{0.5}Co_{0.5}O_{3-d}$.[1,2] The research involves the study of the use of graphite powders as pore former during the membrane support fabrication as well as the study of the obtained microstructural features on the permeation properties of the prepared membranes. Disk and tubular-shaped membranes were successfully fabricated. Results show the obtaining of defects free dual-phase membranes exhibiting excellent perm-selectivity properties for the CO_2 separation at high temperatures (700-900 °C). Moreover, the observed stability and separation properties suggest the use of this kind of dense membranes for membrane reactors applications and therefore the production of syngas ($CO+H_2$).

Keywords: ceramic-carbonate membranes, CO_2 permeation, perm-selectivity, pore former.

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[AMC-226] Frequency response measurements of thin film piezoelectric sensors by photoacoustic method.

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key words: piezoelectric sensor, photoacoustic, KNN, $BaTi_3$

We have grown $K_{0.5}Na_{0.5}NbO_3$ (KNN) and $BaTiO_3$ films on $Pt/TiO_2/SiO_2/Si$ substrates by using pulsed laser deposition (PLD) technique. Some prototypic ultrasonic sensors (build with the KNN-thin film and $BaTiO_3$-thin film, and the platinum-gold electrodes over the Si-substrate) are presented. We implemented the photoacoustic technique using laser pulses for the device characterization (Nd:YAG laser system, Ekspla, model: NL303HT/10-SH @10 Hz, and pulse-width of 5 ns), for sensors excitation, obtaining its time responding, over thin films of 230 nm thick for KNN, and 260 nm for $BaTiO_3$, was found (after a FFT transform) that the resonant frequency of KNN sensor is about 3 MHz, however its extends bandwidth above 20 MHz, and the resonant frequency of $BaTiO_3$ sensor is about 2.8 MHz and the bandwidth is 25MHz. The photoacoustic technique is an easy and versatile method to obtain the frequency response of the piezoelectric sensors.

Acknowledgments:

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[AMC-332] Ferroelectric, Dielectric and Raman scattering studies of BNT system doped with Lanthanum

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The effect of incorporation of Lanthanum into Bismuth Sodium Titanate system (x=0, 0.005, 0.01, 0.015, 0.02, 0.05, and 0.1) were investigated by means of EDS, x-ray diffraction, ferroelectric, dielectric, and Raman scattering techniques at room temperature. Firstly, the powders used to make lead-free dense BNLT ceramics were obtained by the sol-gel method using the acetic acid route. The dried xerogel was calcined at 700°C for 1hr afterwards uniaxially pressed at room temperature using a pressure of 320 MPa for 5 min to obtain 10.14 mm diameter and 0.5 mm thick pellets. Finally, all the samples were sintered at 1150°C for 30 min using an effective encapsulation in order to avoid the losses of volatile elements as Bi and Na. SEM and EDS micrographs show that addition of Lanthanum produces a considerable decrease of the size grain from 4.5 to 0.5 μm and presence of small quantities of secondary phases when the concentration of La is ≥5 at. %, which are not possible to observe by x-ray diffraction. Ferroelectric response in conjunction with x-ray diffraction showed a transition from rhombohedral to pseudocubic paraelectric structure where characteristic hysteresis ferroelectric loop disappears, when Lanthanum is added in large concentrations (≥5 at%). The ferroelectric response (remnant polarization (P_r) and coercive Field (E_c)) of BNLT system shows a maximum at 2 at% (P_r=30 μC/cm^2 and Ec=39 kV/cm) respect to pure BNT. The maximum permittivitye E_{max} and depolarization temperature (T_d) showed a gradual decreasing with the addition of La. Nevertheless, dielectric losses features displayed a diminishing of charge carrier concertation as La concertation increased. The phonon anomalies observed in the Raman spectra at room temperature suggest that the BNT system has a structural evolution as the La doping concentration is increased.

Keywords: sol–gel, lead-free ferroelectrics, dielectrics.

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[AMC-376] Effect of α-quartz addition on the physical and mechanical properties of ceramic prototypes

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The effect of the addition of a-quartz in ceramic prototypes formed by uniaxial pressing and sintered at temperatures that varied between 850 – 1050 °C is reported. Compositions of 90-10%, 80-20% and 70-30% were carried out. The morphology of the specimens was studied using Scanning Electron Microscopy (SEM), the chemical and structural composition was evaluated using X-ray Fluorescence (FRX) and X-ray Diffraction (DRX). Finally, the experimental design showed the behavior of physical and chemical properties such as: absorption, contraction, apparent density, resistance to compression and bending. The shape and size of a-quartz grain was decisive in the properties of the material as well as the temperature and composition used. The properties of the material studied reveals it can be used in electronic applications, masonry units and refractory products.

Key words: a-quartz, ceramic prototypes, mechanical properties, physical properties.

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[AMC-397] Photopyroelectric Response in PZT ferroelectric ceramics doped with Niobium.

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$Pb (Zr_{0.53}Ti_{0.47})_{1-.5x/4}Nb_xO_3$ ceramic samples of PZT family doped with Niobium were prepared by the traditional ceramics process using high purity reagents (better than 99.9%). The ceramic samples were sintered in lead atmosphere at 1250°C during 100 minutes. The photopyroelectric response was measured by photothermal method (in which the A.C, signal is measured due to periodic heating of the sample using the incidence of modulated radiation laser). The samples showed high response pyroelectric signal. The Curie temperature determined by differential scanning calorimetry were from 388°C to 363°C, the transition temperature exhibits a decreasing behavior with the Nb dopant concentration. The relative permittivity as a function of temperature were evaluated with an homemade system, using an Keysight 4990A Impedance Analyzer, a heating cell with a 1ºC/min heating rate in the frequency range of 20 Hz to 1 MHz. Hysteresis loops were evaluated using a Precision LC Radiant ferroelectric test system coupled with a Trek amplifier model 609E-6 at 1-4 kV. The thermal transport measurement were determined from 25 to 500 ºC in vacuum conditions, using a Linseis LFA 1000 Laser Flash equipment. Also the crystalline structure of the samples was analysed using XRD.

Keywords: ferroelectrics, dielectrics, PZT.

Acknowledgements: This research was supported by project CB 240460 and (LIDTRA) LN2015-254119 of CONACYT Mexico. The technical assistance of Q. A. Martín Hernández Landaverde, Tec. Augustin Galindo Sifuentes and I. Q. Ma. Carmen Delgado Cruz, are acknowledged.

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[AMC-410] Dielectric and magnetic behavior of BaFeO ceramics doped with Ti

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Powders of high purity oxides have been mixed and synthetized by a solid state method[1] to obtain $Ba (Fe_{12-x} Ti_x)O_{19}$, x = 0, 0.01, 0.03 and 0.05 and sintered on ceramics pellets to study the effect of titanium addition over its dielectric and magnetic properties[2]. Structural characterization, through by DRX studies, shown the presence of barium ferrite phase. XPS survey and high-resolution spectra were obtained for assessment of total and relative composition, respectively. The total composition in atomic percentages (% at.) for each sample at different values of Ti, are consistent with the expected values for Fe and Ti. The relative composition was evaluated from the high-resolution spectra Ba 3d, Ti 2p, O 1s and Fe 2p, showing the expected substitution of Fe^{3+} ions with Ti^{4+} ions. Dielectric characterization was performed by thermal scanning of dielectric permittivity, from 400 K to 90 K; the curves reveal an anomaly near to room temperature, but it shifts at lower temperatures with the Ti insertion. Magnetic properties were characterized by magnetic susceptibility and magnetization hysteresis curves[3]; the thermal scanning curves of magnetic susceptibility, from 400 K to 50 K, show a change in its behavior in the low temperature side that is more significant with the titanium addition. This behavior is analyzed and discussed in this work.

Key words: *Barium ferrite, dielectric permittivity, magnetic susceptibility, magnetization.*

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[AMC-433] Piezoelectric, ferroelectric, and magnetic properties of iron-doped lithium tantalate thin films.

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In this work, magnetic behavior was induced in a Lithium tantalate (LT) thin film by doping with iron ions. LT is an attractive material to study because of its high pyroelectric coefficient which makes it an excellent candidate to be used as a thermal detector and as of its high piezoelectric coefficient with applications in surface acoustic wave devices for radio-frequency filters [1]. Thin films were deposited by RF sputtering. Structural, ferroelectric, and piezoelectric changes were confirmed. X-ray diffraction showed the formation of a polycrystalline phase of LT. Rietveld analysis revealed a diminishing of unit cell volume. Ferromagnetic measurements presented a saturation magnetization of 4.3 kA/m. Amplitude, phase, and piezoelectric coefficient (d_{33} = 51.53 pm/V) were measured using piezoresponse force microscopy. The unit cell volume contraction and the magnetic behavior will be discussed regarding dopant addition. The ferromagnetic response is understood in term of dilute magnetic oxides theory presented by Coey [2].

Keywords: Lithium tantalate, Ferromagnetism, Dilute magnetic oxides.

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[AMC-542] Piezoelectric material for engineering applications

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Since their discovery, piezoelectric materials have been widely used in many daily life applications, from conventional lighters to ultrasonic devices. Nevertheless, the ongoing progress of technology and system's miniaturization bring new exciting possibilities for further applications, such as sensors, actuators, MEMS/NEMS, medical devices, energy harvesting, among others. The progress of these innovations requires a multidisciplinary approach of several scientific fields, such as the synergy of material science and engineering, in order to boost the development of smart devices taking advantage of the properties of advanced materials.

In this talk, we will present a composite of Nb doped PZT with ZrO particles that we have been recently developing for energy harvesting and aerospace applications. We will then discuss new exciting research directions targeted at engineering applications such as smart micro energy systems, piezoelectric self-powered sensors, self-folding structures, artificial muscles and e-skins.

[AMC-547] High permittivity Li, La doped KNNT ceramics obtained by RTGG

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In the search for a lead-free piezoelectric ceramic to substitute hazardous lead-based compounds for technological applications, the results obtained in the study of $(K_{0.44}\ Na_{0.52}\ Li_{0.04})_{0.97}\ La_{0.01}Nb_{0.9}Ta_{0.1}O_3$ ceramics are presented. The ceramic is obtained by solid state sintering from the precursor $NaNbO_3$ synthetized by the reactive templated grain growth (RTGG) technique. X-ray diffraction studies show the coexistence of two crystal phases, orthorhombic and tetragonal, the last one being the more abundant. Dielectric measurements evince the effect of La doping through a decrease in the transition temperatures with respect to those reported for undoped KNN (tetragonal-cubic $T_{T\text{-}C}$= 264^{0}C and orthorhombic -tetragonal $T_{O\text{-}T}$ = 90^{o} C, in our case). The maximum value for the dielectric permittivity is surprisingly high at 6800 at room temperature and 1 kHz. Ferroelectric hysteresis measurements performed at room temperature give $Pr=20\mu C/cm^2$ for the remnant polarization and Ec=9 kV/cm for the coercive field at kV/cm. Piezoforce microscopy (PFM) shows domain switching areas in response to the applied electric field but also non-switching zones where the polarization is either perpendicular to the applied field or non-existent. The hysteresis loop obtained by PFM gives a piezoelectric coefficient d_{31}=164 pC N^{-1} comparable to the best published values of PZT and KNN ceramics.

This work was partially supported by PAPIIT-DGAPA-UNAM Grants IN110315 and IN105317, and CoNaCyT Grant 280309. The authors thank E. A. Murillo Bracamontes, E. Aparicio, F. Ruiz, and P. Casillas for their technical assistance.

ADVANCED AND MULTIFUNCTIONAL CERAMICS (AMC) POSTER SESSIONS

[AMC-3] Chemical synthesis of CeO2-based catalysts for soot combustion applications

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Due to the dangerous environmental impact that results from the emission of pollutants to the atmosphere such as soot, carbon monoxide (CO) and the so called volatile organic compounds, it is mandatory the development of technologies to both protect the environmental as well as the human healty.

Ceria-based oxides and perovskite like materials are both examples of ionic conductor materials. This kind of compounds show the properties for trap and release oxygen ions at structural level. These particular characteristics are the result of the redox behavior of the cations in the material; for example the Ce^{3+}/ Ce^{4+} transition in ceria. The aforementioned properties give place to the obtaining of oxygen vacancies as point defects in the materials structure and therefore, this kind of materials are able to be used as oxidation catalysts[1,2].

This work is about the advanced chemical synthesis and characterization of a series of ceria-based solid solutions from the CeO_2, CeO_2-ZrO_2 and CeO_2- Y_2O_3 systems.. Furthermore ceria-based phases were decorated with Fe_2O_3 or CuO oxides as active phases. Moreover it is reported the catalysts application and evaluation on the soot combustion reaction.

Keywords: soot combustion, catalytic oxidation, ceria-based ceramics.

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[AMC-15] Study of the thermal stability of lithium zirconate by the combustion method

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Lithium ceramics are applied in different fields of science. However, one of the main fields of investigation of these materials is intimately related to the production of nuclear energy. Some lithium ceramics, such as lithium oxide (Li_2O), lithium aluminate ($LiAlO_2$), lithium silicates (Li_2SiO_3, Li_4SiO_4 and $Li_2Si_2O_5$), and lithium zirconates (Li_2ZrO_3 and Li_8ZrO_6), have been proposed as possible tritium generating materials for the operation of nuclear fusion reactors.

The research effort on these materials has basically focused on four compounds: Li_2O, g-$LiAlO_2$, Li_4SiO_4 and Li_2ZrO_3.

Here, we report the production of lithium zirconate using the modified combustion technique, the precursors that were used for the synthesis of the material were Lithium Hydroxide (LiOH), Zirconium Dioxide (ZrO_2) and Urea (CH_4N_2O) with relation molar 1:1:3 respectively, then an experimental design was carried out in which the obtained powders were subjected to different temperatures (900, 1100, 1300 and 1500 °C) and times (1, 2, 4, 8 and 16 h) to perform the thermal stability study. Its characterization was carried out by means of X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermogravimetric analysis (TGA).

According with SEM, it was observed that the structure of the ceramic is made up of granules that measure between 1 and 2 micrometers of diameter. The XRD results, it was observed that the ceramic has a tetragonal crystalline arrangement and the TGA results showed different processes (dehydration, dehydroxylation and decarbonation) that occur during heating.

[AMC-22] Study of the thermal stability of lithium aluminate with potential application for the generation of tritium

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Lithium ceramics have been applied in different fields of study and one of them is related to the production of nuclear energy and therefore have been proposed as possible tritium generators: Lithium oxide (Li_2O), lithium aluminate ($LiAlO_2$) which has three crystalline forms (a, b y g), lithium silicates ($Li2SiO_3$, Li_4SiO_4 and $Li_2Si_2O_5$) and lithium zirconates ($Li2ZrO_3$ and Li_8ZrO_6). But essentially, the γ-$LiAlO_2$ is one of the most studied materials due to its great stability that reaches high temperatures derived from its thermo physical, chemical and mechanical properties.

Therefore, the following work reports the synthesis of γ-$LiAlO_2$ using the modified combustion method that takes 5 minutes to complete, the precursors used were LiOH, Al_2O_3 and CH_4N_2O at a molar ratio of 2:1:3 and at 1000 °C, according to what was reported with the literature. Se realizó un diseño de experimentos variando la temperatura (900, 1100, 1300 y 1500 °C) con respecto al tiempo de calentamiento (1, 2, 4, 8 y 16 horas) to observe the thermal behavior of the lithium aluminate and find the adequate conditions to produce γ-$LiAlO_2$ maintaining its physicochemical properties for its possible application in the generation of tritium.

The resulting material was characterized by XRD, SEM and TGA. According to the results obtained by X-ray diffraction (XRD), the thermally treated material at 900 ° C showed the presence of two phases, a majority phase of γ-LiAlO2 and another phase of AlO3 in a smaller amount, however, when the temperature reached 1100 ° C, a purer phase of γ-LiAlO2 was observed, but a new phase of LiAl5O8 appeared, of the results obtained by SEM, the sample treated thermally at 1100 ° C presents a morphology of clear, elongated and carved crystals. Finally, through TGA weight losses of γ-LiAlO2 were observed between 100-200 ° C due to dehydration, 400-600 ° C due to dehydroxylation and 600-800 ° C due to decarbonation.

Keywords: lithium aluminate, modified combustion, tritium generation

[AMC-88] Synthesis of lithium silicate by the combustion method with potential applications in the absorption of carbon dioxide

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Lithium ceramics have proven to have favorable properties for their application in science and technology. The latest studies have focused on the application of these materials for the absorption of CO_2. Some ceramic materials such as lithium zirconates (Li_2ZrO_3, Li_6ZrO_7 and Li_8ZrO_6), lithium aluminates ($LiAlO_2$ and Li_5AlO_4) and lithium silicates (Li_2SiO_3 and Li_4SiO_4) have been favorably tested as CO_2 collectors. Specifically, the lithium ortho-silicate ceramic (Li_4SiO_4) has been studied as a potential CO_2 absorber at high temperatures.

Here, we report the synthesis of lithium ortho-silicate using the combustion in solution technique. Li_4SiO_4 was obtained using lithium hydroxide (LiOH), silicic acid (H_2SiO_3) and urea (CH_4N_2O) as precursors. We studied different molar ratios LiOH: H_2SiO_3: CH_4N_2O of 5:1:3 and 6:1:3 and 7:1:3, respectively. The powders obtained were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermogravimetric analysis (TGA). The adequate conditions for obtaining the Li_4SiO_4 phase was a molar ratio of 6:1:3 of the precursors, the obtained powders were heated in a muffle at 1100 °C for 5 min in air atmosphere.

According with the results obtained by XRD, the predominance of the Li_4SiO_4 crystalline phase was observed with small amounts of Li_2CO_3. By SEM a crystalline morphology with grain size of approximately 500 nm was observed. Finally, in the TGA results was possible to identify the absorption process due to a gain in weight due to the absorption of CO_2.

Keywords: lithium silicate, absorption, combustion in solution.

[AMC-98] Synthesis of tungsten trioxide by the modified combustion method with potential application in the degradation of colorants

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Tungsten trioxide (WO_3), also known as tungsten oxide (VI) or volphramic anhydride, is a naturally occurring material in the form of hydrates, which include minerals such as tungstite ($WO_3 \cdot H_2O$), meymacita ($(WO_3) \cdot 2H_2O$) and hydrotungstite (of the same composition as meymacita). WO_3 has several uses, among which it stands out as a pigment in the ceramic and paint industry, in the manufacture of tungstates for X-ray screens, as a gas sensor, as a photocatalyst for degrading dyes in wastewater, among other applications.

Due to the diverse applications of WO_3, the synthesis of this material consist in the recovery of tungsten from incandescent waste bulbs. The filament of the bulbs is made of pure tungsten, it is possible to recover it and at the same time it contributes in the decrease of the waste of bulbs disposed in landfills which contaminate the water, soil and air. The conventional industrial method to obtain WO_3 uses dangerous reagents and long reaction times. Here, we report a novel method called Gelification-Modified Combustion, which is a simple method that does not use hazardous materials since they are used as organic acid fuels (urea, alanine and glycine) and metal nitrates to synthesize metal oxides, this method also uses short reaction times (approximately 5 minutes).

The material obtained was a lemon-yellow powder, which presented the physical appearance of the material of interest. The powders obtained were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). X-ray diffraction (XRD) technique was used to determine the molecular structure of the crystals and identify the various phases obtained, we also performed a scanning electron microscopy (SEM) analysis to obtain information about the morphology and surface texture of the particles, the size distribution of the crystals and the composition of the samples synthesized.

Keywords: Tungsten Trioxide, Modified Combustion Method, Synthesis.

[AMC-191] Synthesis of the (Sr1-x, Yx)2FeNbO6 double perovskite, characterization by diffraction of RX and Mossbauer spectroscopy.

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Polycrystalline samples of $(Sr_{1-x}, Y_x)_2FeNbO_6$ with x=0.00, 0.10, 0.20 and 0.30 were synthesized by the molten salt method [1]. The crystal structure was determined by X-ray diffraction and Rietveld analysis [2]. Mössbauer spectroscopy was used to determine the ionic state of the Fe ions and the internal hyperfine magnetic fields. Considerable reduction of the heat treatment (temperature and time) for the reaction to take place was achieved without the detriment of the quality of the compounds.

[AMC-239] Current effects on atomic displacements and phonon dissipation in hexaboride materials: a Raman Spectroscopy study

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Metal hexaborides are materials characterized by high chemical stability and unique electrochemical behavior. These materials are used as electron field emitters, electrical coatings for resistors, transition metal catalysts, high energy optical systems, and sensors for high-resolution detectors. Due to their unique properties, these materials have been considered for use in several new technologies, including gas storage and separation, as well as solar energy harvesting. In this work, we show the role of an externally applied direct current on the atomic displacements of the boron octahedra in hexaboride materials. We present an analysis of the Raman active modes T2g, Ag, and Eg for single crystals and polycrystalline samples of LaB6 and CeB6. The current applied has a direct effect on the Raman active modes for the four samples, suggesting that the positions of the boron atoms in the octahedra are compromised with the electron flow. Furthermore, at higher currents (I > 3 A), while the single crystals continue exhibiting the same behavior, the polycrystalline samples exhibit higher deformations and phononic dissipation.

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Keywords: Hexaborides, Raman, Electric current

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[AMC-259] Synthesis and characterization Hydroxyapatite (HAp)/metal oxide (TiO2) nanocomposite by sol-gel method assisted by ultrasound in time intervals

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Hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$, (HAp), is a bioceramic material with the ability to chemically bind with bone tissue, making it bioactive. Its similarity with bone, has allowed it to become an alternative as a bone substitute and recent studies show that the incorporation of metal oxides such TiO_2 help improve mechanical properties and adhesion to surface.

The HAp and TiO_2 were obtained by ultrasound assisted sol-gel method, using Ca $(NO_3)_2 \bullet 4H_2O$, $(NH_4)_2$ HPO_4 and $TiOSO_4 \bullet H_2O$ as sources of calcium, phosphorus and titanium respectively. Hydroxyapatite, TiO_2 and composite HAp/TiO_2 powders were characterized by X-ray Diffraction, Raman Spectroscopy, Scanning Electron Microscopy (SEM), Adsorption of N_2 and Tomography. We observed that in all cases the hexagonal and anatase crystalline phases of HAp and TiO_2 respectively are obtained. On the other hand, we found that the ultrasound time to which the material is subjected has a correlation with the increased crystallinity of the samples.

[AMC-324] KNN lead free ferroelectics obtained by high energy milling and sputtering processes

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K0.5Na0.5NbO3 (KNN) is a lead-freematerial with good ferroelectric and dielectric properties[1]. In this investigation, we synthesized KNN ferroelectric ceramics with and without dopants as La3+, Li1+ and Ti4+ to evaluate their dielectric, ferroelectrics and thermal properties in the material. The synthesize process is by mechano-chemical a ctivation of the combination of oxides and carbonates powders and sputtering process deposited on ITO substrate. The chemical precursors for KNN system were K2CO3, Na2CO3, Nb2O5 and the dopants were Li2CO3, La2O3, TiO2. The mechano-chemical process was in two milling stages. Both stages were made in a nylamid container with zirconium balls and pressed in disks of 10 mm, but for the sputtering process a target was pressed in disks of 50.8 mm. Later, the milled powder is calcined at 800 °C for all the materials and sintered at 1080 °C for KNN+ Li1+, 1100 °C for KNN, KNN+La3+ Ti4+ and finally 1120 °C for KNN+ La3+ Li1+ and KNN+La3+. The XRD analysis showed that the samples crystallize in the monoclinic and orthorrombic phases [2]. In ferroelectric properties, we obtained the best value in polarization on the KNN undoped (11.8 μC/cm2) but his relative permittivity value was lowest (302) than the KNN doped (> 302) and showed shifts in Curie temperature. The dielectric permittivity measurements as a function of temperature permit us determine the next crystalline phase transition, monoclinic-orthorhombic (220°C), orthorhombic-tetragonal (280°C) and tetragonal to cubic (410°C). Also the thermal diffusivity were determined as a function of temperature.The films obtained by sputtering showed monoclinic and orthorhombic phases. This films have a thickness around of 250 nm. The transmission-reflection analysis showed semitransparent films with a high transmissionof visible light.

Key words: KNN, lead-free, sputtering.

Acknowledgments

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[AMC-392] Effect of the size of the eggshell particle in the removal of lead, arsenic and mercury in aqueous medium.

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ABSTRACT

Approximately 90% of the chicken egg shell is chemically composed of calcium carbonate ($CaCO_3$), one of the most abundant ceramics in nature produced by living organisms. Its properties have been extensively exploited in recent years in different areas of science. The present investigation made an analysis with particle sizes of 74, 149 and 297 μm of the eggshell and observed the effect on the crystal structure of $CaCO_3$ by X-ray diffraction, the textural properties were characterized by N_2 adsorption where they define adjustments to isotherms of type II and hysteresis of type 3. The functionality in the removal of lead, arsenic and mercury presented better results with a particle size of 297 μm, obtaining removal percentages of 99, 85 and 90% respectively. The adjustments to the models: kinetic of pseudosecond order and isothermal of Langmuir type 2 suggest a chemisorption in a monolayer.

[AMC-438] Sensitive SERS of silice-titania-silver substrate

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Surface-enhanced Raman scattering (SERS) is a powerful tool with high potential for detection of dilute analytes. The developed SERS substrate offers sensitive rapid detection. Nanofibers functionalized by metal nanostructures and particles are exploited as effective flexible substrates for SERS analysis. SERS-active substrates of silicetitania-silver (SiO2-TiO2-Ag) nanofibers were prepared using a simple approach involving sol-gel and electrospinning. We report a simple method for quantitative SERS analysis using SiO2-TiO2-Ag nanofibers as the SERS substrate. Precursors SiO2 and TiO2 were synthetized through the sol-gel method and then incorporated into a polymeric PVP matrix; later they were processed by coaxial electrospinning to obtain fibers with an average diameter of 250 nm. The SiO2-TiO2-Ag structure was demonstrated by Raman, XRD, IR, SEM and EDX. Through infrared spectroscopy it was possible to evaluate the thermal evolution of the sol-gel process. The Titania phase transformation was observed around 800 °C and the hydroxyl group loss was detected between 500 and 800 °C. The presence of two Titania phases, anatase and rutile were analized with DRX. Using Pyridine as probe molecule (1 nM solution), the SERS effect of the scaffold was evaluated, and it was determined that the vibration modes 8a, 8b, and 15 were the most amplified signals with a 3 orders of magnitude factor. With this it was concluded that the Silica-Titania-Silver Scaffold is a feasible as a SERS enhancer.

Keywords: Silica-Titania-Silver, Scaffold, SERS, electrospining.

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[AMC-441] Sol-Gel Synthesis of Lithium niobate Nanofibers by Electrospinning

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Lithium niobate-silica fibers were produced by the combination of the sol-gel method and the electrospinning technique. Two sol-gel solutions starting from niobium-lithium ethoxide ($LiNb(OC_2H_5)_6$) and tetraethyl orthosilicate ($Si(OC_2H_5)_4$) were prepared and then mixed with polyvinylpyrrolidone (PVP); the solutions were electrospun in a coaxial setup. The obtained lithium niobate-silica polymeric fibers had approximately 600 nm in diameter and were then sintered at 800 °C. After sintering the obtained composite, it was characterized by infrared spectroscopy, where the presence of bands corresponding to Si-O, Si-O-Si bonds of silica, and Nb-O bonds of lithium niobate where found. Raman spectroscopy confirmed the composite composition by showing signals corresponding to lithium niobate and silica. The composite was also analyzed by scanning electron microscopy, showing coaxial fibers with a diameter of approximately 600 nm arranged as a fibrillar membrane.

[AMC-518] Low Temperature Magnetic Properties oF Carbon/MnFe2O4 Coreshell Nanofibers

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Key Words: Electrospinning , Manganese Ferrite , Magnetoresistance

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In this work, electrospinning [1] $MnFe_2O_4$ nanofibers[2]were synthesized from precursor solutions composed by 15% wt of polyviniylpirrolidone (PVP), with molecular weight 1300 k, $Fe(NO_3)_3$ 9(H_2O) and $Mn(NO_3)_2$ H_2O in a water and alcohol mixture. As spun nanofibers were calcined at 973 K for 1 h in argon atmosphere to remove the polymer matrix and obtain the desired magnetic Carbon/MnFe2O4 core shell. In order to understand the properties of the Carbon/MnFe2O4, nanofibers were characterized by X ray diffraction (XRD), scanning electron microscopy (SEM), high resolution transmission electron microscopy (TEM) and vibrating sample magnetometry (VSM). $MnFe_2O_4$ pure phase spinel type was found from XRD with crystallite size average diameter of 12 nm. A polycrystalline fiber morphology was determined from the SEM images, with particle average diameter of 34 nm. A high crystallinity was observed from a deep analysis of the HR-TEM images. From the VSM measurements, the magnetic behavior in a temperature range from 50 to 350 K, was determined. The ZFC/FC curves exposed a blocking temperature of 175 K; the hysteresis loops measured at 5 different temperatures showed a characteristic a typical ferrimagnetic behavior, with a maximum magnetization increasing for lower temperature and reaching a value of 84 emu/g. The interest on studying this type of materials arises in manganese ferrite ($MnFe_2O_4$), which is considered highly attractive because it has a high magnetic permeability and high electrical resistance, this last makes it a strong candidate for the electronics and telecommunication industry [3].

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ATOMIC LAYER DEPOSITION SYMPOSIUM (ALD)

Chairmen: Pierre Giovanni Mani González (UACJ)
Edgar López Luna (UASLP)
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ATOMIC LAYER DEPOSITION SYMPOSIUM (ALD)
ORAL SESSIONS

[ALD-208] Daylight white luminescence of GaN thin film synthetized by microwave plasma atomic layer deposition

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Daylight white luminescence of gallium nitride (GaN) thin film deposited in a homemade Microwave Plasma Atomic Layer Deposition (MP-ALD) system are presented. In this work, gallium nitride thin film was synthetized using sequential doses of trimethylgallium (TMG), molecular nitrogen plasma (N_2) and argon such as purge gas. The GaN thin film was grown on silicon wafer (111) at 230 ° C in the walls of growth chamber. The chemical composition of thin film was analyzed by means of X-ray Photoelectron Spectroscopy (XPS), deconvolution of main peaks were performed to identify the different signals of the impurities into the GaN. The band gap was calculated using the results of UV-Vis spectroscopy, assuming that the reflectance in the absorption edge is related to the band gap. The luminescence response was study by room temperature Cathodoluminescence (CL), a broad peak was exhibited which a white emission starting at 390 nm until 760 nm. CIE Chromaticity diagram was used to determinate the correlated color temperature of GaN emission resulting in 5061 K and color purity of 41% for the 564 nm dominate wavelength. A study of the internal signals of the main emission was performed to determine the contribution percentage of luminescence and the defects and impurities which causes these emissions.

[ALD-231] Carbon-Metal Oxides Nanocomposites for Energy and Environmental Applications

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The combination of different nanobuilding blocks in a single heterostructure can lead to materials with improved properties by selecting components with the desired characteristics for a specific application. Carbon-based nanomaterials demonstrated to be highly suitable as support for the elaboration of heterostructures. Atomic layer deposition proved to be a technique of choice for the coating of nanostructured carbon materials. These heterostructures find applications in various areas such as electronics, sensors and energy storage and conversion. Because the chemical inertness of the graphitic carbon inhibits the initiation of ALD film growth, numerous surface functionalization approaches have been investigated in order to provide the required nucleation sites.

The different strategies employed for the ALD onto carbon nanotubes, graphene, graphite and other nanostructured carbon materials (e.g. carbon black, fibers) will be described. The peculiarity of ALD for tailoring the chemical, structural and morphological properties of the deposited material will be discussed.

Finally, in order to highlight the importance of this class of materials, possible applications in energy storage and conversion, catalysis and gas sensing devices are also reviewed.

[ALD-274] Determination of the characteristic times of surface coverage of HfO2 for Si substrates

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Atomic layer deposition (ALD) has been used for electronic devices ensemble. The high quality at the interface and surface allows the use of this technique as a deposition method. But when growing any material, it is important to think in three important points: the aperture-times of each precursor, number of ALD cycles and the surface saturation time. Then, ALD characterization for each material that will be deposit. This work will explain the effect of differente aperture-times of oxygen agent precursor, also the dependence with number of cycles respect to cinetic reaction, and is introduced a basic analytical model to estimate the surface saturation times on thin films produced by ALD procedure. Variying the oxygen agent gives the amount of the active sites for to generate the bond between oxygen and organometallic precursor. The importance of number of ALD cycles is due to the stoichiometric regimen of film and interface. Finally, proposing that the coveraged surface at certain time t, depends on the current density of the number of occupied states, we solve the corresponding set of differential equations which gives us an estimation of the sticking coefficient, depending on the exposure time on each ALD cycle. Then, we contrast our model, cinetic reaction and active sites with previous experimental results in order to validate its effects with the parameters of ALD characterization.

[ALD-277] Characterization of Ta2O5 Growth by ALD

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Thin films deposit by ALD has been growing since this technique offers an exceptional control over the reaction. The precursors are introduced to the reactor trough pulses in defined cycles, the number of cycles allows the thickness control of the deposited film. In addition, this technique offers great uniformity in the deposited film allowing the user to obtain very high quality thin films. Ta_2O_5 is of the interest due its high-K dielectric constant which allows the use of this material in the fabrication of capacitors and many electronic devices used in automotive electronics. The growth of Ta_2O_5 thin films are realized at a temperature range from 275˚C to 450˚C using as precursors Tantalum (V) Ethoxide and H_2O as oxygen source, this kind of deposit depends directly from the inlet pressure of the Tantalum (V) Ethoxide and the temperature which the substrate has in the reactor. The growing rate has been optimized trough the control of the temperature and pressure in the reactor. RAMAN, SEM techniques were used for characterization.

[ALD-378] Structural and Defects characterization of coaxial nanotubes of CNT@ZnO via Atomic Layer Deposition

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The control of impurities or defects generated on nanostructured materials allows the design of materials with desirable properties. Being a wide band-gap semiconductor, zinc oxide (ZnO), and the most attractive 1D nanostructures, carbon nanotubes (CNTs), have been extensively investigated for catalysis and optoelectronic devices. In that sense, this paper reports the synthesis of coaxial nanotubes of CNT@ZnO, by template assisted method and atomic layer deposition (ALD) process, using diethyl zinc as precursor and deionized water as oxidant. Structural and defects incorporation on coaxial tubes CNT@ZnO were studied. XRD, Raman and FTIR were used to validate ZnO deposition on CNTs templates. TEM micrographs confirmed the homogeneous and conformal nanocrystalline coating CNTs surface. Cathodoluminescence shows a low defects concentration, with a NBE emission on as-grown coaxial nanotubes, and a broad low-intensity band, centered at 500 nm, when was annealed in nitrogen atmosphere. By means of HR-XPS, the thermal annealing generates oxygen vacancies on ZnO lattice, as well as chemisorbed oxidized carbon species. The combination of this defects, coupled with a high surface area, gives to this heterostructure a high potential for water remediation which enhance the photocatalytic activity of ZnO.

[ALD-420] XPS characterization and calculation of composition by means of background accurate fitting of HfOx ALD-films nitrided with remote plasma and forming gas

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The understanding of the modification of the structure CMOS of high-k oxides[1] by means of remote plasma characterized by X-Ray photoelectrons spectroscopy (XPS) is a subject of special interest. In previous reports, it has been observed that remote-plasma nitridation improves the electrical properties of CMOS devices of the Si/HfO_xN_y/Altype.[2] With angle-resolved XPS characterization it is possible to observed that soft nitridation with remote plasma replaces an oxygen atom of the hafnium oxide with a nitrogen atom until saturation with composition $HfO_{1.5}N_{0.5}$. Despite these important advances, there is still a problem with a peak in ~403 eV of the N 1s spectrum, this peak that does not correspond to N-Hf bond (~396 eV) and N-Si bond (~399 eV), but it can be attributed to the formation of N-O structures,[3] which are not desirable in the manufacture of devices. We found that forming gas (N_2-H_2@10%) is very promising as a nitridation agent in remote-plasma.[4]

In this work we show the results of nitriding 2nm hafnium oxide films grown by ALD[5]on silicon substrates modified under a remote plasma treatment. The nitridation was carried out with remote plasma LITMAS system coupled with an ultra-high vacuum sputtering system. We studied the effect of time in the incorporation of nitrogen in the hafnium oxide to later characterize it by ARXPS and capacitance-voltage (CV) in a device of the Si/HfO_xN_x/Al type. The best operating condition for the plasma were 2500W of power plasma, 20 sccm of forming gas flow, working pressure of 4×10^{-3}torr and bias -20V.

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[ALD-430] Growth of TiO2 film by ald and peald for use in biomedical implants

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The growth of a homogeneous titanium oxide film on the Ti6Al7Nb alloy was studied for its application in biomedical implants using the tetrakis (dimethylamido) titanium precursor (TDMAT). The growth kinetics, chemical composition, and crystallization behavior of the TiO2 films were compared for combinations of the TDMAT with three different sources of oxygen: a) thermal ALD using H2O, b) plasma-enhanced ALD (PEALD) using H2O and c) plasma-enhanced ALD (PEALD) using O2 plasma at a process temperature of T = 150°C. Excellent step coverage and a clear saturation of growth at 150 °C. was obtained by TDMAT chemisorbed chemical reactions with O_2 and H2O plasma on the surface. Representative growth per cycle (GPC) values at 150 °C were 0.51 Å/cycle for the thermal ALD using water as oxidative precursor. For TiO2-PEALD samples using water plasma and O2 plasma GPC values were 0.71 Å/cycle and 0.52 Å/cycle respectively. The TiO2 films grown using a H2O plasma exhibit the lowest crystallization temperature and have no detectable C impurities. In situ X-ray diffraction measurements were used to test the diffusion barrier properties of the TiO2 layers and proved that all TiO2 films grown using either H2O or O2 plasma are dense and continuous. The same result was confirmed by X-Ray Reflectometry which revealed clear differences between ALD and PEALD samples. From global results, it was possible to infer the main species that can reach the substrate and correlate the as-deposited TiO2 thin film analyses in order to explain the effect of discharge power on film crystallinity and morphology. The global model assumes that the discharge contains several species such as $O^{+\,2}$, O^-, electrons, ground state O_2 and O atoms.

[ALD-454] Effect of substrate polarization on remote-plasma nitridation of TIN/HfO2/Si structures

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It has been demonstrated that nitridation of hafnia in MOS structures improves the device characteristics such as capacitance and leakage current. Photoemission spectra of nitrogen has shown the presence of three peaks at ~ 404eV, 398.4eV and 396eV that can be attributed to N-O, N-Si and HF-N bonds, respectively. The presence of the peak at ~ 404eV has been related to poor electric properties in the metal-oxide-semiconductor devices. It is necessary to find process conditions that could minimize the presence of this chemical species without compromising the density of nitrogen in hafnia.

The aim of this work is to explore the impact on the structural and electrical properties of CMOS structures when different bias voltages are applied to the substrate during remote-plasma nitridation of HfO_2 films. The HfO_xN_y/Si structures were processed in the following way. Standard RCA cleaning was carried out on silicon (100) substrates. Subsequently, a 2 nm layer of HfO_2 was deposited using atomic layer deposition (ALD). The samples were introduced into vacuum to perform the nitriding process. Nitridation of HfO_2 was carried out by remote plasma for 25 minutes, with a flux of 20 sccm, and at 4×10^{-3} Torr. The substrate temperature was fixed at 300 °C; several bias voltages were applied to the substrate (70, 40, 20, -10, -20, -40, -70, -100, -150 & -200 V).

X-ray photoemission spectroscopy experimentation shows that HfO_xN_y/Si samples biased with positive voltages present iron species attributed to contamination from the chamber walls. For negative polarizations, we observed a strong dependence on the voltage of the peaks centered at 396 eV (nitrogen in hafnia) and at 398.4eV (nitrogen in silica); the intensity of the peak at 404 eV remained relatively constant. The composition of the layers of the structure was calculated using the multilayer method, fitting the spectra by means of Voigt line-shapes. Special care was given to the modeling of the background of the Hf 4f spectra, for which the Shirley component was studied in detail.

To evaluate the electrical properties of the film, we fabricate MOS capacitors by means UV photolithography. A 200nm layer of TiN was deposited using sputtering on top of HfOxNy/Si structures followed by wet etching to form $5.625\text{x}10^3$ μm^2 capacitors. Capacitance and the leakage current were measured on the devices.

[ALD-494] XPS study of the composition of HfOxNy films during remote-plasma soft nitridation as a function of nitrogen flow

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High k dielectrics based on transient metal oxides, such as HfO_2, are currently employed for MOS device fabrication. These oxides have excellent properties such as low leakage current, thermodynamic stability, high dielectric constant, large band gap, and compatibility with the current processes used in silicon-based CMOS technology.

It has been reported than species such as In, Ga, and As from InGaAs-based devices migrate from the substrate to the metal gate through hafnia. In this work, soft nitridation of hafnium oxide films using remote plasma was employed to improve its barrier behavior. It has been observed that soft nitridation of SiO_2 films cause the substitution of oxygen by nitrogen to oxygen while keeping its tetrahedral structure. We observed a similar behavior in HfO_2 nitridation.

The silicon p-type substrates (100) were cleaned with the standard RCA process. The oxide film was grown with an ALD Savannah Cambridge 100 tool using tetrakis (dimethylamino) hafnium (TDMA-Hf) and water (Type I) as precursors. The reactor was operated at 250°C with a 20 sccm UHP nitrogen flow as purging gas. Time exposure of TDMA-Hf and water were 0.08s and 0.04s per cycle, respectively [1]. The nitridation process was done using a remote plasma source LITMAS varying the nitrogen flow from 2 to 100 sccm. Our results show a better incorporation of nitrogen in the HfO_2 films at 20 sccm.

X-ray photoelectron spectroscopy (ARXPS) was employed to assess the thickness and composition of the HfO2 films. The analysis required a careful modeling of the background signal. Special care was given to the calculation of the Shirley component of the background of the Hf 4f spectra [2].

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ATOMIC LAYER DEPOSITION SYMPOSIUM (ALD) POSTER SESSIONS

[ALD-40] Photocatalysis time activation of TiOx, TiNx y TiOxNy films growth by atomic layer deposition.

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This work presents an analysis of the photocatalytic time activation and efficiency in TiOx, TiNx y TiOxNy thin films grown by atomic layer deposition (ALD). The study was done using the time-dependent degradation of color units for methylene-blue solutions and inactivation percentages for *E. coli* bacteria, this films have a potential applications in sewage purification. To determine the optoelectronic properties of the films, the optical, structural, surface, and thickness characterizations were carried out by photoluminescence (PL), atomic force microscopy (AFM), and scanning electron microscopy (SEM), respectively.

[ALD-51] Annealing behavior of atomic layer deposited HfO2 films on III-nitrides

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Ferroelectric (FE) materials possess a spontaneous electric polarization that can be reoriented by the application of an external electric field, making them attractive for applications such as non-volatile Ferroelectric Random Access Memory (FRAM), Ferroelectric Field Transistors (FETs) and energy storage/harvesting. Several methods have been reported for achieving the ferroelectricity in HfO_2, such as thermal treatments, growth temperature and cation or anion doping[1]. Another option to obtain the Pca21 orthorhombic phase (ferroelectric phase) is through an epitaxial growth. The lattice mismatch between Pca21 HfO_2 and cubic InN is 1.7%.

In this study, HfO_2 films were deposited on epitaxial cubic III-Nitrides substrates by atomic layer deposition with the substrate temperature varied from 250 to 290°C. After deposition, an annealing in N_2 atmosphere were carried out in order to crystallize the HfO_2 films. Grazing incidence X-ray diffraction (GI-XRD) and Raman spectroscopy were used for the structural phase analyses. The Raman spectrum of HfO_2 films were compared with simulations of the vibrational modes. The thickness of the samples were studied by X-ray reflectivity, and the ferroelectric behavior induced by a polarized coherent light source at room temperature is observed using confocal Raman spectroscopy.

1. Lun Xu, Tomonori Nishimura, Shigehisa Shibayama, Takeaki Yajima, Shinji Migita, and Akira Toriumi, JOURNAL OF APPLIED PHYSICS 122, 124104 (2017)

Keywords: Ferroelectric, ALD, HfO2, epitaxial InN and GaN.

[ALD-62] Atomic Layer Deposition and Characterization of TiO2, TiN and TiN-TiO2 Thin Films for its Applications in Photovoltaic Devices

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The use of hot electrons generated for the decay of the Surface plasmons is a new technology that presents an opportunity for development in technologies of energy transformation.

In the present work, we show the results of a growth and characterization of thin films of titanium oxide and titanium nitride obtained by atomic layer deposition. The thin films were obtained using titanium isopropoxide, ammonia, and water precursors, having 250° C for titanium oxide growth and 325°C for titanium nitride.

The films were grown in a way that we obtained metal-semiconductor and metal-semiconductor-metal junctions. Furthermore, we grew a combination of TiOx-TiN where we used a growth method growing a film of titanium oxide and a separated film of titanium nitride in the same cycle, and so on until the structure was finished. The devices were grown in different substrates including silicon p. type and n-type, showing a better efficiency in the n-type substrate due to recombination in the p-type substrate.

The devices were characterized by Raman spectroscopy, I-V curve, spectral response, external quantum efficiency and scanning electron microscopy. The efficiencies obtained from the data of the I-V curve showed a maximum efficiency of 0.5%. the solar cells exhibited a spectral response in the visible and near-infrared spectrum. We show open circuit voltages between 80 mV and 400 mV with short circuit current between 2uA and 150 uA under one sun.

[ALD-144] Initial growth stages of HfO2 on silicon wafers by ALD and PEALD

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The study Atomic Layer Deposition (ALD) and Plasma Enhanced ALD (PEALD) growth mechanism have the purpose to solve some discrepancies on literature and describe the physical phenomena involved which provide to the thin films reliable electrical properties to apply in semiconductor devices. As is very known, ALD promotes good interfacial properties, as very thin interfacial layer thickness less than 1nm and low density of trapped charges. Nevertheless, the usual deposition temperatures are about 200°C making difficult to use this technique in polymer substrates. In some cases, thin film bulk stoichiometry is not good as consequence of relative oxidant agent low reactivity. PEALD (remote or direct plasma) promotes the reduction of vacancies in bulk thin films because of the high reactive plasma radicals, decrease the deposition temperature or increases the growth per cycle (GPC) at the same temperature of thermal ALD. In Direct Plasma mode increases the crystallinity but has the disadvantage of generate thicker interfaces as consequence of energy interchange between positive ions and surface, lowering the thin film electrical quality. In this work the initial growth stages of HfO_2 using ALD, PEALD and mixed layers with both techniques were studied on silicon wafers cleaned with the RCA procedure and dipped in HF aqueous solution to eliminate the surface native oxide. The resulting treated wafers were exposed to O_2 plasma and water vapor for different oxidizing pulse times in ALD reaction chamber to determine the effect of oxidant agents in the silicon wafer surface. The prevalence of hydrophobic behavior is characteristic of a Si-H surface finished where no native oxide is present, while hydrophilic behavior is related to Si-OH bonds present when native oxide is on the surface. For this reason, contact angle between surface silicon wafer and droplet water is a very good indicator of the surface state and additionally, C-V and I-V response of MOS capacitors were analyzed to find the relationship of trap density, interface layer, bulk stoichiometry and surface roughness of samples taking account the synthesis process and the resulting surfaces at the initial growth stages.

[ALD-161] Aluminum doped ZnO thin films through an unsaturation approach by atomic layer deposition

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Al doped ZnO (AZO) has been currently studied as an alternative transparent conductive oxide in optoelectronics. It shows an *n*-type conductivity, a direct bandgap of ~3.35 eV, and a transmittance >80%. In addition, the availability and low cost of its constituent elements make it suitable to replace In_2O_3:Sn (ITO). AZO thin films have been deposited by different methods, among them; ALD has shown excellent conformality and uniformity due to the self-limiting mechanism of reaction and the surface saturation, which make it attractive for microelectronics. However, one of its disadvantages has been the deposition of complex and unpurified systems. In this work, we used a different operation mode of ALD to explore the current limits reached in the electrical properties of AZO obtained with the conventional ALD nanolaminates doping. This different approach is based on the generation of unsaturated surfaces to promote reaction sites availability for the Al atoms to substitute the Zn positions in the wurtzite structure. This novel growth technique has been called atomic partial layer deposition (APLD). The electrical analysis was developed through Hall Effect measurements to compare differences between conventional ALD and APLD processes. For APLD samples was observed a charge carrier concentration of $3.91\text{x}10^{19}$ cm^{-3} and mobility of 16.1925 cm^2/Vs, with a resistivity of $9\text{x}10^{-3}$ Ωcm^2 of the AZO films, in comparison with the AZO films obtained through ALD nanolaminate, ($\rho=3.1\text{x}10^{-2}$ Ωcm^2, $\mu=9.51$ cm^{-3}, $n= 2.76\text{x}10^{18}$ cm^2/Vs) and the undoped ZnO ($\rho=6.3\text{x}10^{-1}$ Ωcm^2, $\mu=3.74$ cm^{-3}, $n= 2.14\text{x}10^{19}$ cm^2/Vs). These results show that unsaturation approach favors the substitution of Zn^{2+} ions by Al^{3+}. This behavior was related to the presence of free charge carriers as a consequence of the Al incorporation in the wurtzite. The presence of free charge for APLD samples was also confirmed with the optical transmittance measurements for which lower values were obtained in the NIR region. The surface topography was studied using atomic force microscopy along with Kelvin probe force microscopy for surface potential mapping. Clear differences on the surface, compared with the conventional ZnO/Al_2O_3 ALD nanolaminates confirm the ZnO-$Al2O_3$ APLD growth. The incorporation of Al suggests a more complicated mechanism of the doping process by this approach, which could have a great impact on the optical properties, and the chemical stability of the films.

[ALD-325] Effect of oxidation states on Si/Ta2O5 by XPS

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In this work we realized an analysis of X Ray Photoelectron Spectroscopy (XPS) data corresponding to tantalum pentoxide (Ta2O5) through AAnalyzer software. We extracted the information of Ta 2p core level with doublets signal. The analysis revealed four signals which were associated with each oxidation-reduction state of tantalum, namely the oxidation states were 1+, 2+, 3+, 4+, 5+. This work was carried out with the aim of obtaining the quantitative contribution of each atomic species which helped to estimate the stoichiometry of several samples. This analysis gives us an idea about innovation and technology for augmented reality devices or solar cells of Ta2O5.

[ALD-351] Study of ALD reaction mechanism in Si/Ta2O5 by DFT

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In this work we realized a simulation with Gaussian View 5 software through density functional theory (DFT) proofs and varying three Becke parameters and also the Lee-Yang-Parr (B3LYP) correlation for structure optimization to finally obtain Raman frequency. In this reaction mechanism the analysis of tantalum organometallic was obtained using tantalum (V) ethoxide ((CH_3 CH_2 O)_5 Ta), with (H_2 O) as a precursors. The principal purpose was broken ethoxide group (CH_3 CH_2 O) bond of organometallic tantalum and was fixed the water molecule in replace the rest of organometallic molecules. For the separation of ethoxide functional group was fixed so close water molecule for to breaking bond by chemical reaction. This was made to put out tantalum bond of ethoxide group. If water molecule can not bond with the tantalum is possible that there is not a correct reaction mechanism. Also water molecules were added slowly one by one. This due to if the water molecule add so fast the reaction will not correspond to tantalum products at the surface of silicon.

[ALD-355] HfO2-TiO2 Nanolaminates grown by Atomic Layer Deposition

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Well-known applications for HfO_2 and TiO_2 are optical coatings [1, 2]. However, in the last few years these materials have been studied as high-k dielectrics for applications in CMOS technology[3]. Atomic Layer Deposition (ALD) is a novel technique that allows to deposit oxides, metals and nitrides with high quality and control thickness [4]. HfO_2-TiO_2 nanolaminates were grown using Tetrakis(dimethylamido)hafnium(IV) and Tetrakis(dimethylamido)titanium(IV) as precursors and H_2O as oxidant-agent using the sequence Hf-O-Ti-O in function of substrate temperature (150 °C, 200 °C and 250 °C) to increase dielectric properties. In this work, stoichiometric of the films were analyzed with depth profile X-Ray Photoelectron Spectroscopy (XPS) from each sample and found carbon and nitrogen trace through nanolaminates due to partial decomposition from precursors and determined optimal growth temperature.

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[AMC-557] Multiferroic properties at room temperature of KNbO3 doped with Co

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Polycrystalline samples of the complex oxide $KNb_{1-x}Co_xO$, a potassium niobate doped with Co, with x = 0, 0.03, 0.05, 0.07 and 0.10 were prepared by the standard solid-state reaction technique with high-purity powder precursors of $K_2CO_31.5H_2O$ (98.5 %), Nb_2O_5 (99.95 %), and Co_2O_2 (99.9985 %). Powders in the proper proportions to obtain a given desired stoichiometry, and doping level, were mixed to get 0.5 g of the compound. Homogeneous mixtures were pressed into 0.5 cm φ and 0.5 mm thickness pellets at a pressure of 3 Ton. The pellets calcined in air at 600 °C for 6 hours, and then sintered for six hr. at 1000 °C (undoped samples) and 800 °C (doped samples) at heating and cooling rates of 3 °C/min. The crystal structure of pellets was analyzed by X-ray diffraction using CuKα radiation in a θ-2θ configuration. XRD patterns showed that all compounds were single phase with the polycrystalline perovskite structure of the $KNbO_3$ phase. It is observed that the peaks of Co doped samples are shifted to higher angles compared to the peaks of the undoped samples. Scanning electron microscopy observations evidence that crystallite size increases with the Co content. Measurements of polarization as a function of the applied electric field for all samples evidence a hysteretic feature characteristic of the ferroelectric materials. Magnetic properties were measured with a Vibrating Sample Magnetometer. The measured remnant polarization was 3.51 $\mu C/cm^2$ for the undoped sample and decreased with doping level to 2.35, 1.53, 1.07, and 0.71 $\mu C/cm^2$ for x = 0.03, 0.05, 0.07 and 0.10 respectively. Undoped samples are paramagnetic, however, doped samples exhibit weak ferromagnetism. Interactions between bound magnetic polarons are considered as a possible mechanism to explain the appearance of the ferromagnetic signal in the Co-doped samples [1, 2].

Keywords: Ferroelectricity, Ferromagnetism, $KNbO_3$

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BIOMATERIALS AND POLYMERS (BIO)

Chairmen: César Marquez Beltrán (BUAP)
Amir Maldonado Arce (USON)

BIOMATERIALS AND POLYMERS (BIO) ORAL SESSIONS

[BIO-37] Physico-chemical properties, thermo-rheological behavior and thermoplastic films mechanical characterization of three varieties of Triticale starch

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Nowadays, starch is a good biodegradable option for the replacement of synthetic polymers to avoid contamination. In this work, triticale starch from three varieties (Faraón, Peteroa and Aguacero) was isolated and the physico-chemical and thermo-rheological properties were evaluated. Also, mechanical properties of thermoplastic films using this starch were assessed. From the physico-chemical analysis it was found that the moisture, protein and lipids contents were slightly different among starches. Amylose value was similar. Thermo-rheological behavior measured by Mixolab® revealed that initial water uptake was higher for Faraón variety due to the grain morphology observed by Scanning Electron Microscopy (SEM). Values for gelatinization temperature obtained were 82.2 °C for Faraón starch, followed by Peteroa (72.0 °C) and finally Aguacero (65.6 °C). From mechanical properties, Faraón thermoplastic starch (TPS) films showed the highest value of Young's modulus for composition 50/25/25 (1.90 ± 1.09 MPa). The highest elongation at break (64.77 ± 14.14 %) was obtained for Peteroa composition 50/35/15. Then, triticale mainly used to feed animals more than for human consumption, can be a good alternative for preparing biodegradable films.

[BIO-106] Chitosan-hydroxyapatite nanocomposites for bone tissue engineering

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The aim of this work is to investigate the new physical effects in chitosan-hydroxyapatite nanoparticles (CS-nHAp) films related to mechanical and dielectric percolation effects. Structure, dielectric and mechanical properties of composites and their dependencies on the hydroxyapatite concentrations are investigated by SEM, TGA, FTIR, nanoindentation and dielectric spectroscopy measurements. Hardness, elastic modulus and dielectric constant exhibit a strong dependence on nanoparticles concentration such that maximum values of referred properties are obtained at 30-40 wt. % of nHAp. This maximum can be related to cluster agglomeration of nHAp above percolation threshold (*ca.* 30-40 wt. % of nHAp). The properties of CS-nHAp nanocomposites films have been interpreted using a three-phase model which includes: 1) CS matrix, 2) nHAp particles, and 3) interfacial layer between nHAp and CS matrix which appear due to strong interactions between chitosan's side groups with PO_4^{3-} of hydroxyapatite. Results of fitting using the three-phase model demonstrated good correlation with experimental results. We have obtained chitosan-hydroxyapatite nanocomposite with hardness higher than those values for bovine cortical bone. We believe that our methods and interpretation proposed in this work can be used for design polymer nanocomposites for bone tissue engineering applications.

[BIO-149] Obtaining, preliminary phytochemical study and encapsulation of aqueous extract of Agave potatorum zucc.

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The results of the obtaining, preliminary phytochemical characterization and encapsulation of the aqueous extract of *Agave potatorum zucc* leaves with antioxidant potential are presented. The extraction was carried out by the extrusion method from the leaf of *Agave potatorum zucc*, from which 8 grams of lyophilized aqueous extract were obtained. From the phytochemical study it was possible to identify secondary metabolites such as saponins, sterols and flavonoids. The encapsulation of the extract was very successful using the drip method and as an encapsulating polymer to the aginate. By varying the polymer concentration it is possible to control the structural properties of the alginate shell. Thicker and more compact (less porous) hearts were necessary for higher concentrations of alginate, in contrast, at lower, smaller and poorer concentrations of stronger alginate. The characteristics of controlled release of the extract in the function of the structural properties of the polymeric shell were evaluated using UV-vis spectroscopy, optical and electronic microscopy.

[BIO-204] Effect of different carbon sources in biogenic calcium carbonate production by Bacillus subtilis 168.

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Calcium carbonate ($CaCO_3$) is one of the most widely inorganic compounds used in several industries, such as plastics, cosmetics, pharmaceutic, construction and paper. Also, is one of the most abundant mineral in nature, being part of several geocycles, both in marine and lake sediments [1]. $CaCO_3$ mineralization by bacterial metabolism is a promising biotechnological environmental friendly technique to develop new biomaterials. Bacterial $CaCO_3$ mineralization is a phenomenon that occurs in sediments, in caves and even in monuments and buildings [2], [3], [4]. The ability of bacteria to nucleate calcium ions and form minerals is due to the production and nature of exopolymeric substances (EPS) and biofilm geometry [5]. Several investigations have reported differences in mineralizing yield, crystallinity and polymorphic products in different growth condition and species dependence (e.g., strains of *Bacillus licheniformis* and *Lysinubacillus sphaericus* (*B. sphaericus*)) [6]. The purpose of this work is to determine the conditions of $CaCO_3$ crystals production by *Bacillus subtilis* in a semi-solid media supplemented with different carbon and calcium sources.

$CaCO_3$ crystals formation was performed in semisolid media supplement with different carbon source, 2 calcium linked, (calcium acetate and calcium lactate) and 2 calcium not linked, (glucose + $CaCl_2$ and glycerol + $CaCl_2$). Crystals were observed in all conditions since the third incubation-day in semisolid media. The largest produced crystals were observed in glycerol + $CaCl_2$ medium (228±43nm) in contrast to calcium-acetate, glucose + $CaCl_2$ and calcium-lactate media. Diffraction data show that calcite was the prevalent polymorphism in all conditions. The four conditions influenced the crystallinity and the quality of the crystal formed. Crystallite size calculated by Scherrer's equation shows a final crystal grow of 36, 24, 26 and 30 nm for glucose, glycerol, lactate and acetate respectively. Crystallinity index was calculated by mean calcite diffraction peak integration, the highest IC at 9 days was 91% in glucose media. EDS quantification analysis evidenced presence of Ca, O and C as main elemental components, however FTIR analysis show amides, phosphates and sulfur functional groups presence. Those are functional groups constituents in biofilm and exopolymer proteins, amyloids, phospholipids and phosphates sugars [7]. This material surrounds the obtained crystal in all carbon sources, nevertheless, biofilm does not modify mineralized composition. The thermogravimetric analysis showed a difference in the amount of amorphous material produced in all carbon sources, results show that crystals obtained in glycerol carbon sources have the major weight loss (~20%) starting at 296.5 °C. Weight loss indicates organic matter decomposition and probably amorphous calcium carbonate melt point. In all conditions, a second weight loss is observed at 700°C-800°C, which is attributed to $CaCO_3$ decomposition to CaO. Finally, it was determined that *B. subtilis* produces more calcium carbonate crystals, 85% mineralized calcium, in calcium-acetate medium. This work demonstrates that use of different carbon sources coupled to *Bacillus subtilis* 168 can be used as a biological system that can produce calcite with different crystallinity and micromorphology characteristics, that implies an advantage for the applications of $CaCO_3$.

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[BIO-313] Thermoplastic starch materials: effect of formulation and extrusion process conditions

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Synthetic polymers or plastics are almost everywhere, from fabrics to food containers, these materials are essential for our everyday life. However, most of the plastics are petroleum-based polymers that consume about 10% of the supplies of petroleum, which is not renewable. Their production also come with high CO_2 emissions related to climate change and global warming. On the other hand, some plastics also take a hundred years to degrade, generating huge problems towards the environment. In this scenario, bioplastics could be an alternative, being biodegradable, renewable and in some cases, even edible and biocompatible. The purpose of this research was to develop biodegradable thermoplastic (TPS) materials based on starch and polylactic acid (PLA) for biotechnological applications.

The TPS were formulated using: native corn starch, glycerol as a plasticizer in a ratio of 30 to 50% (w/w) and citric acid (1.0%, w/w) as a crosslinker. The thermoplastic material was mixed with polylactic acid (PLA) [0-50%, w/w]. The material was obtained by extrusion, using a single screw extruder (CICATA-IPN, Mexico). Samples previously ground were characterized by different techniques: Scanning Electron Microscopy (SEM), Differential Scanning Calorimetry (DCS), Fourier Transform Infrared Spectroscopy (FTIR) and X-Ray Diffraction. Finally, the mechanical properties evaluated were the Young modulus, tensile resistance and elongation to break. All treatments were performed randomly and the data were analyzed by Response Surface Methodology.

Results showed that biodegradable TPS materials with similar physicochemical properties of plastics were developed by extrusion. The maximum tensile strength of these materials was 8.6 MPa for 28% (w/w) of PLA at temperature of 213 °C in the last two heating zones of the extruder. The maximum Young's modulus of these TPS materials was greater than 730 MPa. High concentrations of glycerol (45%) and low concentrations of PLA (12.5%) gave the maximum elongation percentage for the TPS. A decrease in the crystallinity of the materials obtained by extrusion was found compared to pure PLA and native corn starch. No significant effect was observed from the screw speed of the extruder.

Overall, extrusion process showed potential for developing TPS materials base on starch and PLA presenting advantages over the conventional processes such as process time and low water consumption without generating effluent pollutants.

[BIO-338] Analysis of the mechanism of functionalization of LaMnO3 nanoparticles doped with Sr and Ca by folic acid and chitosan conjugate

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The present investigation focuses on the use of a conjugate of folic acid (FA) and chitosan (CS) for the functionalization of lanthanum manganite (LaMnO$_3$) doped with Sr and Ca. The use of conventional cancer treatments such as chemotherapy are known for having adverse effects on the overall health of patients suffering from this type of diseases due in most part to their lack of specificity. During the las two decades nanoparticle systems have been studied thoroughly to be used as tools for the development of targeted cancer treatments. The use of FA-CS conjugates has emerged as a promising alternative. However, the study of the mechanism of functionalization of nanoparticles of LaMnO3 doped with Sr and Ca, with conjugates of FA, has not been fully addressed. Due to this, the interactions between the conjugates of FA and the surface of LaMnO3 nanoparticles doped with Sr and Ca, as well as the effects of said functionalization on their structure, morphology, and magnetic properties, have not been previously identified. The lack of studies that address this kind of analysis represents a problem since there is currently a great interest in the development of nanoparticle systems synthesized with alternative materials to magnetite Fe$_3$O$_4$ which can distinguish between healthy cells and cancer cells and bind to cancer cells to achieve greater effectiveness in cancer treatment and reduce the negative effects on healthy tissues. In this study, a conjugate of FA-CS was prepared to coat the surface of LaMnO$_3$ doped with Sr and Ca, previously synthesized through the sol-gel method and characterized with SEM and XRD. The FA-CS conjugate was prepared by mixing a CS 1% solution with a solution of FA activated with dicilohexildiimide (DCC) and N-Hidroxisuccinimide (NHS). We hope to identify the effects of the functionalization on the structure, morphology, and magnetic properties of the LaMnO3 nanoparticles doped with Sr and Ca, by characterizing the coated nanoparticles using SEM, FT-IR and XRD.

[BIO-431] A case of study: Titanium alloy for medical implants.

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Nowadays it is important for everyone to have the certainty that a product meets the specified requirements or properties of a material. This condition become more important if the topic in question is a medical implant or a device for some treatment. The goal of this study was to conduct a metallographic characterization of a proximal femoral nail. Using a proximal femoral nail, made of a titanium alloy designed for medical implants (Ti-6Al-4V) a metallographic characterization of the casting process was performed by analyzing its influence on the microstructure of commercial implant alloy: Ti-6Al-4V using scanning electron microscopy (SEM), energy dispersive X-ray spectrometry (EDS).

[BIO-439] Antimicrobial activity of polycaprolactone- silver fibers on against Gram-positive and negative bacteria

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Nanotechnology has played an important role in the search for new ways to prevent and treat infections, including the use of metallic nanoparticles with antibacterial properties. The adhesion ability and adaptability of bacteria, coupled with constant use of the same bactericides, have made the increase in the diversity of treatments against infections necessary. In this study, we worked on the design of a composite of silver nanoparticles (AgNPS) embedded in poly-epsilon-caprolactone nanofibers and evaluated its antimicrobial properties against various Gram-positive and Gram-negative microorganisms associated with drug-resistant infections. Antibacterial activity of PCL-AgNPs nanofibers against *E. coli, S. mutans, K. pneumoniae, S. aureus, P. aeruginosa,* and *B. subtilis* was evaluated. Results showed sensibility of *E. coli, K. pneumoniae, S. aureus*, and *P. aeruginosa*, but not for *B. subtilis and S. mutans.* This antimicrobial activity of PCL-AgNPs showed significant positive correlations associated with the dose-dependent effect. The antibacterial property of the PCL/Ag nanofibers might have high potential medical applications in drug-resistant infections.

BIOMATERIALS AND POLYMERS (BIO) POSTER SESSIONS

[BIO-4] Synthesis and characterization of hydrogel with Ag nanoparticles for 3-d printable prosthetics

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The objective of this work is the synthesis of a hydrogel with Ag nanoparticles, like a biopolymer (hydrogel/Ag), as well as its characterization, to be used in prosthetics in 3D printing.

Hydrogels are of great interest due to their unique properties such as high content of water, softness, flexibility and biocompatibility. Some of the applications of these materials are the delivery of drugs, pesticides and tissue engineering. Silver nanoparticles are used in biomedical applications for their antibacterial property. The purpose of an anti-bacterial hydrogel is that, in addition of being biocompatible, it avoids prosthetic infection.

To get Hydrogel, Laponite was dispersed in water in a proportion of 3% by mass. MBBA (cross-linker), I2959 (initiator), and the monomer AMPS were added later, under rigorous agitation. Ag nanoparticles, previously synthesized by the method of Turkevich, were added to the solution obtained. The Hydrogel/Ag obtained was used to build a model piece with a 3D printer, finally held a curing through UV radiation to provide it rigidity.

We proposed to characterize the mechanical properties of tension, compression, and rigidity. As well as the viscosity to hold in a range of 14.48-37.22 kPa, to ensure the viability in 3D printing. The morphology was characterized by scanning electron microscopy (SEM). The composition and antibacterial activity were characterized by Raman Spectroscopy and Gram test, respectively.

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[BIO-75] Preparation and characterization of zinc doped hydroxyapatite for possible use as a photocatalyst

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Hydroxyapatite HAp is one compound from a family of calcium phosphates. An important element of this structure is that it allows a great number of substitutions without the change of the crystallographic structure. The possibility of controlling the material stoichiometry and its ion substitutions make the hydroxyapatite a very attractive material, especially the development of catalysts with specific properties.

In the present work hydroxyapatite and zinc doped hydroxyapatite were synthetized via co-precipitation at low temperature. The properties of the samples obtained were characterized using XRD, SEM-EDS and BET surface area. XRD confirmed the formation of hydroxyapatite with hexagonal structure and the surface area of the powders varied from 189 to 272 m^2/g.

[BIO-84] Heavy metal removal from wastewater by nanofibers with Fe0 and CeO2 nanoparticles

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Polyacrylonitrile (PAN) nanofibers with Fe0 and CeO2 nanoparticles were obtained by electrospinning technique using a natural surfactant in order to disperse Fe^0 nanoparticles. The nanofibers obtained by coaxial technique were subsequently submerged in the wastewater treatment for the removal of Cr (VI) and As (V). Textural and chemical characterizations of the nanofibers were carried out by analysis of scanning electron microscopy and X-ray diffraction. From the adsorption equilibrium studies were used Langmuir isotherm model and SEM analysis, it was found that the removal mechanism of the target metals are functionalized in polymer surface impregnated with nanoparticles. The $Fe^0/CeO_2/PAN$ nanofibers showed effective adsorption affinity for both Cr (VI) and As (V), achieving maximum capacities in order to comply the norm the water establishes the maximum permissible levels of heavy metals in the NOM-001-ECOL-1996 (0.05mg/L).

[BIO-103] Synthesis and characterization of metal matrix composites Ti-TiB2 for biocompatible implants

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Metal matrix composites (MMCs) combine the metallic properties (ductility and toughness) with the ceramic characteristics (high strength and modulus), improving sometimes also their corrosion and wear resistance. Titanium (Ti) and titanium alloys are known for their excellent biocompatibility and strength-weight ratio, but minimal studies have been done for MMCs with a Ti matrix reinforce of Titanium-Boron (TiB2) ceramic particles, processing by Spark Plasma Sintering (SPS).I n this work, we present MMCs system (Ti-TiB2) synthesized viaSPS , and its characterization concerning the wear resistance, corrosion resistance in a Simulated Body Fluid (SBF) environment and hardness. This characterization was performed with the use of a Tribometer, Potentiostat and micro-indenter respectively. Finally, we analyzed the samples by Scanning Electron Microscope (SEM), Atomic Force Microscope (AFM), X-ray Diffraction (XRD) and Raman Spectrometer (RS) with the finality of observing the microstructure, wear track, corrosion and indentation prints. It has been observed that as the amount of TiB2 increases, the hardness and friction coefficient of the samples improves. Application of Ti-TiB2 MMCs synthetized via SPS in biocompatible implants are reviewed taking in consideration its mechanical, corrosion and tribocorrosion properties in comparison to reported in the literature.

[BIO-114] Influence of polyelectrolyte chains on surface charge and magnetization of iron oxide nanostructures

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The layer-by-layer (LbL) technique was employed to encapsulate maghemite (γ-Fe2O3) nanoparticles with natural and synthetic polyelectrolytes, with a view to producing magnetic nanoplatforms as a tool to improve remotely assisted delivery/release of hydrophobic drugs and to address their low cargo capacity. Magnetic nanoparticles (MNPs) were synthesized by coprecipitation and functionalized with the layer-by-layer (LbL) assembly of polyelectrolyte multilayers. Simultaneous conductimetric and potentiometric titrations were utilized in order to find the optimal pH for the deposition of four intercalated layers of polystyrene sulfonate (PSS)/ polyallylamine hydrochloride (PAH) or sodium carboxymethylcellulose (CMC)/chitosan (CHI) polyelectrolytes. XRD, TEM, DLS, TGA and FTIR techniques were utilized to access structural, morphological and surface properties. Charge reversals after each deposition confirmed a stable LbL assembly adsorbed on a multiparticulate nucleus (~64 nm) of 8.8 nm-sized MNPs. Polymer layers of increasing thickness ranging from 4 to 15 nm (PSS/PAH) and from 21 to 48 nm (CMC/CHI) were estimated as MNPs were successively coated with polyelectrolytes. All the systems exhibited superparamagnetic-like behavior. Surprisingly, a stronger reduction was observed in the saturation magnetization of MNPs coated with synthetic polyelectrolytes (thinner shells) than in the system layered with natural polymers (thicker shells). Magnetization results suggest that synthetic polyelectrolytes adsorbed on the nanoparticle surface appear to have a stronger cooperativity than that of biopolymers, which could differently affect the interaction of spins located in the magnetically disordered regions in the nanoparticle surface

[BIO-157] Synthesis, characterization and evaluation of a nanostructured composite of chitosan-magnetite-banana peel for adsorption of heavy metals

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This work is immersed in a current problem, water pollution; specifically, heavy metal contamination and presents a method that uses chitosan and banana peel as adsorption agents for the metals and magnetite to facilitate their recovery of the composite from the effluents. This paper reports a method of synthesis of a composite that improve adsorption and mechanical properties, respect to existing materials based in chitosan and magnetite, these improvements in the new composite are provided by banana peel. Additionally, to the synthesis, an estimation of the life time of the material under controlled conditions that take the material to the saturation which will allow to establish an optimal use according to the real conditions of an effluent.

[BIO-162] Synthesis of silver nanoparticles with green extracts

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Key words: Synthesis, silver nanoparticles, plant extracts, Green method

Abstract

One of the main limitations that arise during the synthesis of nanoparticles is the use of chemical reagents for the reduction of the precursor salts of the metal nanoparticles to be synthesized, which besides being toxic, are usually of a high price. Taking into account the above, and that certain plants (which have functional groups capable of reducing metal salts and give stability to the formed nanoparticles) can be used as a reducing agent for metal salts for obtaining silver nanoparticles. Silver nanoparticles (NPs) present an attractive field of research, currently, it is sought to implement synthesis routes by green methods, due to environmental pollution and generation of toxic waste from chemical synthesis, where the purpose is to replace the use of chemical solvents by a natural medium from plant extracts. In this work the synthesis route is shown via green from *Opuntia ficus-indica* and *Aloe vera* extracts. To obtain the nanoparticles, the extract of both plants was first prepared, which was incorporated into an AgNO3 solution and kept under constant temperature agitation. The nanoparticles obtained were analyzed by X-ray diffraction (XRD) showing the characteristic peaks of silver reflection for both extracts, located at 2θ = 38 °, 44 °, 65 ° and 78 °, indicating the obtaining of silver nanoparticles (NPsAg), later by scanning electron microscopy (SEM), it was observed that the morphology is quasi-spherical and that the sizes are approximately 60 nm. On the other hand, using the DLS (dynamic light scattering) methodology, nanometric sizes were confirmed. Finally, with the obtained results, it is possible to confirm the obtaining of silver nanoparticles by means of green syntheses using extracts of *Opuntia ficus-indica* and *Aloe vera* being this a simple, effective and sustainable method with the environment.

[BIO-163] Synthesis of polymer nanocomposites based on PVA / PVP and silver nanoparticles

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Key words: PVA, PVP, crosslinking agents, silver nanoparticles, extracts of Rosmarinus officinalis and Citrus cinensis

Abstract

In this work films of polyvinyl alcohol (PVA), polyvinyl pyrrolidone (PVP) and crosslinking agents such as glutaraldehyde or citric acid additivated with silver nanoparticles (NPAg) synthesized by extracts of *Rosmarinus officinalis* and *Citrus cinensis* were prepared. To obtain the films, the PVA and the PVP were first dissolved separately in H2O, to then mix these two solutions maintaining a ratio of 80-30% respectively. The crosslinking agents glutaraldehyde and citric acid are separately added because the films without this agent are soluble in water. The silver nanoparticles were added when a homogeneous mixture was observed between the polymers and the crosslinking agent. The films were characterized by FT-IR, swelling percentage and crosslinking percentage. The results of FT-IR show that the incorporation of the silver NP does not alter the molecular structure of the polymersThe swelling values are above 100%, indicating that the films can swell, but they do not lose their molecular structure. The percentages of crosslinking of all films showed values above 95%.

[BIO-168] Mechanosynthesis of a dimida-diácida and its application in nanotechnology

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Mechanosynthesis is one of the methodologies that has a great interest, due to the economic and environmental advantages it offers: it does not require the use of solvents, and it allows to obtain solid oxides with a high homogeneity and smaller particle sizes than those obtained by other methods

In the present work, a dimida-diácida (DIDA) was synthesized in solid phase, from trimellitic anhydride (TMA) and 1,4-phenylenediamine (p-FDA), using 1,4-diazabicyclo [2,2,2] octane. (DABCO) as a catalyst. Subsequently, the compound was characterized by nuclear magnetic resonance of proton (RMN1H) and infrared (ATR).

Finally, the obtained product was used for the formation and stabilization of Au nanoparticles, synthesized by colloidal method; Proliferation monitoring was carried out by ultraviolet and visible spectrophotometry (UV-VIS).

[BIO-169] Synthesis of a Dimida-Diácida used for the formation of gold nanoparticles (Au NP's)

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For the present work, a dimida-diacida (m-DIDA) was obtained by means of mechanosynthesis of "environmentally friendly reactions", which works as an electrolyte in the elaboration of gold nanoparticles (Au NP's) by chemical reduction. For solid phase synthesis of m-DIDA, it was used 1,2,4-benzenetricarboxylic anhydride (TMA) previously dry at 120 ° C for 2h, m-phenylenediamine (m-FDA) and 1,4- Diazabicyclo [2.2.2] octane (DABCO) for a grinding time of about 2 hours. The obtained reaction product purified by sublimation, was used for the synthesis of the Au NP's at different concentrations with a chloroauric acid solution, the characterization was carried out by UV-vis at different time intervals to identify the characteristic plasmon revealed at approximately 550 nm.

[BIO-173] Synthesis of a nanostructured membrane of collagen-calcium alginate by electrospinning for application in hemostasis.

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The progressive importance of attention to chronic wounds and injuries with hemorrhages caused by accidents has led to the search for novel materials of high biocompatibility that hastens the process of hemostasis, also known as coagulation. It is known that collagen not only has a structural and physiological function in tissues, but also plays an important role in hemostasis, where it acts in processes such as aggregation, adhesion and platelet activity. In addition, it acts on mechanisms of the coagulation process; besides, calcium ions are also part of the platelet activation process during hemostasis. The electrospinning technique has been widely used during the last years thanks to the possibility of creating fibers in micro and nanometric scale for a wide variety of applications within the biomedical area, it is used because it provides characteristics such as: large area per unit of area, porosity and multiple mechanical properties.

[BIO-192] Influence of addition of two silanized clays on the flexural modulus of a experimental dental resin

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Increased filler loading generally increases physical and mechanical properties that determine clinical performance and durability, such as compressive strength, tensile strength, modulus of elasticity and toughness. A low modulus causes a deformation and a dimensional change in the occlusal surfaces due to the constant tension to which they are subjected, which produces a greater wear of the material. As the volume fraction of filler approaches approximately 70%, abrasion and fracture resistance are raised to levels approaching those of tooth tissue, thereby increasing both clinical performance and durability. On the other hand, the marginal seal between filling material and tooth substance may be destroyed if the material is able to undergo elastic deformation under loading. A high value of modulus of elasticity is therefore beneficial. The significantly lower value of modulus of elasticity for the microfilled materials may have clinical significance. These products may potentially deform under stress, leading to a breakdown of the marginal seal. For these reasons, the objective of this work was to investigate the influence of the addition of two silanized clays, separately, on the modulus of elasticity of a composite resin. Two different groups were prepared: BIs-GMA/TEGDMA and silanized montmorillonite (MMTsil) and BIs-GMA/TEGDMA and silanized bentonite (BENsil) and compared to the control (Bis-GMA/TEGDMA without clay), using five concentrations for each group (0.1, 0.2, 0.3, 0.4, and 0.5 phr). Silanized clay was first handly mixed with Bis-GMA and photo initiator system (camphorquinone/ ethyl 4-dimethylamine benzoate) was dissolved by in TEGDMA, then TEGDMA mixture was added to Bis-GMA mixture. Subsequently, silicon dioxide nanometric was added to form a paste with which the specimens were made for the three point flexural test. ANOVA and Tukey test with a $p \leq 0.05$ were applied to both groups; it was determined that the value of the flexural modulus in the control group (3306.4 MPa) and the MMTsil group with a concentration of 0.1 phr of silanized clay (3855.4 MPa) are significantly lower than the other concentrations reinforced with this clay; while for the group reinforced with BENsil in all its concentrations, the control group (3306.4 MPa) is significantly lower. Considering the limitations of this study, it can be concluded that the silanized clays incorporated into the Bis-GMA / TEGDMA / SiO2 system improve the elastic modulus of the resin based- composite, due to the interaction of the clay with the organic matrix.

[BIO-218] Automatization of a low-cost pneumatic fatigue testing machine for bone cements fatigue damage assessment

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The human body is constantly under complex load requirements which may induce multi-axial stress to some specific bones and body articulations. Repeated and variable load events sustained by a body could result in the accumulation of damage in some bones or articulations. Partial or total replacement of a bone by biocompatible materials, makes necessary the evaluation of the mechanical behavior of these materials, in order to estimate their lifetime under different circumstances. In this sense, it is necessary the use of machines that can reproduce experimental conditions close to the reality. However, the cost of fatigue testing machines is very expensive, so designing and manufacturing equipment with the same testing capabilities is an excellent opportunity to build new and reliable laboratory infrastructure. This work presents the design and implementation of a pneumatic fatigue testing machine, in which is possible to carry out cyclic load testing in bending, axial and multi-axial loading. The equipment was designed to perform tests of bone cement specimens with dimensions according to ASTM D-790. The effects of the work pressure on the load and the stress applied in acrylic bone cement specimens, doped with carbon nanotubes, are presented.

[BIO-236] Cellulose acetate membranes for effective dye discoloration under exposure natural

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Cellulose acetate (CA) membranes were obtained by electrospinning and their properties were analyzed by scanning electronic microscopic (SEM), Fourier-Transform Infrared spectroscopy (FTIR), X-ray diffraction (DRX), differential scanning calorimeter (DSC) and thermogravimetric analysis (TGA). The potential of polymeric fibers for the discoloration of dye aqueous solutions under dark and sunlight irradiation was assessed by using UV-Vis absorption and photoluminescence spectroscopies. The results revealed that the dye molecule discoloration with CA fibers mesh was better in the sunlight irradiation that under the dark conditions. The absorption band maxima (664 nm) of methylene blue decreased with the time in absence and presence of polymer under solar natural exposition. The presence of CA fibers increased in 20% the discoloration effect of MB solution, as compare with the experiment without polymer, after 6 h of solar irradiation. The FTIR and TGA showed the interaction of dye organic or sub-products generated with the polymeric component. This work provides a method simple for the discoloration of wastewater effluents.

Keywords: electrospinning; cellulose acetate; methylene blue; sunlight

[BIO-243] Synthesis of nanoparticles of methyl methacrylate / methacrylic acid by the semicontinuous heterophase polymerization method.

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The synthesis and characterization of nanoparticles made of the methyl methacrylate / methacrylic acid copolymer synthesized by semicontinuous heterophase polymerization is presented here. This polymerization method consists in the dosage of monomer at a determined rate to produce starved monomer conditions. This procedure allows incorporate a large amount of monomer, using a small surfactant concentration. Also, by controlling the dosing rate, the particle size can be controlled and the chain growth, in addition to which high conversions from monomer to polymer is obtained.

The obtained nanoparticles were characterized by differential scanning calorimetry and infrared spectroscopy to confirm the synthesis of the copolymer, which turned out to be of the random type; the conversion was studied by gravimetry, obtaining conversions of the order of 93%, and the particle diameter, as well as the morphology of the particles, were determined by quasi-elastic light scattering and transmission electron microscopy, respectively, which allowed to identify the particles as semi-spherical in the order of 5 to 8 nm, of narrow distribution.

[BIO-261] Electrospinning of nanofiber membranes doped with zerovalent nickel nanoparticles for polluted water cleansing

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Nowadays, the implementation and widespread of nanotechnology sciences in the market for environmental applications has been obtaining greater interest especially in recovery processes, water treatment, ecological packaging and oil absorbers. Including the study, design, synthesis, manipulation and application of such materials, devices and functional systems through the careful control at the nanoscale. The metallic nanoparticles incorporation in such devices as nanofiber membranes have taken great relevance at present, given its ease and low cost of fabrication.

In this study we present the production, characterization and chemical evaluation of zerovalent (ZV) nickel (Ni^0) nanoparticles incorporated in electrospun nanofiber membranes. It will be presented the influence of the type of polymer (PVP or PAN) and its solution concentration, as well as electrospinning parameters, such as distance, voltage, flux; and furthermore the single versus coaxial electrospinning system. It will be shown that a wide range of nanofiber diameters can be carefully attained, from 200 to $\approx$ 1000 nm, suitable for hosting and holding of zerovalent nickel (Ni^0) nanoparticles. These electrospun nanofibers were subjected to controlled experiments of Cr(VI) adsorption, by means of Ni^0 and potassium dichromate interaction and retain efficiency adsorption. The global outcome of these tests will show the potential of such electrospun nanofiber membranes with ZV-Ni^0 nanoparticles for heavy metal ions cleansing of drinking and/or potable water.

[BIO-299] Electrospun cellulose acetate fibers sputtered with silver nanoparticles: Characterization and antibacterial properties

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In this work, cellulose acetate electrospun fibers were prepared and subsequently sputtered with silver nanoparticles. Cellulose acetate fibers were obtained using a vertical electrospinning setup. Magnetron sputtering equipment was used to obtain silver nanoparticles. Sputtering deposition was carried out at different time periods at room temperature. The morphology and composition of the electrospun nanofibers and composite membranes were examined by electron microprobe. The micrographs show cellulose acetate nanofibers full covered with silver nanoparticles with uniform size and homogeneous distribution. The crystalline structure of the films was studied by X-ray diffraction (XRD) measurements obtained with a Rigaku Dmax2100 Xray diffractometer, spectra were recorded for 2θ 10-80. XRD show four well defined diffraction lines at 38°,44°,64°,77° which correspond to (111), (200),(220),(311) reflections for metallic silver with face centered cubic (fcc) structure. This pattern is agreeing with metallic silver reference JCPDS No. 04-783.

Antibacterial activity of cellulose acetate nanofibers sputtered with silver nanoparticles was tested with the agar diffusion test using the ghramm-positive *Staphylococcus aureus* (ATCC 6539P) and the gramm-negative *Escherichia coli* (ATCC 25922). The electrospun cellulose acetate nanofibres were used as a negative control and antibiotic cefoxitina 30 ug/uL as a positive control. The inhibition zone formed around the coated nanofiber membrane was measured and recorded as the antibacterial efficacy.

[BIO-345] Synthesis of silver nanoparticles and evaluation of the incorporation to acrylic resin of dental application

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Introduction: One of the main disadvantages of polymers when used in applications in contact with soft tissues is that they are very susceptible to microbial colonization. Currently silver nanoparticles have received greater attention as new antimicrobial agents, due to its broad spectrum of action and nil bactericidal resistance, as well as antifungal. The introduction of silver nanoparticles into conventional polymers results in new materials with improved properties. *Objective:* To synthesize silver nanoparticles and evaluate the incorporation to commercial acrylic resin termocurable and autocurable based on PMMA for the application of dental prosthesis. *Materials and Methods:* Colloidal silver nanoparticles were synthesized using an aqueous solution of AgNO3 as a precursor, polyvinylpolyrridone (PVP) was added as a reducing agent and polyethylene glycol (PEG) as a stabilizer, evaluating with different pH values, subsequently it was brought to a state of boiling at 80 ° C for 2 hrs and allowing to cool to room temperature. Finally, the nanoparticles were added in situ to the thermostable and self-curing PMMA, evaluating the properties of the nanoparticles before and after, using UV-Visible Spectrum, TEM and Raman. *Results:* Spherical silver nanoparticles are obtained, average size between 10 and 30 nm, with a pH of 6.5 to 7, remaining stable in the acrylic resin. *Conclusions:* The particles of acrylic resin with silver nanoparticles were analyzed showing the characteristic bands of the vibrations of the molecule of PMMA and Ag, however, other evaluations should be carried out.

[BIO-424] Elaboration of biodegradable films from modified starches and glycerol for possible use in food packaging

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Plastic packaging is the most common material to store and transport of organic (foods) and inorganic materials; however, in recent years, it has become a global concern, since inadequate disposal of disused plastic leads to contamination of the environment. There is great interest from governments and research centers for the development of new biodegradable materials as an alternative to synthetic polymers. In the present work, biodegradable films were elaborated from modified starches and hydrolysates of rice, corn and potatoes, mixed with a plasticizer. The films were fabricated by thermoplastic extrusion with a temperature of 125 ° C and an output of 70 ° C with a flat matrix of 0.5 mm, a ratio of 1: 1 screw and 30 rpm speed. Four types of films with characteristics similar to a polyethylene were obtained. The resistance of the material obtained was measured with Texture Analyzer TA-TX2 equipment. Also, a SEM analysis was carried out to observe roughness and small invoices and to verify the homogeneity of the films. The mechanical and microscopic analyses showed the best results with samples fabricated with modified rice and potato starches.

[BIO-457] Efecto piezoeléctrico de esmalte humano

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La piezoelectricidad en el esmalte humano fue medida usando tanto el proceso de forma directa como de forma inversa. El efecto piezoeléctrico en forma directa se registra cuando una fuerza es aplicada a la muestra y se ésta produce un voltaje. El efecto piezoeléctrico medido en forma inversa aparece cuando se aplica un campo eléctrico a la muestra. En este caso, el efecto piezoeléctrico es detectado por el sistema PFM, en donde un sensor piezoeléctrico trasforma el movimiento mecánico de la punta del PFM en una señal eléctrica. El efecto piezoeléctrico fue Los resultados indican que existe el efecto piezoeléctrico en la dentina humana, y en menor proporción en el esmalte humano. Además, se observó que el valor de la constante piezoeléctrica es diferente en diferentes zonas del diente tanto en el esmalte como en la dentina. Los resultados de PFM indican que los cristales del diente humano presentan tanto el grupo espacial $P6_3/m$ como el grupo espacial $P6_3$ en diferentes proporciones

[BIO-478] Therapeutic prototype for the treatment of epicondylitis, through the use of infrared LED's

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Phototherapies have been increasingly used in several applications as such as the control of the pain and inflammatory process. The present work, exposes the methodology to develop a therapeutic system that works by emitting focused infrared light, using the emission of light generated by LEDs.The tests to reach its maximum functionality, were performed on phantoms, which emulate the optical characteristics of the biceps brachial, skin and adipose tissue. The phantoms were made using PEO with coffee, milk and ink by the process Spin coating and Doctor Blade. The optical window obtained in the phantom characterization was used to the design and construction of the first prototype.

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[BIO-479] Fibers composed of polypyrrole particles with polylactic acid as biomaterial

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The synthesis of new materials acquires interest in the area of health. Only the plasma configuration has been reported, that polypyrrole regenerate lesions in the central nervous system because it has functional groups related to our system. In this context, this paper presents a study on the dispersion of polypyrrole particles (PPy) in solutions of polylactic acid (PLA) to form electrospinned fibers for their possible application as a biomaterial.

For this, the conjugation of properties was carried out in two steps: The first was to synthesize by plasma polymerization the fractions: soluble, insoluble and particles that are obtained according to the conditions of synthesis and the configuration of the reactor. Subsequently, different solutions of PPy particles were prepared with PLA dissolved in chloroform in a PLA/PPy=10 mass ratio, considering the voltage, distance and roller speed variables, obtaining composite PLA/PPy fibers by means of the electrospinning technique. Finalmente, las fibras compuestas de PLA/PPy se caracterizaron estructural y morfológicamente para determinar la presencia de grupos funcionales afines al sistema nervioso central. Finally, the fibers composed of PLA/PPy were characterized structurally and morphologically to determine the presence of functional groups related to the central nervous system.

[BIO-481] Effect of the solvent and electrospinning conditions for the synthesis of polyethylene oxide fibers

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Polyethylene oxide (PEO) is a biodegradable and biocompatible polymer that is applied in the release of medicines. The PEO has mechanical properties and elasticity to form microfilled fibers of micrometric size. However, one of the disadvantages during the synthesis of the fibers with homogeneous diameters and lengths is the control of the electrospinning conditions that involves different variables such as: roller speed, voltage, distance, needle diameter, among others. In addition to that the viscosity plays an important role.

Considering the above, in this work a study is made on the influence of the solvent H_2O and $CHCl_3$ on the formation of PEO fibers in a ratio of 0.5/10. Subsequently, they were injected into the electrospinning equipment, maintaining the injection and roller speed constant with 0.01 mL/h and 350 RPM, respectively. The needle diameter was 0.6 mm and the voltage was 12.2 kV. The distance between the electrodes was varied with values of 5, 7, 10 and 12 cm.

With the morphological characterization of PEO dissolved in water, continuous and homogeneous fibers were observed with the formation of some pearls that grow on fibers. In contrast, a non-homogeneous surface and different fiber lengths were present in the PEO/$CHCl_3$ fibers. This indicates that the distance between the electrodes and the type of solvent influences the homogeneity of the fibers.

[BIO-515] Optical and structural characterization of micronized shrimp shells used as a matrix of entomopathogenic microorganisms

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In this work we have characterized micronized shrimp shells free of organic residues. We have used several techniques to characterize optically and structurally after the biopolymer of shrimp shell has suffered mechanical milling. We have study the morfology of the micronized chitin trough Scanning Electronic Microscopy (SEM), but also we have used Energy-dispersive X-ray Spectroscopy in order to get the chemical content (EDS). We have obtained the absorption spectrum by the Photoacoustic Spectroscopy (PAS). Through the optical properties we have detected some compositional content of carotenoids. Infrared and Raman spectroscopies gave us the structural information and also the degree of deacetylation. The purpose of this work is to study the surviving of entomopathogenic microorganisms among them Metarhizium anisopliae, Beauveria bassiana and Bacillus thuringiensis on these microparticles used as a substrate; which would be applied as biological control of plant pathogens.

[BIO-540] Fibrous silica-hydroxyapatite composite

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New silica-hydroxyapatite nanocomposite membrane was fabricated by electrospinning. The composite proposed the incorporation of glass to counteract the brittleness of HA in a composite formed by coaxial fibers which will be used for bone replacement. Precursors of hydroxyapatite and silica were synthetized through the sol-gel method and then incorporated into a polymeric PVP matrix; later they were processed by coaxial electrospinning to obtain fibers with an average diameter of 538 nm. Chemical and physical characterization of the membranes evidenced fibers in a coaxial disposition with a glass core and hydroxyapatite cover. The microporous fibers have many potentials uses in the repair and treatment of bone defects, drug delivery and tissue engineering.

[BIO-559] Preparation and Characterization of Self-assembled Multilayered κ-Carrageenan/Chitosan Nanocapsules

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The preparation of multifunctional nanocapsules with stability and good release properties is still challenging. In this work, we study the natural polymers κ-carrageenan (κ-CAR) and chitosan (CS) deposited onto olive oil-DTAC (in water) nanoemulsion droplets (NE) via layer-by-layer (LbL) self-assembly.

Size and surface charge data were obtained by dynamic light scattering (DLS) and zeta potential (ζ-potential) measurements. Chemical elements and functional groups of the polyelectrolytes were identified by x-ray energy dispersive spectroscopy (XEDS) and Fourier transform infrared spectroscopy (FTIR). The morphology of the nanocapsules was observed by transmission electron microscopy (TEM) and scanning electron microscopy (SEM).

The ζ-potential data collected evidence the stability and the successful formation of polyelectrolyte assemblies on the liquid NE colloidal template (less than -30 mV or more than +45 mV) presenting a surface charge inversion after each deposited polyelectrolyte layer. FTIR and XEDS analyses also have proven the presence of characteristic elements and functional groups of each polymer after they were deposited. Spherical and smaller particles were observed by transmission electron microscopy and scanning electron microscopy; their dimensions were compared to the hydrodynamic diameter obtained by DLS analysis of the systems. The NE yielded an average diameter size of 291 nm which increased 21 nm after the adsorption of four polymer layers.

[BIO-560] Influence of the Number of Layers on Drug Release Kinetics and Transport Mechanisms of Biopolymer Multilayered Emulsions

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CHARACTERIZATION AND METROLOGY (CHM)

Chairman: Roberto Machorro (CNYN-UNAM)

CHARACTERIZATION AND METROLOGY (CHM) ORAL SESSIONS

[CHM-94] Experimental Results of Gold Grating-Coupled Surface Plasmon Resonance

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Scientific literature refers to the diffraction grating technique to excite surface plasmon polaritons, using light sources with wavelengths greater than the pitch of the diffraction grating. This condition forces the angles of the diffracted orders to be greater than 90^0. That is, all light energy is coupled to the boundary between two surfaces (metal-dielectric). Some authors point out that this technique favors the nanophotonic applications, such as the construction of plasmonic circuits. However, this technical consideration is not indispensable in other applications, such as in the design and manufacture of sensors. On the contrary, a sensor requires a certain configuration of the optical system to perform the measurements on the reflected light intensity curve. That is, by emulating the configurations of Otto and Kretschmann and Raether, with the diffraction grating method, and under certain conditions, we could avoid the use of costly techniques for its manufacture (e.g. interferometry, scanning electron microscope). Likewise, it would no longer be necessary to use costly equipment to carry out the measurements on the variations of the intensity of the light signal within the surface boundary. To test the above, an optical prototype was fabricated to perform measurements of surface plasmon polaritons in light beams diffracted at angles of less than 90^0. Experiments were developed to identify the excitation resonant angle of surface polariton plasmons by a diffraction grating with a pitch greater than the wavelength of the light signal. In the laboratory tests, measurements of the intensity curve of the diffracted light signal were carried out in the +1 and -1 orders. The experimental results were consistent with the theoretical approach. Based on the above, it is concluded that it is possible to excite surface plasmon polaritons, using the technique of the metallic diffraction grating with a wavelength shorter than the space frequency of the grid. The achieved optical prototype turns out to be very flexible for future applications in the measurement of plasmons. This is possible thanks to the speed at which it is possible to modify the frames and their assemblies for the alignment of the optical elements: laser diode, rugged metallic surface, linear polarizer. Likewise, the absolute control in the incident angle apparatus, and the ease of exchanging the light source and the rough metal surface, open wide possibilities for testing new hypotheses for the excitation conditions of surface plasmon polaritons.

[CHM-128] Temperature influence in the synthesis of zeolites from fly ash applied to removal of metals in waste waters

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Zeolites were synthesized from fly ash obtained from combustion of coal by a hydrothermal process varying the temperature of synthesis and using sodium hydroxide as precursor for crystallization. The morphological study and structural characterizations were carried out using electron microscopy (SEM) and X-ray diffraction (XRD). The chemical characterization was carried out using scattered energy spectroscopy (EDS) and X-ray fluorescence spectroscopy (FRX) techniques. Finally, the cation exchange capacity was evaluated by determining the percentage of metals removal (Cr, Ni, Cd, As, Pb, Cu and Hg) in the test water before and after adding the synthesized zeolites with different dosage. It is evident how the temperature in the synthesis influences on morphology and type of zeolite obtained. High efficiencies are reported in terms of removal of As, Hg and Pb at the highest dose of material. It was possible to obtain a good percentage of Cu removal. However, the synthesized materials are not efficient to remove Cd and Ni.

[CHM-175] Novel Applications of Inelastic Background Analysis: HAXPES and 3D Imaging

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Technological applications of nano-structured materials are steadily increasing and to create materials with optimized properties, it is of utmost importance to have non-destructive techniques to characterize elemental depth distributions at the *nm* depth scale.

A widely used technique[1] consists in analysis of the energy distribution of inelastically scattered photoelectrons which depends strongly on the depth distribution dependent transport of the photoelectrons to the surface. Nano-structures can be studied up to depths of ~ 8 inelastic mean free paths[1] which with conventional XPS is ~ 5-10 *nm*.

With HAXPES, where synchrotron generated photons with energy ~ 10 keV are used, the potential probing depths increases to ~ 100 *nm*. In this respect it was recently demonstrated from analysis of practical samples that *nm* thin structures buried at depths ~ 70 *nm* [2] and in some cases up to 150 *nm* [3] can be studied with this method.

With the smaller lateral size of industrial devices there is also a need for non-destructive 3D-imaging of nano-structured samples. For this, automated data analysis is mandatory due to the huge number of spectra. An algorithm well suited for that was developed ~10 years ago[1]. With conventional XPS it was demonstrated[4] that 3D-imaging with sub-*nm* depth resolution is possible with a lateral resolution of ~ $10^{\mu m}$. With HAXPEEM it should be possible to eventually obtain 3D images with better than 100*nm* lateral and 1*nm* depth resolution. Such work has been initiated[5]. Here spectral noise is also an issue due to the small areas probed and Principal Component Analysis has proven[4] to be extremely effective for noise reduction.

Very recently, high energy lab X-ray sources[6] have become commercially available[7] and with these it is now possible to perform HAXPES and HAXPEEM in the lab. This opens up for practical industrial applications of these advances in inelastic electron background analysis of deeply buried nano-structures.

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[CHM-316] Application in fingerprint analysis using TOF-SIMS

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Time-of-flight secondary ion mass spectrometry (TOF-SIMS) has been used in imaging of small molecules (<500Da) in fingerprints, such as gunshot residues and illicit drugs. However, identifying and mapping relatively high mass molecules are quite difficult owing to insufficient ion yield of their molecular ions. In this report, graphene oxide (GO)-enhanced TOF-SIMS was used to detect and image relatively high mass molecules such as poison, alkaloids (>600 Da) and controlled drugs, and antibiotics (>700 Da) in fingerprints. Detail features of fingerprints such as the number and distribution of sweat pores in a ridge and even the delicate morphology of one pore were clearly revealed in SIMS images of relatively high mass molecules. The detail features combining with identified chemical composition were sufficient to establish a human identity and link the suspect to a crime scene. The wide detectable mass range and high spatial resolution make GO-enhanced TOF-SIMS a promising tool in accurate and fast analysis of fingerprints, especially in fragmental fingerprint analysis.

[CHM-407] Honey bee characterization by THz and Raman spectroscopy for quality certification purposes

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Honey is the natural sweet substance produced by honeybees mainly from the nectar or secretions of living plants, which the bees collect, transform by combining with specific substances of their own, deposit, dehydrate, store and leave in honeycombs to ripen and mature. In our daily life, bee honey is a unique sweetening agent that has been used without processing, and it provides significant nutritious and medical benefits. It is a rich source of readily available sugar, organic acids, amino acids, enzymes, in addition to being a source of many biologically active compounds such as flavonoids enzymes, amino acids, organic acids, antioxidants, vitamins and minerals and so on. Today the apiculture represents an important economic activity, being Mexico the third source of foreign exchange of the subsector livestock. Therefore, the main concern of producers to continue maintaining the acceptance of honey in the national and international market is to guarantee its authenticity. Adulteration practices through the addition of corn, rice or maltose syrup and falsification of single pollen honeys for lower quality products are not unusual. Besides honey deterioration due to its inadequate handling and storage may conduce to consumer health complications. Therefore, for producers and customers, it is important to characterize the quality of honey produced. In this work, THz and Raman spectroscopies were employed in order to investigate fast and non-destructive mechanisms to analyze the authenticity of the honey produced. Commercial brands and an artisanal bee honey were analyzed. As a figure of merit honey samples provided by the Instituto Mexicano de Apicultura (IMA, Mexican Institute of Apiculture) were used. THz time-domain spectroscopy (THz) presented characteristic honey absorption peaks. Nevertheless, the low-frequency region (0.35 -0.6 THz) seems to be more sensitive to quality or adulteration. At first glance, there are differences in the honey's color, which is related to biological and nutritive properties, and consequently to honeys quality. Dark honeys are quantitatively richer in minerals, and it is known that the honey bee color depends in the plants or region where the honey is produced from, so it is thought that these THz absorption lines are associated with minerals. [1-2] In addition, Raman spectroscopy with the 785 nm excitation line was used to characterize the samples. Low-quality honey bees showed the absence of several resonant modes, for example 778, 863, and 982 cm-1. The 863 line is associated to vibration of CH and C(1)H, CH2, while the other modes are still unknown. [3] Additionally, all the samples showed Raman signals around 1461 cm-1 caused by a combination of bending vibration of CH2 group (major) and the vibration of COO group. [3] Also an analysis of fluorescence was carried out. Taking the IMA honey as reference we found that the its fluorescence intensity is from 1.2 to 4.5 times greater than that observed for samples of poor quality. However, analyzing the Artisanal honey it was found that it presents an increment in the background fluorescence near to the 21%, which could be related to a better quality of the homemade product.

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[CHM-419] Exploring quantitative modeling of the Shirley background in photoemission spectra

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In quantitative chemical studies with X-ray photoelectron spectroscopy, the total background signal is well described as the sum of two terms, one originated from inelastic electron-energy losses and another that is described by the empirical Shirley method [1,2]. The inelastic part is very well quantified by the Tougaard theory proposed in 1982 [3]; the Shirley part, in the near-peak region, can be quantified by the method illustrated by Proctor and Sherwood [4]. Since the Tougaard background meets the experimental signal at binding energies ~ 50 or 100 eV above the peak, the Shirley contribution must banish at those energies. Therefore, the Shirley signal begins as a step-like function at the peak position to then vanish at higher binding energies (examples of the Shirley-signal in the entire range will be presented).

We showed that the Shirley part of the background is related to the capture of photons by deeper levels [5]. The physical process can be described as interchannel coupling [6] but adding a strong involvement of the valence band, i.e., a process resembling off-resonant participator photoemission with the generation of a shake-off type signal. Based on this model, we will explore an approximate method to estimate the Shirley signal in the near-peak region.

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[CHM-460] The photoemission spectra of copper sulfide thin films obtained by a chemical bath deposition route

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Copper sulfides have many applications in nanoscience and recent developments in catalysis, solar cells, supercapacitors, etc., require a comprehensive understanding of the photoemission spectra of these materials. Interestingly, the chemical state determination of copper sulfides is rather controversial and there is no clear consensus in the matter. Unlike copper oxides which bear distinctive satellite structures,[1,2] the Cu 2*p* spectra of copper sulfides do not show or the satellite structure is weak.[3,4]

The present work shows a detailed analysis of the photoemission spectra of copper sulfide thin films obtained by a chemical bath deposition route. The as-deposited films show photoemission spectra that are characteristic of a Cu^+ oxidation state, but the assessed composition does not correspond to the stoichiometrically expected Cu_2S compound. This apparent incoherency is possibly related to the amorphous nature of the as-deposited films. In addition, after annealing in an inert atmosphere, the as-deposited films turn into crystalline covellite whose chemical formula implies a Cu^{2+} state, however, the photoemission spectra show a mixed Cu^+/Cu^{2+} state; thus, calling for a revision of the state assignation in copper sulfides.

The shape of the photoemission spectra, chemical composition estimation, and structural analysis shows that the chemical state determination of copper sulfides must be done with caution and with the support of both photoemission and structural characterizations.

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[CHM-509] Morphological study of quartz grains after heating treatment

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The morphological, chemical and structural characteristics of quartz grains coming from the micro-casting waste are reported. By performing standard laboratory tests, such as optical microscopy, scanning electron microscopy (SEM) and X-ray diffraction (XRD), the porosity and fractures present in the grains are identified. In addition, a qualitative and quantitative analysis of the mineralogical phases is carried out, determining the majority phase and comparing it with the phases present before the thermal treatment to which the material was subjected. In the analysis it was possible to identify the presence of small pores caused by the evacuation of gases, in addition, the drastic temperature changes that occur during the microcasting process, which can exceed 1200 ° C, greatly affected the surface giving origin to grains formed by the union of various sizes of quartz with transit of binder.

Keywords: siliceous sands, microcast, microstructure, crystallinity, amorphous structure.

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[CHM-516] Effect of the Al-Cu inter-diffusion on the surface properties of Cu alloys for aerospace applications

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Cupper alloys with high concentration of Fe and Al are used in aerospace applications due to its extraordinary mechanical properties and its resistance to oxidation and corrosion in saline mist atmospheres. This kind of alloys are mainly used in the aeronautical industry for pump blocks, rings, bushings, and in bearings for landing gears. In this investigation, the thermal diffusion, phase transformation and resulting improved surface properties on a superficially treated Cu alloy (10%Al - 3% Fe), are analyzed. Samples of this alloy were Aluminum coated by cold spray process followed by thermal treatments at three different temperatures, and times. The Al coat interphase microstructures and surface properties were analyzed by optics and SEM metallography, EDX and microhardness. Results exhibited a systematic high hardness/corrosion resistance layer consisting of different phases generated by the Al-Cu–Fe inter-diffusion

[CHM-561] Quantification of the sulfidation extent of Mo in NiMo HDS catalysts with XPS

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A quantitative study was carried out on the surface of hydrodesulfurization (HDS) catalysts-based Ni-Mo supported on alumina by using X-ray photoelectron spectroscopy (XPS) technique. The performance of the Ni promoter on the catalyst Mo and S was evaluated from the assessment of proper areas using state of the art methods for background removal. These includes the use of an approximation for background modelling called active approach, in which the background and intensity are optimized during fitting and allows the use of different types of backgrounds as was required for Mo 3d-S 2s and the S 2p –Si 2p regions. Both regions contain two elements overlapped, making fundamental a distinction between them. In these cases, was used a slope background in conjunction with Shirley-Vegh-Salvi-Castle (SVSC), with which is possible to have a clear distinction between the different strengths of backgrounds arising from the overlapped peaks Mo 3d - S 2s and S 2p – Si 2p through the assignation of particular values to their components.

From the resulting fitting were obtained the areas and was performed composition assessment on the catalyst MoS2. The results were compared with composition obtained using the traditional (static) approach. With these results, was obtained a fundamental parameter that indicates the performance of a hydrodesulfurization catalyst: Mo4+/MoTotal.

CHARACTERIZATION AND METROLOGY (CHM) POSTER SESSIONS

[CHM-20] Implementation of the Piezoresponse Force Microscopy Technique on an AFM System

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This work presents the implementation of piezoresponse force microscopy (PFM) technique on an atomic force microscopy (AFM) system using the lock-in amplifier principle. PFM measures the local electromechanical surface displacement of a ferroelectric material as consequence of an external sinusoidal *ac* signal sent though a conductive probe. The probe operates at a frequency close to its contact resonance to enhance the sensitivity and it acts as a movable upper electrode. To close the circuit, the ferroelectric material is generally deposited or grown on a conductive substrate or film, which functions as the bottom electrode. The electromechanical surface displacement is transmitted through the tip transforming into deflection or torsion of the cantilever. These probe movements are detected by the optical lever method, where a laser beam is reflected by the cantilever on a position sensitive four-quadrant photodetector. The deflection or torsion of the probe, *i.e.*, the out-of-plane or in-plane displacements, respectively, are acquired from the photodiode signal. As the tip slides across the ferroelectric sample, the photodiode detector follows the vibration of the probe and sends the signal to a lock-in amplifier where the signal is amplified and filtered using the frequency of the *ac* signal as a reference. The lock-in amplifier allows obtaining the amplitude and phase signals that are returned to the AFM system to form the typical PFM images. The necessary requirements for the implementation of PFM in other AFM systems are presented and discussed.The implementation of this technique in our AFM system will allow us to evaluate the piezoresponse of new ferroelectric and piezoelectric materials.

[CHM-26] Time resolved study of optical properties and microscopic dynamics during the drying of TiO2 films by spectral diffusing wave spectroscopy

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We present a combined experimental, theoretical and numerical study of photon transport and microscopic dynamics in rigid and drying turbid thin films. Our setup is based in multi-speckle diffusing wave spectroscopy and is adapted for frequency sweep of the illuminating source. The spectral diffusing wave spectroscopy (SDWS) technique, is a useful tool used to characterize optical properties of random turbid solids. We apply our approach to simultaneously monitor the changes in optical properties and microscopic dynamics of turbid thin films of rutile TiO2 powder dispersed in ethanol during the full drying process. Accordingly, we introduce an extension of the photon diffusion model for spectral speckle intensity correlations to account for system microscopic dynamics We find that our results are well described by the model, where parameters required as the time-dependent sample thickness and transport mean free path are obtained from experiments. Furthermore, our findings are validated by numerical simulations of speckle dynamics based on the copula scheme. We consider that our scheme could be useful in time-resolved physical characterization of time-evolving turbid thin systems.

[CHM-113] The effect of welding on mechanical properties inmersion in biofuel on micro alloy steels

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This work presents an experimental study in the behavior on the mechanical properties of welding on of micro alloy steel under inmersion in biofuel. The specimens were welded into the central part with electric arc, later they were immersed in biodiesel in four conditions with immersion ranges of 20 to 56 days at temperature of -9°C.

For each condition, the specimens were subjected to monotonic uniaxial tensile tests by ASTM E8-03 and Rockwell C indentation according ASTM E10. A microstructure characterization was evaluated using optical microscopy (OM) and scanning electron microscopy (SEM).

The microstructure observed in the base material is formed of ferrite and perlite and in the welding zone, there are phases of acircular ferrite, lamellar cementite and perlite constituents. The hardness of the base material to the welding zone was obtained in a range of 9 to 15 HRC.

Finally, the mechanical properties influences on the day inmersion decrease with increase the day inmersion and the fracture surface were observed by scanning electron microscopy (SEM) with ductility fracture in all condition.

[CHM-174] Thermal Characterization of a Solid State Synthesized Monomer

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In the present work, the bisimide compound was synthesized by solid phase reaction using mechanochemistry, from 1,4-phenylenediamine (FDA) and phthalic anhydride (AF), using DABCO as a catalyst. The reaction was carried out in a period of approximately 4 hours, then successive washes were made in ethyl alcohol, followed by a vacuum drying at a temperature of about 150 ° C for the elimination of residues. It was characterized by infrared spectroscopy (ATR) to show that the bisimide was obtained satisfactorily.With the purified product, the phase change transitions (melting temperature and enthalpy of fusion) were determined experimentally by differential scanning calorimetry (DSC) and theoretically through the group contribution method.

[CHM-182] Low thermal emissivity filter design with alternative material for architectural glass pane

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A low thermal emissivity filter (low-e) coated on glass reduces the amount of heat coming from solar light into the building, thus the expenses in electricity for air conditioning are reduced 30% [1,2]. They are characterized by high transmission in visible region about 80%, but a low thermal emissivity in the infrared (IR) about 30% [3]. The standard low-e filters contain a silver (Ag) layer between two dielectric thin films due to its high reflectance of infrared wavelengths; however, silver layer has chemical and mechanical weakness which reduced the filter mean lifetime and react with the environment. In this work, we report the study of aluminum (Al) as an alternative material to be replacement of Ag, so the filter becomes more ambient resistant by a more stable metal, although keeping similar comparing their optical performances and durability. Theoretical designs are shown with e Low-e construction with 3 and 4 layers, with the measure of sensibility of each layer and feasibility of carrying it out the low-e filter.

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[CHM-184] Inhomogeneous optical interference filter

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Inhomogeneous thin films have a great potential in optical thin film filters. Its theoretical foundation begins since 1972 [Sossi, Dobrolowsky, Southwell, Bovard]. Due to technical difficulties, they are not in practical use at this moment. In this references is shown that transmittance is related to the Fourier transform of the refractive index profile, opening an infinite number of possibilities. The problem arises when we try to create a film with a refractive index changing continuously, as a function of thickness, according to a prescribed profile.
In this work we demonstrate de possibility to fabricate an inhomogeneous film, controlling the stoichiometry of the material, thus the refractive index, using optical emission spectroscopy (OES). For this purpose we capture the plasma light produced during sputtering deposition, relate the Ar spectral lines with the target and reactive gases emission lines, to obtain a sensitive line ratio indicator of the film composition.
From our previous experience, the use of OES provides a sensitive tool to make a diagnostic of the plasma, and from this information estimate the film performance. We are able to generate a film with a given refractive index with high repeatability, managing the reactive gas flux in the chamber, controlling via OES. We report our results on this matter.

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[CHM-203] Evaluation of Mechanical Properties of Polymer with Different Density Obtained in 3D Printing

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In this paper we evaluate the mechanical properties of 3D printing polymers with different densities. The densities were obtained by molten material modeling (FDM) with a 45° oriented hollow hexagonal infill pattern for PLA (Poly Lactic Acid) and carbon fiber (FC) filament with 80% ABS, with a infill geometry densities of 40%, 80% and 100%.

Tensile strength tests under ASTM-D638-02a were performed on a Shimadzu AG-X universal testing machine. The results obtained from yield stress with ranges of 35.06-39.57 MPa and 37.85-38.50MPa for PLA and FC, respectively. Mechanical properties influence the 3D print density.

Likewise, the results obtained were validated and compared using a finite element, which will allow the design of mechanical elements with the application of external prostheses and robotic elements to be generated and specified.

[CHM-210] Morphological, chemical and microstructural characterization of the coatings produced with the technique of electric wire arc spraying

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In this research, the dissimilar coatings 140MXC-530AS and 140MXC-560AS were produced, applied on an AISI / SAE 4340 steel, with the technique of electric wire arc spraying. Four deposit parameters were used: current (I), voltage (V), primary air pressure (AP) and secondary air pressure (AS), using the Taguchi experimental method (fractional and factorial orthogonal arrangements) $L_9(3^{4-2})$.

Characterization was carried out using conventional optical microscopy (COM), scanning electron microscopy (SEM), atomic force microscopy (AFM), energy dispersive spectroscopy (EDX), X-ray fluorescence spectroscopy (XRF), spectroscopy Auger electronics (AES), X-ray photoelectron spectrometry (XPS) and X-ray diffraction (XRD).

The 140MXC-530AS mixture had a porosity of 13.5%, an average thickness of 432 μm, an approximate particle diameter of 15 μm and a surface roughness of 390 nm; while for the 140MXC-560AS mixture the porosity was 9%, the average thickness of the deposits 390 μm, the particle size 6 μm and 200 nm in its roughness. The EDX and XRF techniques showed the elemental chemical composition of the coatings and the AUGER and XPS techniques allowed to see the surface behavior and the electronic structure of the elements that make up the coatings. The microstructural condition of these deposits was marked by the influence of elements such as Cr, Nb, Mn among others on characteristic peak of Fe in the XRD spectra.

[CHM-223] Study of LaFe13 type alloys for magnetocaloric applications

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During the last years, the requirement for a clean enviroment have searched for new technologies and materials in this way the magnetocaloric materials have emerged to develop efficient cooling systems and environmentally friendly. Currently, different types of materials for magnetic cooling have been used, and depends strongly on device operational conditions and material properties, such as work-cycle at room temperature, magnetic field applied, and not hazard, corrosive or expensive materials. The LaFeCoSi alloys fulfill with above mentioned criteria where Cobalt concentration allows a shift on Curie temperature, while keeping a large isothermal entropy variation. The purpose of the present work was to characterize comercial base LaFeCoSi alloys, with different concentrations of Mn and Al, and Hydrogen incorporation. These commercial samples are provided by Vaccumshmelze GmbH & CO., mainly for refrigeration system purpose. X-ray diffraction was used to identify the phase and crystalline structure, where we observed a cubic type $LaFe_{13}$ structure which is characteristic of these intermetallic compounds. The morphological properties were measured by Scanning Electron Microscopy observing a distribution of phases with different oxidation grade. Measurements using differential scanning calorimetry show Curie temperatures around 23°C to 60°C, showing that hydrogen incorporation is not determinant in Curie temperature. Results of Vibrating Sample Magnetometry were used to obtain magnetic properties; hysteresis loops from 1-3 T showed soft materials which implies that the intermetallic compound is magnetized and demagnetized easily, obtaining low coercitive fields between 28-87 Oe. The influence of the magnetic field and the Curie temperature, show important magnetic properties which are crucial for applications in the industrial sector showing that this type of alloys since of their temperatures of magnetic transition and ferromagnetic characteristics are appropriates for magnetic cooling applications.

[CHM-225] Development of Low-emissivity optical filters using double cannon sputtering

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The implementation of Low emissivity (Low-E) filters in windows for buildings reduces de energy costs employed to compensate the thermal interchange in the structure, hence saving up to 30% of the energy used to keep the building's temperature. The actual designs of this filters use a silver layer between two protective layers, which is expensive and can be easily oxidized when it gets in contact with the atmosphere, also when moisture reaches the thin silver layer, an agglomeration effect is produced due to the migration of the silver to the surface, causing peeling and losing its low emission property (Ando and Miyazaki, 1999).

The aim of this work is the construction of a Low-E filter made up of stack layers: glass/Si_3N_4/Al/Al_2O_3/Si_3N_4, with a high transmittance in the visible region > 80% and high reflectance in the infrared region. This filter has the novelty of employing aluminum (Al) instead of silver (Ag) as a reflector of IR to obtain a cheaper, efficient and durable Low-E filter. The Al is protected with silicon nitride (Si_3N_4) for hardness, high density, and high refraction index (Signore, et al, 2012), furthermore, alumina (Al_2O_3) is a protective layer for the aluminum, and that quality is exploited to enhance its durability.

The Low-E filter is grown using reactive sputtering technique with double cannon; the reason for this is to be able of synthesizing the whole stack without opening the chamber, hence of avoiding different layers interact with the atmosphere. With this procedure, we can ensure the intended optical properties of the filter. Plasma optical emission spectroscopy and in-situ spectroscopic ellipsometry are employed to find the optimal deposition conditions for each layer and also control and monitor the stack fabrication process for its reproducibility (Abundiz, 2013).

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[CHM-266] Effective thermal conductivity of Al2O3 and TiO2 coatings performed by thermal spraying process on ceramic substrates

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The effective thermal conductivity (K_{ef}) at room temperature of alumina powder (α-Al_2O_3 Sulzer Metco® 105SFP) and titanium dioxide (TiO_2 Sulzer Metco® 102) coatings produced by oxyacetylene thermal spray on ceramic tablets is reported. The substrates were sintered at 1100 ° C from atomized red clay powders. The process of preparation of the coatings was carried out using the ARESTE oxiacetylene thermal projection chamber, which has a Terodyn 2000TM (Eutectic Castolin) torch and a vibratory system (Tumac CHTB 10), which allows the incorporation of the powders to be projected on the substrate, a highly oxidizing flame with an oxygen fuel ratio of 1: 4 was also used. Three different thicknesses were grown, which were determined by the variation in the cycles (5, 9 and 14 cycles respectively) of projection of the torch on the substrate. The morphology of the coatings was carried out by scanning electron microscopy (MEB, FEI Quanta FG 650), while the room effective thermal conductivity, was measured using the TPS 2500 equipment, which uses the physical principle of the plane source (TPS), or hot disk method. The results for the coatings of TiO_2 report values between 0.842 (W/mK) and 0.860 (W/mK), on the other hand, those of Al_2O_3 oscillated between 0.743 (W/mK) and 0.816 (W/mK). These results contribute to the development of ceramic coatings with high value added, which can be used in various technological applications.

[CHM-404] Electrocardiographic signal analysis tool for research purposes

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This paper presents the implementation of a biomedical system for research purposes in the area of biomedicine, specifically in the field of Electrocardiography, with which different types of electrocardiographic (ECG) signal analysis can be performed, through the acquisition and ECG type signal processing, based on a Texas Instruments processing tool, its main operation is based on converting the cardiac signal into an electrical potential, through an amplification stage of instrumentation and filtering stages for signal conditioning, the main method consists of implementing an algorithm that has the ability to determine some dimensional characteristics of the ECG type signal, from the obtained measurements statistical results are generated with which there is the possibility of being able to determine the existence of some type of cardiac pathology.

[CHM-405] Characterization of Mexican Amber by Raman Spectroscopy

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Amber is a natural resin resulting from a polymerization process of millions of years. In Mexico, the pieces of amber are up to 23 million years old, this is found in the State of Chiapas, while in regions like the Baltic Sea amber is around 65 million years old. Within its main structure are polymers of labdanoid diterpenes, which have functional groups that characterize them. These are carboxylic acids and ester groups, as well as methyl exocyclic, the latter is of great importance for the identification of the degree of maturity of the resin, since the more unsaturation present the molecule its degree of maturity is lower. For our study, 12 varieties of Mexican amber pieces obtained from the amber museum of Chiapas were analyzed. They have different colors, such as yellow, orange, reddish, red, cognac, mossy, black, etc. By means of Raman spectroscopy, the characteristic bands of the ester groups were identified in 1031 cm^{-1} corresponding to the C-O bond, likewise, the band corresponding to the C = C double bond of the methyl exocyclic was identified in 1651 $cm^{-1.}$ Relating the intensity of this band with respect to the intensity of the C-H band at 1444 cm^{-1} (I^{1651} / I^{1444}) which indicate the change in unsaturation, is that the degree of maturity of the resin can be determined. Values were obtained within the range considered for mature resin (Amber) however there are variations according to the type of sample.

Acknowledgements

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[CHM-418] Chemical state assessment of cobalt oxide thin films via quantitative photoelectron spectroscopy

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The diverse applications of cobalt and cobalt oxides in the fields of catalysis, energy, electronics and especially in nanotechnology requires detailed and proper quantification of the chemical state of these compounds. This valuable information can be extracted from the X-ray photoemission spectra of the present compounds; however, the analysis is not straightforward because there exist many complications, like, an intense background and many overlapping peaks that render many attempts of quantification to be inaccurate.

Therefore, this work presents a detailed analysis of the photoemission spectra of cobalt oxides using state-of-the-art peak-fitting methods[1–3] and a set of parameters to accurately peak-fit the Co 2*p* photoemission spectra are presented. The analyzed samples consisted of cobalt ultra-thin films prepared by thermal sublimation, that were subsequently oxidized through time and pressure-controlled exposures to oxygen at room temperature.

The photoemission spectra show several satellite peaks that reveal that the oxidation of cobalt thin films, in fact, results in CoO. The proposed set of parameters and a proper background modeling employing the *active background*[3] approach enables a close experimental data reproduction and accurate peak area estimations. The shape of the spectra and the assessment of the chemical composition using the assessed peak areas and a multilayer model[4] also strongly indicate that the oxide is CoO and that it grows in a layer-by-layer fashion.

The results strongly suggest that the parameters employed to assess the intensity of the photoemission signals and the use of the *active background*[3] approach to accurately model the background are accurate and can overcome the inherent complications of resolving the Co 2*p* photoemission spectra. Thus, the proposed analysis methodology can be employed to assess cobalt oxides and can possibly be transferred to other cobalt compounds with relative ease.

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[CHM-422] Analysis of the extra-cavity pulses generate by thermo-cavitation in natural dyes.

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We present the analysis of extra-cavity pulses generation by thermo-cavitation induced by a CW laser beam (at 532 nm) focused into a liquid solution of Hibiscus Sabdariffa dissolved in ethanol. The high absorption of the natural dye produces a heating which gives origin and implosion of bubbles, during the bubble formation time the light go through the material and blocks it when the bubble collapses, this is visualized in the form of pulses. For the acquisition of this pulses, the sample is moved around the focus of lens, this modifies the frequency rate of thermo-cavitation and the amplitude of pulses. The frequency rate and the amplitude of the pulse was measured, as a result we observe that the average frequency decreases and the average of amplitude increases when we move the sample away from the focus.

[CHM-470] Early stages of the oxidation of silver films

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The increasing scope of transition metals and their oxides in nanostructure-related applications in turn increases the relevance of their characterization through X-ray photoelectron spectroscopy (XPS). The latter provides information about the chemical structure and film thickness. In this work, we report the characterization by angle resolved (ARXPS) of different silver oxidations to quantitative study the oxidation state and the oxidation mechanisms of metallic silver films.

Metallic silver films were deposited through sublimation using a background pressure of 1.5×10-7 Torr and a sublimation pressure of 1.1×10-6 Torr. The film was characterized with an XPS instrument with a monochromatic X-ray aluminum source (XR5, from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher).

Metallic silver films have shown a 3d peak with multiplet structure. It has two satellites in the positions of 1110 and 1116 eV. Special care was given to the modeling of the background of metallic and its oxide. The precise composition of the thin oxide layer will be reported for various oxidations levels.

[CHM-473] Design and construction of a microabrasion machine for material evaluation

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In the area of material science, many physical phenomena converge to determine the behaviour and properties of materials. Abrasion is of special care due to the adverse effects it can generate in the short, medium and long term, causing failures of different kinds such as shouting, fatigue, and even promoting corrosion phenomena. There are many applications in which materials are exposed to abrasion or corrosion wear and this is where we focus our work, on tribology.

In this project, we build a machine to evaluate different materials in terms of microabrasion of three bodies. We use a loaded sample, an abrasion ball and a microabrasive suspended in a liquid solution. A material shall be subjected to microabrasion tests and the surface of the material shall be characterised before and after the process, to look at the influence of the test on its tribological and morphological properties. We re-designed and old machine taking into account some concepts of design, materials, wear, loads, angles, and also with a biomaterials evaluation in mind. For that, we are evaluating the possibility of simulate human fluids and some joint movements of the human body. We can simulate the movements of a joint such as the shoulder, where its range of motion is 230 degrees and even lower or higher angles.

[CHM-490] Study on the generation of correlated photon pairs in silicon nitride optical waveguides

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Efficient non-classical light sources with tailored quantum entanglement properties and implemented in integrated photonic circuits are essential for the development of quantum technologies. The generation of correlated photon pairs is feasible from the implementation of the spontaneous four wave mixing (SFWM) process in optical waveguides fabricated by photolithography techniques and based on materials that exhibit high third-order non-linearity, such as Si_3N_4, and that can be synthesized in the form of thin films by ionic erosion, laser ablation and atomic layer deposition techniques.

In this work, we propose the implementation of SFWM in ridge waveguides of Si_3N_4 on substrates of Si and SiO_2. Si_3N_4 is a transparent material at optical wavelengths and exhibits a third-order electrical susceptibility higher than that of SiO_2. Using the MODE Solution package from LUMERICAL, the propagation constant of the fundamental mode of waveguides with rectangular cross-section were calculated. The waveguide dimensions were varied in the ranges 0.2 - 0.8 microns (waveguide height, the film thickness) and 0.6 - 3.0 microns (waveguide width). From the calculated waveguide dispersion, the phasematching properties required for the SFWM process were studied. It was found that in the considered parameter ranges become possible to generate SFWM photon pairs and in different spectral regions (determined by the waveguide cross section). In particular, it was identified that a waveguide of 0.5 microns x 1.5 microns constitutes an optimal medium for the generation of photon pairs (with a photon tuned in the visible and its sibling in the telecommunications band) exhibiting different spectral correlation properties. The specific degree of correlation is determined by the excitation wavelength, which can be accessed from a tunable Ti: Sapphire laser.

The present work constitutes the basis for the development of integrated quantum devices with applications in quantum information processing.

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[CHM-493] Quantitative ARXPS study of the oxidation of chromium

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Chrome is widely employed in industry because of its catalytic properties and its attractive lustrous appearance when its surface is polished. Chromed surfaces retain the metallic appearance giving a protection layers against oxidation and corrosion.

We prepared thin chromium metal films through sublimation employing a tungsten filament with metallic chromium (99.995% pure Sigma Aldrich). The background pressure in the processing chamber was 1.5×10^{-7} Torr and the pressure during sublimation was 1.1×10^{-6} Torr. The growing rate (measured with a MASTEK TM-350) was 0.1 Å/s and the total thickness was 30 nm. The film was characterized with an X-ray photoelectron spectroscopy (XPS) instrument with a monochromatic X-ray aluminum source (XR5, from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher) assembled by Intercovamex.

We present four samples of chromium films that were oxidized at different conditions, two of them at atmospheric air for 15 min and 48 hours and the other two under oxygen-controlled environment at 1350 L and 594 GL.

The quantification of the composition of clean metallic chromium exposed to oxygen was done employing XPS data. We use the block method [1] to analyze the Cr 2*p* oxidation by considering the differences on background properties between pure metallic and oxidized chromium. It was found that, in contrast with most metals, the oxidation does not take place through the formation of an oxide layer. State of the art analysis showed that, even at long exposures, a fraction of the chromium retains its metallic nature even at the top surface. Both Cr3+ and Cr6+ species coexist with the metal throughout the probing depth of XPS. We employed the multilayer method [2] to analyze the angular dependency to obtain the chemical depth distribution. The results show that a thin layer of oxide is not formed on the surface of the chromium film as is normally assumed, but instead the metal and the oxide are distributed equally throughout the entire material.

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[CHM-499] User-friendly software for the assessment of the structure of multilayered films from ARXPS data

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A quantitative study of the surface of ultrathin films can be carried out by characterization through angle-resolved X-ray photoelectron spectroscopy (ARXPS). It provides information on the chemical structure and thickness of the film using physical parameters such as the cross section of the photoelectric and the effective attenuation length of the electron. This characterization technique is highly recommended for quantitative assessment of the composition of ultra-thin films. This paper presents a Labview®-based user-friendly software to perform these calculations employing the intensity of the peaks of the relevant core-levels. The fit of the XPS spectra is done through the software AAnalizer®; it allows an optimal modeling of the background and provides, in this way, accurate peak intensities. The calculations are based on the MultilayerModel (MLM), which can consider the differences on effective attenuation lengths as the electrons travel through the various layers. The method has proven to be accurate in many other materials. The objective of this software is to facilitate the analysis of ultrathin films by ARXPS.

[CHM-521] Matrix and nano substrate enhanced fluorescence yields for the x-ray fluorescence trace analysis of biomedically important ions

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Introduction: Ions of several elements in the periodic table play an important role in the physiology of living organisms, and indeed are vital to life. Relatively new advancements in x-ray fluorescence (XRF) technology such as Total Reflection XRF (TRXRF) and Polarised Energy Dispersive XRF (PEDXRF) spectrometries have emerged as mature and reliable techniques for non-destructive quantitative elemental analysis over a large dynamic range (trace to percentage levels) of biomedical samples [1]. However the detection of elements with $Z<13$, particularly in the air ambient, and the quantification of volatile elements (e.g. Se) are inhibited. In the former case, the fluorescence yields are intrinsically low as well as the fact that the low energy characteristic x-rays are absorbed by the intervening medium, while in the latter, complications arise out of real-time compositional changes. Surface effects such as surface plasmon resonance, the lightning-rod effect' (concentration of the electric field on the sharpest points of the surface), and grazing geometries as well as bulk matrix enhancements (proximity of high-Z elements), could augment the fluorescence yields [2,3]. Calculations estimate that sample thicknesses of a few nm would result in an almost 200 fold enhancement [2]. We hypothesize that elemental fluorescence yield can be enhanced by nano particle (NP) surfaces and by matrix effects of the substrate. NPs with sharp ends such as carbon nanotubes (CNT) or high-Z element NPs such as precious metal NPs, as well as matrices with relatively larger high-Z elemental content, would be particularly suitable. We report our results on the PEDXRF analysis of Na and Mg in a high-Z element containing ceramic bulk sample and the general scheme of the first nano surface enhanced TRXRFS analysis of Se, Mg, K, Cl and I ions adsorbed onto multiwalled CNT (MWCNT) and on mesoporous TiO_2 (mTiO2), and Au nanoparticles (Au-NP) fabricated in our laboratory.

Materials and method: Details of the PEDXRF analysis on the bulk soil and ceramic samples are given in [3]. Ions of Se, Mg, K, Cl and I are adsorbed onto a few mgs of MWCNT, mTiO2 and Au-NPs from stock solutions of Se, $MgCl_2$ and KI whose concentrations are constituted in such a manner as to yield a final estimated concentration of the adsorbed ions close to human physiological concentrations. The functionalised NPs and Controls are analysed by the Bruker S2 Picofox TRXRF spectrometer. Peak characteristics are determined by the on-line software as well as off-line through peak deconvolution programming by ORIGINLAB 9.0.

Results: Figure 1 shows the spectral enhancement factor of the PEDXRF spectrum of the low and medium Z elements of the powder soil standard GSS-1 of particle size < 50 um, pelletized to a disc of 24mm diameter [3]. An enhancement of 160% was achieved for the lightest element, Na. The enhancement factors gradually decreased with Z. The matrix contained several high Z elements, notably Fe. The enhancement was attributed to secondary fluorescence of the low-Z elements caused by multiple photoelectric absorptions of the characteristic x-rays from the substrate´s high-Z elements, effectively increasing the fluorescence yield of the former.

Conclusion: Matrix effects such as the multiple or enhanced excitations of low-Z atoms by substrate composition and topography, can be used to advantage for increasing the sensitivity of the measurement of medically important light ions by TRXRFS, PEDXRFS and related advanced bench-top XRFS techniques.

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Figure 1. Enhancement factors of the PEDXRF peak areas for the elements of atomic numbers (Z) 11 to 14 in the sample GSS-1 due to fluorescence yield increases caused by the matrix containing high Z elements, notably Z=26 (Fe).

[CHM-523] Scattering anisotropy in AlGaAs/GaAs (631) MQWs as a function of As pressure and widths of the wells

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The III–V compound semiconductors are very important in electronics and optoelectronics applications. For example, AlGaAs/GaAs heterostructures have been widely used in the fabrication of visible light-emitting diodes, laser diodes, and solar cells. Self-assembly on high-index (HI) substrates is a promising technique that has been used in the last few decades for achieving QWRs with high density and high optical quality. In this technique, the planes that are energetically unstable tend to break up into low index facets to minimize their surface energies and under appropriate growth conditions uniform nanoscale step arrays has been obtained in the homoepitaxial growth of GaAs(631)A. Quasi-two-dimensional behavior can be produced in structures where a thin layer of GaAs is sandwiched between layers of a compound with a larger gap (e.g., $Al_XGa_{1-x}As$), with the electrons and holes generally both confined in the low gap layer. In the present work, It was studied the scattering anisotropy of corrugated AlGaAs/GaAs(631) heterostructures by Raman spectroscopy (RS) measurements with the 532-nm as the excitation source. The AlGaAs/GaAs MQW heterostructures were grown as a function of the Arsenic beam equivalent pressure P_{As} and with different QW widths Lw. The MQW heterostructures consist of five periods of 10 nm AlGaAs barriers. For the GaAs wells Lw = 2, 3 and 4.5 nm we used. Furthermore, for each L_w the P_{As}/P_{Ga} ratio was diversified to achieve distinct corrugation order and through this propitiate the formation of quantum wires. Both transversal optical (TO) and longitudinal optical (LO) phonons are allowed when backscattering from a perfect GaAs(631) crystal, where the intensity of the TO phonon (I_{TO}) is larger than the LO (I_{LO}) phonon. Therefore, a high I_{TO}/I_{LO} ratio in the Z(YY)-Z configuration would reflect the degree of order on flat (631) GaAs layers, which may differ from faceted surfaces. Atomic force microscopy images of the samples showed superficial 1D corrugation ordering after the deposition of the heterostructure, suggesting the formation of embedded quantum wires at low P_{As}/P_{Ga} ratio. The evidence of the 1D character of the samples was also studied by Raman spectroscopy. As it is known the confinement effects cause wavenumber redshifts of optical phonon modes. So, this information was extracted by Lorentz fittings of spectra LO and TO modes. Both of the GaAs TO and LO confined modes present wavenumber shifts, in which larger shifts were observed for the LO modes, independent of the Raman configuration and P_{As}/P_{Ga} ratio.

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LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS (LPM)

Chairmen: Salvador Carmona Téllez (CICATA LEGARIA-IPN)
Gilberto Alarcón Flores (CICATA ILEGARIA-IPN)

LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS (LPM) ORAL SESSIONS

[LPM-7] Role of Li+ ion in improved crystallization and the luminescence enhancement of upconversion

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Upconversion emission enhancement with the addition of Yb^{3+} and Li^{+} ions in nanocrystals of $Y(OH)_3$: Er and Y_2O_3: Er under excitation at 980 and 1532 nm, synthesized by the hydrothermal method are reported. We have extensively investigated the luminescence evolution with the addition of ions co-dopants and calcination temperature. The Li^{+} incorporation in Ln^{3+} - Y_2O_3 phosphors with thermal treatment at 1100 °C increase the luminescence 1758, 76, 124 times in the emission green, red and infrared respectively. XRD shows thermally treated Yttrium phosphors have to changes in the crystalline structure. SEM micrograph exhibit a changed in the morphology with the addition of ions dopants. FTIR spectra were used to monitor the incorporation of Li-species in the phosphors.

[LPM-12] Sol-gel synthesis of calcium-deficient hydroxyapatite: Influence of the pH behavior during synthesis on the structural, chemical composition and physical properties

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This work analyzes the influence of the pH on the physical-chemical properties of calcium deficient hydroxyapatite synthesized by the sol-gel method. The pH evolution in the course of the synthesis is followed during the drop-by-drop adding of the calcium source to the phosphorus source, at different drip rates. The structural, morphological and textural characterizations demonstrate that increasing the drip rate up to values of 10 ml·s-1 increase the crystallite size and the specific surface area; while the chemical and optical characterizations show that higher drip rates also increases the calcium and oxygen vacancies, related to an increase in the energy of the optical band gap. However, for the sample synthesized at a drip rate of 17 ml·s-1, the conjunction of higher calcium and oxygen vacancies have an opposite effect in the optical properties, in comparison to the observations in the synthesized samples at lower drip rates. Finally, the thermal characterization shows that, for all cases, the thermal diffusivity values agrees with the reported values elsewhere.

[LPM-27] Thermoluminescence from Cu Doped Lithium Tetraborate Irradiated with X-ray and γ using 137Cs Radioactive Source

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In this paper the lithium tetra borate ($Li_2B_4O_7$) was prepared by used water/solution assisted synthesis method. After finished the Synthesization, Copper (Cu) were used to doping material with $Li_2B_4O_7$ in order to enhance its thermo luminescent properties. The heating temperature parameters were 750°C for 2 hr and 150°C for 2hr. The samples produced by water assisted method were doped at different doping percentage (0.02%, 0.04%, 0.06%, 0.08%, 0.1%, and 1%) of Cu. The characteristics and identification of $Li_2B_4O_7$ (undoped and doped) were determined in four tests. The luminescent and morphological characterizations were performed by X-ray diffraction (XRD), Scanning electron microscope (SEM), Photoluminescence (PL), and Ultraviolet-visible spectroscopy (UV-Vis). XRD and SEM analysis of intrinsic and doped materials confirmed the obtained $Li_2B_4O_7$ structure and show its morphology. XRD patterns of the $Li_2B_4O_7$ matched a tetragonal crystal structure. Crystals of $Li_2B_4O_7$ of an average size of 50 nm were obtained. The presence of the copper dopant was confirmed in crystals of $Li_2B_4O_7$: Cu by SEM-EDS (energy dispersive spectroscopy X-ray). The emission spectrum of Cu doped $Li_2B_4O_7$ showed a prominent peak at 367 nm, while the main UV-Vis absorption was observed from 240 nm to 300 nm due to Cu^+ ion $3d^{10} \rightarrow 3d^9 4s$ transitions. The thermoluminescent (TL) response was studied for both γ radiation and X-ray. A 661.7 keV γ radiation using a ^{137}Cs source at doses of 50, 100, 200, 300, 400 and 500 mGy was applied to $Li_2B_4O_7$:Cu (0.1 wt%) pellets. An X-ray source was used at doses of 600, 800 and 1000 mGy to irradiate pellets of $Li_2B_4O_7$:Cu (0.02, 0.04, 0.06, 0.08 and 0.1 wt%). A linear TL response was observed for both X-ray and γ radiation. The order of kinetics (*b*), frequency factor (S) and activation energy (*E*) or the trapping parameters were calculated using peak shape method. Especially $Li_2B_4O_7$: Cu(0.1%) presents good glow curve in all kind of doses. The experimental results showed that this $Li_2B_4O_7$: Cu could have good potential applications in radiation dosimetry. The main purpose of this paper is to determine the effect of synthesis on the TL properties of doped lithium tetra borate $Li_2B_4O_7$.

[LPM-58] Incorporation of Quantum Dots in Borate Glasses for its application in Dosimetry

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Borate glasses doped with Dy^{3+} ions, silver nanoparticles (SNPs) and containing Quantum Dots were synthesized in the present work. We report photoluminescence characterization by absorption and emission spectra. The effect of Quantum Dots on the thermoluminescence (TL) glow curves was studied. The scanning electron microscopy (SEM) shows the Quantum Dots in the matrix glass. Absorption spectra of the samples show the influence of the Quantum Dots and SNP in the bands 350 nm at 425 nm associated with the Dy^{3+}, in the same spectra we can see the bands 750, 800, 875, 1098, 1278 nm and 1675 nm belonging to the Dy^{3+}. Emission spectra show two prominent bands at 480 nm and 574 nm and one faint band at 665 nm corresponding to ^{4}F9/2 → ^{6}H15/2, ^{4}F9/2 → ^{6}H13/2 and ^{4}F9/2 → ^{6}H11/2 transitions, respectively. All bands under 364 nm pumping, and the fluorescence in the 550 nm and 590 nm spectral range enhanced. The photostability of the samples was also studied in the UVA (315–403 nm) and UVB (280–315 nm) ranges. TL due to ultraviolet radiation (UVR) was studied; the glow curves show significant dependence of the TL intensity with the increment of SNPs and Quantum Dots in the samples. These results show the Borate glasses doped with Dy^{3+} containing SNP and Quantum Dots as a potential candidate to be use in solid-state illumination and retrospective dosimetry.

[LPM-61] Photo-, radio- and thermoluminescence emissions of Tm3+ doped strontium pyrophosphate

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In this work, luminescence emissions of Tm^{3+} (0.5, 1, 3, 5, 8 and 10 mol%) doped strontium pyrophosphate ($Sr_2P_2O_7$:Tm^{3+}) were studied by photoluminescence emission (PL) and excitation (PLE) spectra, radioluminescence (RL) and UV-blue thermoluminescence (TL). The synthesized $Sr_2P_2O_7$:Tm^{3+} powders were analyzed by energy dispersive spectroscopy (EDS), scanning electron microscopy (SEM) and X-ray diffraction (XRD) for obtaining its chemical composition, surface morphology and crystalline structure, respectively. PLE and PL spectra showed band emissions around at 298 ($^3H_6 \rightarrow {}^1I_6$), 369 ($^3H_6 \rightarrow {}^1D_2$), 451 ($^1D_2 \rightarrow {}^3F_4$) and 467 nm ($^1G_4 \rightarrow {}^3H_6$) corresponding to Tm^{3+} transitions. PL quenching concentration was observed in the $Sr_2P_2O_7$:Tm^{3+} samples doped at 3 mol%. RL emissions of $Sr_2P_2O_7$:Tm^{3+} (10 mol%) are composed by two bands centered at 371 and 463 nm which are according to PLE emissions of Tm^{3+} ions. UV-blue TL emissions were stimulated by a ^{90}Sr beta particles and they were measured from room temperature to 400 °C with a 2 °C/s heating rate. UV-blue TL glow curve of the $Sr_2P_2O_7$:Tm^{3+} (1 mol%) samples exhibited at least four overlapped maxima at around 63, 165, 207 and 331 °C. An acceptable repeatability of 2.6%, a linear dose-response range of 0.05-1 Gy and a fading of 21% after 82 days of storage in the dark at room temperature were obtained in the $Sr_2P_2O_7$:Tm^{3+} (1 mol%) samples. The complex UV-blue TL glow curve was thermally bleached from 80 to 350 °C with 10 °C steps for analyzing in detail the TL maxima.

[LPM-74] Photoluminescence of Hydroxyapatite/MWCNT composites

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Hydroxyapatite ($Ca_5(PO_4)_3OH$) is naturally found in coral and in the vertebrates' skeleton. Actually is one of the most studied materials for its compatibility with the hydroxyapatite shown in the humans' bones and in others elements of the body, despite this, it isn't the only aplication one can find; there are others like in photocatalysis, sensors, semiconductors, etc.

However, the material lacks of some physical, chemical and biological properties no matter which aplication have been chosen, whereby reinforcing the material with carbon nanotubes one could improve those properties, since carbon nanotubes have higher strenght, contact surface and sorption capacity.

In this work hydroxyapatite and composites of hydroxyapatite/carbon nanotubes were synthesized by a miscellaneous method consisted of coprecipitation of the hydroxyapatite's precursors with the addition of carbon nanotubes, after that the materials were subject to ultrasound bath irradiation and at the end fallowed microwave irradiation.

The resulted materials was characterized for DRX, Raman and FTIR spectroscopies and for Photoliminescence. The results of DRX show that the material have a hexagonal structure, while Raman spectroscopy identified the main phononic modes of hydroxyapatite, with FTIR spectroscopy was observed the fingerprint of the compounds, and finally photoluminescence for each material was obtained, the hydroxiapatite luminescen in the region of 380-450 nm, while the composite showed luminescence in the region of 355-700 nm.

[LPM-79] Characterization of a SiO2-PMMA hybrid matrix doped with terbium ions

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Using the sol-gel technique a SiO_2-PMMA hybrid matrix was synthesized by the simultaneous hydrolysis of tetraethyl orthosilicate (TEOS) and the polymerization of methyl methacrylate (MMA). The hybrid material was doped with terbium ions for it's luminescent properties for applications in thin film devices, sensors and as a active laser media. The optical properties of the material were characterized by UV-vis and photoluminescence spectroscopy. Surface morphology of the material and mechanical properties were observed using atomic force microscopy and the material's composition was studied using Raman spectroscopy. Distribution of the dopant inside matrix was analyzed by confocal microscopy. Measurements indicate that an homogeneous, non-porous composite was obtained with the terbium ions retaining their luminescent properties with good optical transmission across all the visible spectra.

[LPM-87] Luminescence in ZnO-Eu doped nano-structures produced under a sequential ALD-Hydrothermal method

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It is desirable to manipulate the structural and electronic characteristics of some materials. Among them, thin films of compounds that possess luminescent properties. A prominent material in this regard is zinc oxide; which can be modified electronically by means of the inclusion of elements that increase its luminescent signal, or that extend its emission spectrum. With that purpose $Zn_{(1-x)}Eu_{(x)}O$ nanostructured arrays with different aspect ratio were synthesized by means of ALD technique on silicon substrates (100). The working conditions of the textured films were made through the decomposition of diethylzinc (DEZn) at 190˚ C and 3.29 ´10^{-4}atm. Subsequently, the growth of nanostructures was performed carrying out one 2^3factorial design using the solvothermal microwave-assisted method (MASM). The experimental levels for every considered factor were Eu^{3+}concentrations of 0.02 and 0.06 (atomic %), temperature of 80˚ and 120˚ C and time of 30 and 50 min. The reagents used for solvothermal synthesis were $Zn(NO_3)_2 6H_2O$ and hexamethylenetetramine (HMTA) as promoters. The Europium doped ZnO nanostructures (ZnO-NS) were produced using $Eu(NO_3)_3 5H_2O$ as doping agent. Each synthesis products were characterized through X-ray diffraction (XRD), scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). Thus, it is demonstrated that is possible to produce nanorods with specific size or shape as a result of every condition proposed in the experimental design. Also, it was found that luminescence could be modulated in this way.

Keywords: Thin Films, Nanorods, ZnO, doped.

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[LPM-156] Is the origin of the red emission in Pr3+-doped titanates, metal-to-metal or ligand-to-metal in character?

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Until very recently, the exceptionally efficient $^3P_0$-$^1D_2$ nonradiative decay process that gives place to the characteristic red emission in Pr^{3+}-doped titanates, had been attributed to a Pr-to-metal charge transfer state model. Briefly, in this model $^3P_0$-$^1D_2$ nonradiative decay takes place through electron transfer from the $^3P_0$ state of Pr^{3+} to a Ti^{4+} of the host, which leads to an intermediate metal-to-metal charge transfer (MMCT) state ($Pr^{3+} \rightarrow Pr^{4+}/Ti^{4+} \rightarrow Ti^{3+}$), followed by an electron back-transfer from the Ti^{3+} to the remaining Pr^{4+} ion that leads to a Pr^{3+} in the $^1D_2$ state. This intermediate state was initially labeled as the intervalence charge transfer (IVCT) state. Despite many experimental results supported this interpretation -though not ruling out other possibilities- direct proof of the MMCT character of the intermediate state in Pr^{3+}-doped titanates was never found. In this work, new experimental evidences supporting an alternative mechanism for the $^3P_0$-$^1D_2$ nonradiative decay, which is based on an intermediate O^{2-}-to-Ti^{4+} ligand-to-metal charge transfer (LMCT) state, is presented. To demonstrate its feasibility, luminescent and reflectance spectra are measured in different compositions of the $Sr_{0.9955}Pr_{0.003}Ti_{1-x}Zr_xO_3$ (SPTZO) solid solution. The resulting spectra are analyzed using a foundational approach of the host-dopant interaction given by the chemical shift model (CSM). The substitution of Ti^{4+} by Zr^{4+} in the solid solution results in an increase in the energy of the transition associated with the host. Following the CSM, it is natural to ascribe that transition to the $O^{2-} \rightarrow Ti^{4+}$ LMCT state; furthermore, the CSM allows also to explain many additional features of the photoluminescence response of the Pr^{3+} ion along the entire SPTZO solid solution. In spite of the consistency of the previous results, and that recent state-of-the-art ab initio calculations also point out to the $O^{2-} \rightarrow Ti^{4+}$ LMCT state as being responsible for the $^3P_0$-$^1D_2$ nonradiative decay process, some concerns about how a non-localized state (from the point of view of the activator) can operate, seem reasonable. To overcome this issue, equivalent experimental results in Yb^{3+}-doped SPTZO solid solution are showed. Since the Yb^{3+} does not tend to oxidize, the presence of an $Yb^{3+} \rightarrow Ti^{4+}$ MMCT is ruled out. On the other hand, the presence of an $O^{2-} \rightarrow Yb^{3+}$ LMCT gives a clue about the differences on the luminescence features when energy is being transferred to the activator center from a localized and a non-localized state. Finally, the importance of these results regarding the color control of Pr^{3+}-activated phosphors is emphasized.

[LPM-214] Spectroscopy evaluation of crystalline and amorphous Cd2V2O7 as blue phosphors

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$Cd_2V_2O_7$ compounds in crystalline and amorphous phases were fabricated by the melt-quenching process. Characterizations such as X-ray diffraction, Raman spectroscopy and photoluminescence were performed. X-ray diffraction patterns of the crystalline sample showed peaks associated with a pure $Cd_2V_2O_7$ monoclinic structure, in agreement with the Raman vibrational spectrum. In the case of the amorphous sample, X-ray diffraction patterns only exhibited a broad band, typical of a glassy structure, whereas its Raman spectrum displayed two broad vibrational modes centered at 350 and 850 cm^{-1}, attributed to stretching vibrations of VO_3 groups. In spite of the structural differences, both samples presented similar photoluminescence features, consisting of a wide band in the 375–525 nm range with two peaks at 411 and 432 nm, associated respectively with the $^3T2 \rightarrow {}^1A1$ and $^3T1 \rightarrow {}^1A1$ electronic transitions in the VO_4 tetrahedron, under 340 nm excitation. Thus, blue light emission with CIE1931 chromaticity coordinates x~ 0.200 and y~ 0.145, and color purity of 62–63%, is achieved from the crystalline and amorphous $Cd_2V_2O_7$ compounds. The emission decay time profiles were well fitted to a bi-exponential function from which the calculated average lifetime values resulted to be 112 ± 13 and 99 ± 4 ns for the crystalline and amorphous $Cd_2V_2O_7$ samples, respectively. Theoretical calculations based on the density of electronic states revealed that the photoluminescence arises through charge transference processes from *3d* orbitals of four-fold coordinated vanadiums to *2p* orbitals of three-fold coordinated oxygens in the VO4 tetrahedron, being the basic unit of $Cd_2V_2O_7$ in crystalline and amorphous phases.

[LPM-233] Optically active point defects in fluorescent boehmite hybrid nanoparticles

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A simple route to design high-efficient white LED by combining a commercial UV-LED chip (InGaAsN, 390 nm) and boehmite (γ-AlOOH)-based organic-inorganic hybrid material as white down-converting phosphor was reported.[1] We demonstrated the possibility to sensitise the emission from boehmite point defects by a light harvesting chromophore leading to an enhancement of the emission quantum yield and to a lowering of the excitation energy. This is achieved by the development of hybrid organic-inorganic nanoparticles based on boehmite prepared by a one-pot non-aqueous approach. Boehmite hybrid nanoparticles exhibit emission properties that cover most of the visible region of the electromagnetic spectrum. The materials also display high emission quantum yield due to an efficient and synergic energy transfer between the benzoate ligands and the defects of the boehmite nanoplates. This is due a synergic energy transfer between the triplet levels of the organic-phase and the defects of the inorganic phase. In this communication we will concentrate on the study of the nature of the surface defects and the energy transfer mechanism taking place in this novel class of hybrid materials.

[1] X. Bai, G. Caputo, Z. Hao, V. T. Freitas, J. Zhang, R. L. Longo, O. L. Malta, R. A. S. Ferreira, N. Pinna Nature Comm. 2014, 5, 5702

[LPM-534] Luminescent characteristic of hybrid self assembled Eu-TTA luminescent complexes and composite styrene-butadien copolymer films

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A highly luminescent europium complex obtained with two different ligands, succinimide (SI) and 2-thenoyltrifluoroacetone (TTA); was synthetized with different TTA concentrations. The photoluminescence (PL) emission from these materials corresponds to the characteristic inter-electronic energy level transitions of the Eu^{3+} ions. However, the excitation spectrum is strongly dependent on the presence of TTA, having an optimum response when 0.75 mmol of this compound is added to the EuL$_3$(H$_2$O)$_3$ complex.

The quantum yield obtained by these powders were around 72% ± 1:7% indicating an optimum sensitization of these complex. The EuL$_3$ TTA complex with the best PL properties was embedded in a styrene butadiene copolymer (SBC) film, produced by the drop casting method, obtaining similar PL behavior at different concentrations, the highest intensity was observed at 1.2% (w/v) of EuL$_3$TTA complex and the quantum yield of these composite films was 60:5% ± 2%. These films were exposed to continuous UV irradiation and after 141 h no photo-bleaching effect was observed in contrast with the EuL$_3$TTA complex that exhibited a noticeable photoluminescence intensity degradation at much shorter exposure times. The use of these composite films on photovoltaic response of a Si-based solar cell will be discussed as well.

LUMINESCENCE PHENOMENA: MATERIALS AND APPLICATIONS (LPM) POSTER SESSIONS

[LPM-54] The effect of the reduction of Eu3+ to Eu2+ in the thermoluminescence emissions of Eu3+ doped strontium pyrophosphate exposed to 90Sr beta particles

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In this work, Eu^{3+} doped strontium pyrophosphate ($Sr_2P_2O_7:Eu^{3+}$) was exposed to ^{90}Sr beta particles and its thermoluminescence (TL) emissions were analyzed. The $Sr_2P_2O_7:Eu^{3+}$ powders were synthesized by the solvent evaporation method and they were doped with 0.5, 1, 3, 8 and 10 mol% of Eu^{3+}. The incorporation of the Eu^{3+} ions into the $Sr_2P_2O_7$ host was confirmed by the $^5D_1 \rightarrow {}^7F_{1,2}$ and $^5D_0 \rightarrow {}^7F_{1\text{-}4}$ emissions observed in the photoluminescence emission (PL) and the $^7F_0 \rightarrow {}^5H_5$, $^5D_4$, $^5G_3$, $^5L_7$ and $^5L_6$ transitions displayed in the excitation (PLE) spectrum. Also, a charge transfer band (CTB) between O^{2-} and Eu^{3+} ions was exhibited in the PLE spectrum. The $Eu^{3+} \rightarrow Eu^{2+}$ reduction processes were studied in the $Sr_2P_2O_7:Eu^{3+}$ powders using radioluminescence (RL) and cathodoluminescence (CL) spectra which showed an intense UV-blue emission band around of 427 and 417 nm related to Eu^{2+} emissions, respectively. Orange-red Eu^{3+} emissions were also observed in the CL spectrum of the $Sr_2P_2O_7:Eu^{3+}$ powders. After CL analyses, UV-blue (Eu^{2+}) and orange-red (Eu^{3+}) emissions were observed in the $Sr_2P_2O_7:Eu^{3+}$ samples using PL spectrum. In this sense, the $Eu^{3+} \rightarrow Eu^{2+}$ reduction process affected drastically the Eu^{3+} TL emissions in the orange-red region and, therefore, it improved the UV-blue Eu^{2+} TL emissions in ^{90}Sr irradiated $Sr_2P_2O_7:Eu^{3+}$ powders. Finally, the chemical composition, surface morphology and crystalline structure of the $Sr_2P_2O_7:Eu^{3+}$ powders were analyzed respectively by energy dispersive spectroscopy (EDS), scanning electron microscopy (SEM) and X-ray diffraction (XRD).

[LPM-68] Effect of pH on the optical and structural properties of HfO2:Eu3+, synthesized by hydrothermal route

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In this work, the influence of the pH of the precursor solution on the optical and structural properties of hafnium oxide (HfO_2) doped with europium (Eu^{3+}) are reported. The synthesis was conducted by hydrothermal route at a temperature of 200 °C, with a reaction time of 80 minutes and a concentration of 3 mol% of europium, in relation to hafnium in solution. In order to study the influence of acidity on the kinetics of reaction, the pH of the precursor solution was varied in the range of pH=4 to pH=12. X-ray powder diffraction patterns showed that the materials crystallized better under alkaline conditions with pH=11, observing a good crystallinity in the material doped with Eu^{3+} ions. The characteristic rhombohedral microstructure of HfO_2 in the monoclinic phase was observed in alkaline media. Photoluminescent spectra showed the characteristic peaks of the emissions of Eu^{3+}, where the intensity of the luminescent emission increases by increasing the pH. On the other hand, it was found that radiative life kinetics of the dopant is related to the kinetics of crystallization, and therefore, to the acidity of the precursor solution.

[LPM-122] optical and structural properties of SrO and SiOC films obtained by the HFCVD technique

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The luminescent dielectric materials have been recently attracted attention due to the need for efficient silicon-based optoelectronic devices. Thus, dielectrics materials as Silicon Rich Oxide (SRO) and Silicon Oxicarbide (SiOC) have been studied due to their Photoluminescence (PL) in the visible region from 370 nm-900 nm, making possible candidates for the development of light emitting devices. In this work, we present results about optical and structural properties of SRO and SiOC films obtained by Infrared Spectroscopy, Photoluminescence and X-ray Photoelectron Spectroscopy (XPS). The results show that carbon concentrations in SiOC films are critical in terms of obtaining a high emission in the violet-red region (370-724 nm), so that an intense emission is obtained for carbon concentrations less than 10% at. In the case of SRO films, the silicon (Si) concentration is important, and the PL intensity in red region around 827 nm is improved. Thus, Si concentrations less than 5%at are optimal for obtaining a high emission. The different emission mechanisms in the SRO and SiOC films are explained and attributed to the formation of Si nanocrystals and radiative defects.

[LPM-136] Optically Stimulated Luminiscence Response of Calcium Dialuminate

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Currently carbon-doped alumina (Al_2O_3:C) is used commercially for radiation dosimetry using the optically stimulated luminescence (OSL) and thermoluminescence technique. However, the interest to develop new materials applicable in OSL dosimetry to provide alternatives to the reference material continues. Therefore, this work presents the OSL response of intrinsic calcium dialuminate ($CaAl_4O_7$) and doped material ($CaAl_4O_7$:Cr) after an exposure of electrons from a source of ^{90}Sr in the range of 0.25 to 30 *Gy*. The continuous wave technique (CW-OSL) with a blue stimulation source (458 ± 5 *nm*) and a detection window of 365 ± 25 *nm* was implemented to obtain the response. Dose response, reproducibility and fading tests were performed. Intrinsic Calcium dialuminate shows three orders of magnitude more intense than that of $CaAl_4O_7$:Cr, and the dose response test presented a linear function for both materials. The results of the reproducibility study showed a relative error of 0.012 for $CaAl_4O_7$ and 0.004 for $CaAl_4O_7$:Cr.

Keywords: OSL, Dosimetry, Aluminates

[LPM-154] Synthesis and characterization of nanoscintillator and gold nanohybrids for the potential application in theranostics

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Theranostic nanomedicine is an evolving and promising field in therapeutics. This new nanomedicine paradigm enables the integration of different functionalities, such as cell targeting, sensitive imaging, and therapy, on a single platform. In this work, we present the synthesis, morphological and, structural characterization $LiGa_5O_8$:Cr (LGO:Cr) and $Bi_4Ge_3O_{12}$ (BGO) nanoparticles synthesized by Sol-gel process. The gold (Au) nanorods were synthesized by seeding approach. Finally, the Au nanorods were conjugated on the surface of the luminescent nanoparticle by thiol coupling. The morphological and physiochemical properties of LGO:Cr@Au and $Bi_4Ge_3O_{12}$@Au composite nanomaterial were studied by scanning and transmission electron microscopy, Fourier transform Infrared spectroscopy and UV-Vis spectroscopy. The results suggest that the Au nanorods were successfully functionalized on the surface of luminescent nanoparticles. These nano-composites will be further analyzed for the plasmonic photothermal efficiency of attached Au rods upon excitation with 808 nm laser [1]. Moreover, this nanocomposite systems will be studied for the luminescence imaging to determine their potential application as a theranostic agent.

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[LPM-189] Terbium-doped yttrium hydroxide nanorods synthesized by the microwave assisted hydrothermal method

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$Tb:Y(OH)_3$nanorods were synthesized by the microwave assisted hydrothermal method. Samples morphology and photoluminescent properties were studied as a function of the relative concentration of terbium: 0%, 3%, 4%, 5%, 6% and 8%; as well as the concentration of hexamethylenetetramine (HMETA) in the start solution: 0M, 0.025 M, 0.05 M and 0.075 M. The Anton Paar microwave oven parameters were set at 200 °C held by 30 min with magnetic stirring at 1000 rpm and a heating rate of 6 °C/min. The structure of the material was analyzed by SEM and HRTEM, while the photoluminescent spectra were recorded with a spectrofluorimeter. From the analysis it is concluded that the final structure depends strongly on the presence of the dopant concentration: showing nanorods of different sizes; as well as HMETA concentration: the sample obtained without it showed shapeless polycrystalline cumuli, whilst the samples obtained with it present cumuli consisting of 160 nm diameter and 1 to 5 mm long rods. The photoluminescence analysis indicates that the emission increases as the dopant concentration is raised, presenting a maximum emission intensity at 6 at.% of dopant concentration, and being quenched at 8 at.%. The effect of HMETA in the emission is barely perceived, yet those samples synthesized with it present a stronger emission compared to those without it; this is attributed to the differences in morphology.

[LPM-195] Aluminium carboxylate metal-organic framework MIL-96(Al) functionalized with fluorescent molecules

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The interest in porous materials results from their outstanding properties and their vast applications. Research on porous solids and their functionalization has been one of the most studied topic. Over the last decade porous materials, known as metal-organic frameworks (MOFs), have increased their study because of their high surface area, properties and structural design, which made them suitable to be used in gas storage, drug delivery, as adsorbents, catalysis and electrochemical applications. As a result of the physico-chemical properties of MOFs, they have been used as immobilization matrices for active species such as fluorescent molecules. MOFs are synthetized in solvents like *N, N*-dimethylformamide, dimethylsulfoxide or mixed solvents. As far as green chemistry is concerned, volatile organic solvents have many implications as environmental pollutants. Therefore, a synthetic route that can mitigate the problems associated with solvents, save time, and produce less waste liquid is highly desired for the preparation of MOF. On the other hand, the studies on the functionalization of MOFs are ever growing because in this way the properties of the material is improved. In this work we describe a methodology to synthesize the aluminium trimesate MIL-96(Al) using a green methodology in relatively short reaction time. Further exploring functionalization of aluminium carboxylates MOF, we prepared a series of hybrid materials based on MOFs with rhodamine, fluorescein and phthalocyanin. The obtained solids were monitored from the fluorescence properties of the dye and by the X-ray diffraction pattern to evaluate the cristallinity of the materials. The products were characterized by powder X-ray diffraction patterning, scanning electron microscopy, thermal gravimetric analysis and gas adsorption.

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[LPM-206] Luminescent dynamics of porous silicon infiltrated with rare earths

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In this work, we study the luminescent properties of rare earths (RE) in porous silicon (PS) structures. Theoretical and experimental studies will be carried out in order to understand the luminescent dynamics. We will develop a microscopic model that models the individual behavior of each ER ion inside of SP. The fundamental understanding of the optical behavior of PS:RE will be very useful for the design of electronic systems that are capable of transmitting electrical and optical signals simultaneously. Recently there has been a growing interest in luminescent silicon, in both, basic and applied research. Since microelectronic devices are mainly made of silicon, the possibility of fusing microelectronics and photonics in the same chip is a real possibility. In this way, the understanding of the luminescent behavior of PS doped with rare earth is a current theme. From the technological point of view, in the commutation signal area, for example, it is of great interest not only to control, but also to predict the luminescent behavior. Three of the most important luminescent properties are: the luminescent intensity (quantum efficiency), the color coordinate and the lifetime. The luminescent intensity refers to the amount of light emitted by the material, the materials with high efficiency are able to convert the incident energy into emission efficiently. The color refers to the wavelength of the signal transmission. Finally, lifetime determines the time between pulse and pulse of the optical signal.

Here, we study the dependence of the emission intensity of with the porosity and the concentration of RE inside the samples. Different samples were prepared by electrochemical etching of p^+-type crystalline silicon wafers followed by simple impregnation with rare earth ions and subsequent high temperature annealing in air. The samples exhibited room temperature photoluminescence and the excitation spectra present a wide excitation band around 233 nm which can be associated to the charge transfer band transitions.

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[LPM-211] Photoluminescent Studies of SiO2 Activated with Eu3+ y Tb3+ and SiO2:Eu3+:Tb3+

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Monoliths of SiO_2 with Tb^{3+} (0.1% mol) and Eu^{3+} (0.1% mol) optically activated have been successfully synthesized through sol-gel method. Fluorescence, energy transfer and composition properties of as-prepared samples were systematically analyzed using photoluminescence spectroscopy (PL) and NIR. The results showed that under ultraviolet excitation, the SiO_2:Ln^{3+} (Ln = Eu, Tb) showed characteristic red and green emissions corresponding to f-f transition of Eu^{3+} and Tb^{3+}, respectively. Moreover, the luminescence emissions of the samples can be tuned from green to yellow, orange and red by doping the SiO_2:Tb^{3+} and SiO_2:Eu^{3+} ions into the host due to the efficient dipole–dipole transitions under 377 nm and 393 nm light excitation, respectively. Additionally, in the co-doped samples the strongest emission intensity at 612 nm increased up under annealing treatment at 900 ºC of SiO_2:Tb^{3+}:Eu^{3+} co-doped samples and under the excitation of 368 nm, 377 nm and 487 nm. The energy transfer studies of the co-doped samples were recorder under excitation of 368 nm and 377 nm, corresponding to absorption transitions of terbium, and were found the energy transfer emission peaks centred at 578, 591, 597, 613, 654 and 703 nm own to europium ions. The energy transfer processes between the relevant excitation levels of Tb^{3+} and Eu^{3+} ions and the energy transfer efficiency were discussed. The obtained results indicate that Tb^{3+} can be an efficient sensitizer for Eu^{3+} to enhance emission at red laser transition for sensors at NIR emission at 612 nm for optical communication applications and colour display fields.

[LPM-215] Analysis of Mexican quartz sand to identify surface defects that prevent its use as foundry core sand

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Quartz sand is a key commodity to prepare core molds for metals casting; it should satisfy specific features such as grain shape, size grain distribution, high silicon oxide content and low impurity level. Mexican foundries use high quality foundry sand from the USA due to round shape grains and at least 98% quartz content. Core sand molds are prepared glueing sand grains with polymeric resin, hence, round shape grains are preferred because more interface contact points between adjacent grains. However, the chemistry of the interface between the grains and resins might play a key role in the bonding between polymeric resins and sand.

In this research, first results about analysis of quartz sand samples from Mexico with Thermoluminescence (TL) and other techniques provide useful data to infer the nature of defects in the sand and the low strength of the core molds test obtained with this samples. The studied samples were S-00 from the US, used as reference, and three from Mexico, S-01 (Nuevo Leon), S-02 (Durango) and S-03 (Baja California Norte). Characterization of sand samples included mineralogy by DRX, morphology by SEM, chemical composition by EDS, and type of defects by TL. The Computerized Glow Curve Deconvolution (CGCD) analysis of the samples in study using mix order kinetic model (MOK) shown that R values were greater or equals than unity, therefore trapping process is predominant, finally the assumption of mixed order kinetics (MOK) comparing with other models, as general order kinetics (GOK), is more useful due to the fact that the MOK has a physical basis.

The samples were washed with distillated water then dried at 100 ºC. In addition, the sample S-01 was processed by attrition using sodium hydroxide, sodium pyrophosphate, oxalic acid, citric acid or hydrochloric acid, then washed with distillated water and dried at 100 ºC. The last assays included preparation of specimen of core molds with national samples S-01, S-02, S-03 and S-00 to measure the strength according to AFS regulation. The results showed that strength of specimen of core molds prepared with national sand samples were lower than the specification, 170 psi for immediate strength and 230 psi for strength after 1h. SEM images showed that bonding of polymeric resin in the S-01 were shorter than those in S-00. Chemical composition showed that Al and Ge, and other metallic oxides impurities in S-01, S-02 and S-03 were higher than in S-00, and TL glow curves help to identify some peaks around 105 ºC and 150 ºC, related to substitutional defects due to Ge and Al replacing Si. This defects due to Al and Ge would result in bonds in the sand-resin interface weaker than those obtained with Si.

[LPM-216] Photoluminescence and electro-optical characterization of Nd-doped (ZnV2O6, Zn2V2O7)

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By using the melt-quenching method, ZnV_2O_6 and $Zn_2V_2O_7$ vanadate compounds were prepared and simultaneously doped with Nd^{3+}. X-ray diffraction patterns indicate the polycrystalline character of both materials, which are acting as a host matrix of Nd^{3+}. The crystallinity of the two vanadate compounds was also verified by Raman scattering, where different vibrational modes assigned to ZnV_2O_6 and $Zn_2V_2O_7$ were detected. The electron dispersive spectroscopy analysis shows an homogeneous doping of Nd throughout the ZnV_2O_6 and $Zn_2V_2O_7$ host materials, of the order of 1.0 ± 0.2 at %. The micrographs acquired by Scanning Electron Microscopy, show that Nd-doped ZnV_2O_6 is constituted of microrods and irregular crystalline blocks. In the case of Nd-doped $Zn_2V_2O_7$ only irregular crystalline blocks were observed. The band gap energy was calculated from optical absorption data, the values were E_g = 2.24 and, E_g = 2.86 eV for ZnV_2O_6:Nd and $Zn_2V_2O_7$:Nd, respectively. By means of two points dark conductivity measurements, values in the 10^{-4}-10^{-6} $(\Omega\ \mathrm{cm})^{-1}$ range for ZnV_2O_6:Nd and in the 10^{-6}-$10^{-8}$$(\Omega\ \mathrm{cm})^{-1}$ range for $Zn_2V_2O_7$:Nd were registered. From photoluminescence spectra, multiple emissions assigned to electronic transitions of Nd^{3+} ion were detected. For instance, in Nd-doped ZnV_2O_6, the $\{^4F_{5/2}, ^4F_{3/2}\} \rightarrow {}^4I_{9/2}$ electronic transitions were observed. Concerning to Nd-doped $Zn_2V_2O_7$, the $\{^4G_{7/2}, ^4F_{7/2}, ^4F_{5/2}, ^4F_{3/2}\} \rightarrow {}^4I_{9/2}$ transitions were identified. All these results suggest that a successful doping of vanadates was obtained by the melt-quenching growth technique.

[LPM-252] Luminescent MOF films deposited by ultrasonic spray coating

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The deposition of high quality MOF films is still challenging but offers potential applications in gas storage, catalysis, sensing, lighting and solar energy harvesting. This work reports a simple, fast and inexpensive method for in situ synthesis and deposition of crystalline luminescent Tb(BDC) (Tb = terbium) (BDC = 1,4-benzenedicarboxylate) MOF films using ultrasonic spray deposition on top of hot glass substrates. The films were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), profilometry, infrared (IR) and luminescence spectroscopies. As expected, the emission spectra present high-intensity characteristic emission bands of the sensitized terbium luminescence for all the films. Nevertheless, the temperature of the substrate during deposition played a crucial role on the final structural and morphological characteristics of the MOFs, which in turn, greatly modifies the excitation features. The studies suggest that this synthesis method can be extensive to other MOF structures.

[LPM-280] Thermoluminescence and glow curve analysis of erbium niobate exposed to beta-radiation

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The family of rare earth orthoniobates and orthotantalates, $REYO_4$ (RE=La–Lu, Y=Nb, Ta), are suggested to be an excellent host for luminescent materials, in which the $ErNbO_4$ (NEr) has attracted considerable attention in the past several decades due to their wide applications and interesting optical and luminescent properties[1]. Thermoluminescence (TL) is a phenomenon that occurs when a semiconductor or insulating material, which was previously irradiated, emits light when heated[2]. TL is widely used to measure ionizing radiation doses, such as X rays, gamma radiation, and beta particles[3]. In this work, erbium niobate (NEr) was synthesized via solid state reaction[4]. It was characterized with powder X Ray Diffraction, scanning electron microscopy, and energy-dispersive spectroscopy, and its TL properties were assessed by exposure to beta radiation from a 90-Sr source. The TL response to the dose was evaluated between 10 Gy and 10 kGy, displaying saturation starting at 6 kGy. The response's linear region was located between 10 and 400 Gy. The glow peaks showed a maximum at 315 °C and a shoulder at ~224 °C, whose intensity increases as the dose augments until it becomes a very intense maximum. The glow curve deconvolution obtained at 100 Gy employing a general order model[5], and the experimental data from the initial rise revealed at least 4 peaks : 116 °C (E = 0.66 eV), 167 °C (0.73 eV), 243 °C (0.82 eV) y 313 °C (1.04 eV). NEr showed both good fading behavior in 48 h and reproducibility of the TL signal. These results suggest that NEr is a new phosphor material with potential application in TL dosimetry.

***Keywords**: Erbium niobate; Beta radiation; Dosimetry.*

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[LPM-284] Synthesis and Characterization of Luminescent Films of SrAl2O4:Tb3+, Eu3+ y Tm3+ deposited by the Spray Pyrolysis Technique

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The synthesis and characterization of strontium aluminate ($SrAl_2O_4$) films optically activated with europium (Eu^{3+}), terbium (Tb^{3+}) and thulium (Tm^{3+}) ions are described in this work. These films are deposited by the spray pyrolysis technique, where the deposition temperature is 550 °C and the precursor solutions are chlorides; later they receive a heat treatment at 800 °C for 16 hours. These films are characterized by means of: X-ray diffraction (XRD) to determine their crystalline structure; to observe the surface morphology is used the scanning electron microscopy (SEM); X-ray photoelectron spectroscopy (XPS) is utilized to quantify the elemental composition and binding energy of the chemical elements present, and finally the luminescent properties are studied by means of photoluminescence and cathodoluminescence. These films exhibit the characteristic colors induced by these dopants: red due to europium, green by the terbium and blue from the thulium, and some of the combinations of these colors such as yellow, orange and colors very close to white.

[LPM-289] Luminescent and structural analysis of yttrium oxide doped with different percentages of terbium and dysprosium, to obtain different shades of green to yellow

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The structural and luminescent results of nondoped, terbium and dysprosium doped, and codoped Y_2O_3 powders are presented. Different percentages of the rare earth ions were employed. The powders were obtained by means of the solvent evaporation technique and were annealed at 1100°C for 2 h. The emission spectra of these samples are associated with the characteristic intraelectronic energy levels that are related to the Tb^{3+} and Dy^{3+} ions transitions. The maximum peaks of emission are located at 542 nm with λ_{exc}= 274 nm for terbium that is associated with the $^5D_4$ to $^7F_5$ transition; for dysprosium, the maximum is at 573 nm, when excited with λ_{exc}= 210 nm, corresponding to the $^4F_{9/2}$ to $^6H_{13/2}$ transition; the emission spectra of the Y2O3:Tb4%:Dy3% and Y2O3:Tb4%:Dy0.75% phosphors were also obtained, and the emissions of these two ions are observed when excited with λ_{exc} = 260 nm, suggesting that these ions are near neighbors, giving place to energy transfer between these two ions. When the sample of $Y_2O_3:Tb^{3+}$ is excited with λ_{exc} = 274 nm, a single exponential decay is observed with τ=2.95 ms; when the $Y_2O_3:Dy^{3+}$ is excited with λ_{exc} = 210 nm, there is decay time with τ= 0.89 ms; and when excited with λ_{exc} = 274 nm, the phosphors of $Y_2O_3:Tb^{3+}:Dy^{3+}$also have a single exponential decay with τ0 2.04 ms. The Commission Internationale de l'Eclairage diagram coordinates obtained for different relative contents of these lanthanide ions are given. X-ray diffraction analyses of these phosphors indicate a polycrystalline cubic yttrium oxide structure with a grain size running from 37 to 45 nm.

[LPM-300] Luminescent and structural properties of microwave synthesized HfO2:Eu3+, Tb3+, Ce3+, Tm3+ nanopowders

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HfO_2:RE^{3+} (RE^{3+}: Eu^{3+}, Tb^{3+}, Ce^{3+}, Tm^{3+}) nanopowders were synthesized in a microwave reactor at temperature of 180 °C and a precursor solution of 0.05 M. Hafnium chloride ($HfCl_4$), and hydrated europium, terbium, cerium, thulium chloride (Eu, Tb, Ce, Tm: $Cl_3{\cdot}6H_2O$), were employed as precursors and ethanol and deionized water as solvents. Different ratios of RE^{3+} to Hafnium were considered; (RE^{3+}/Hf * 100). The synthesis of the powders lasted about 25 minutes, with 600 rpm agitation and a temperature ramp of 10 °C min^{-1} for all samples. The structural and luminescent characteristics of the powders were determined by XRD, SEM, EDS, and PL measurements. The powders resulted polycrystalline with the HfO_2 monoclinic phase, independently of the amount of RE^{3+} in solution. The average size of the crystallites resulted in the nanometer range. Photoluminescence spectroscopy of the powders revealed the incorporation of RE^{3+} into the monoclinic crystalline structure of HfO_2, showing a maximum PL emission in powders synthesized from solution with 10.0 % for europium and terbium, when is excited with λ = 395 and 250 nm, respectively; and 5.0 % of cerium for λ = 378 nm and 2.5 % of thulium for λ = 369 nm. The corresponding colors red to europium, green to terbium, and blue to Cerium and thulium in chromaticity diagram, suggest that the nanopowders might have potential applications as highly efficient RGB emission materials considered in the White Led´s technology.

[LPM-335] Thermoluminescence response of LiF:Dy obtained by coprecipitation chemistry method to exposed to beta radiation.

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LiF:Dy particles have been obtained by co-precipitation method. The thermoluminescence characteristic and structural properties of these phosphors were studied. The samples were exposed to beta irradiation source of 90Sr. The TL characterization includes the TL dependence on role of dopant concentration, reusability, temperature and sintering time, dosimetry and fading. Glow curves were obtained for 80 mg mass pellets-samples. The glow curves of LiF:Dy shows two maxima those located at 100 and 230 ºC at a heating rate of 5 ºC/s, with the intense signal well defined over 230 ºC. The TL peak located between 200 and 250 ºC are suitable for dosimetry, because they are very stable under standard conditions. The results show a low fading, a good reusability and lineality in the range of doses studied. Keywords: LiF, Thermoluminiscence, Co-precipitation

[LPM-347] Up and down-shifting emission properties of novel Er3+-doped CdO-V2O5-P2O5 glass system

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Er^{3+}-doped $CdO-V_2O_5-P_2O_5$ novel glass samples, with high amount of CdO (90 %mol), were fabricated by the melt-quenching method. The glassy structure was confirmed by X-rays diffraction patterns and Raman spectra. A detailed analysis of the Raman Spectra showed that these samples are mainly constituted by amorphous $Cd_2V_2O_7$ and PO_4 units. By optical absorption, band gap *(E_g)* values in the 2.44-2.63 eV range were determined, depending on the Er^{3+} concentration. Upon 980 nm diode laser excitation, the up-conversion spectra displayed the well-known $(^4S_{3/2},^2H_{11/2}) \rightarrow {}^4I_{15/2}$ and $^4F_{9/2} \rightarrow {}^4I_{15/2}$ transitions in the 510-575 and 640-690 nm range, whereas the down-shifting emission spectra in the near infrared (NIR) region showed a broad band extending from 1440 to 1650 nm, attributed to the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition. Both spectra reached the highest intensity at 2.5 %mol of Er^{3+}. For higher Er^{3+} concentrations, the emission intensities were gradually reduced, which is associated with non-radiative cross relaxation processes. The NIR emission decay recorded under 980 nm pulsed laser excitation was shortened as the Er^{3+} concentration increases. This fact was attributed to cross relaxation processes between $^4I_{13/2}$ and $^4I_{15/2}$ levels. The mechanism involved in such processes was analyzed by fitting the emission decays with the Inokuti-Hirayama model, which revealed that dipole-dipole electric interactions might dominate the cross-relaxation processes within Er-Er clusters.

[LPM-349] White and color emission of recycled LDPE thin films deposited by ultrasonic spray method

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A new scheme of recycling plastic bags wastes made of low density poly ethylene (LDPE) is reported in this work. Ultrasonic spray method at low temperature was used in order to deposit plastic thin films on Corning glass substrates from a polymeric solution precursor. Any signals of degradation were not observed, as revealed by FTIR spectroscopy. Different fluorescent inorganic and organic pigments (FIP and FOP´s, respectively) were incorporated as a luminescent additive on these polymeric thin films; As a result, these films showed different emission colors. By mixing red and green FOP´s, we obtained yellow color emitting LDPE thin films, which were deposited onto electronic chips obtained from blue light emitting diodes. These devices exhibited a white light emission, which chromaticity coordinates CIE 1961 was X=0.3030 and Y=0.3020. Measured thicknesses of these polymeric films were close to 1 µm. Optical (photoluminescence, UV-Vis spectroscopy) and structural characterization (Scanning electronic microscopy and infrared spectroscopy) were carried out.

[LPM-357] Effect of Ag incorporation on luminescence properties of the ternary system CdO-V2O5-P2O5:Er3+

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Glasses with molar composition wt.% (90-5-5: 2.5) of $CdO-V_2O_5-P_2O_5:Er^{3+}$ respectively, were prepared by the melting quenching method. The effects of Ag incorporation on structural and luminescent properties were studied. The X-ray diffraction and Raman spectroscopy patterns indicate that all samples were amorphous. Despite of the addition of Ag, absorption bands presented the same form and a little change in the band gap until 5%wt. of Ag. Photoluminescence spectroscopy shows energy transfer from the VO_4 units to the Er^{3+} ions, due to the overlapping between emission spectrum of the matrix and the absorption of Er^{3+}. Emission spectra in the visible range under excitation at 488 nm show that the Er^{3+} related emission intensity increases, reaching the maximum intensity at 1%wt of Ag. Such effect is associated to a distortion of the crystalline field around the Er^{3+} ion. In a similar way, the NIR Er^{3+} emission under excitation at 521 nm, the intensity reaches the maximum at 1%wt of Ag.

[LPM-384] Upconversion and Downshifting luminescent properties in Nanocrystals of (HfO_2)(SiO_2) co-doped with (Tb)^(3+)-(Yb)^(3+).

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In this work we present the synthesis and luminescence properties of $(HfO_2)(SiO_2)$ using the spray pyrolysis technique, hollow spherical particles with a diameter ranging from a few nanometers to a couple of microns were obtained. The shells, nevertheless, have a few nanometers thick and the distribution of diameters have a maximum of around 700nm. XRD analysis shown that the particles are mainly composed by nanocrystals of hafnium oxide domains with sizes of about 14.36nm.

The luminescent properties of the material allow it to be excited with a wavelength of 270nm and have a maximum of emission at 545nm and another at 973nm with this same excitation, it is also possible to excite with a wavelength of 980nm and obtain a maximum of excitation at 545nm which is known as the upconversion process. Whenthe decay times were measured and adjusted, the cooperative process of excitation and emission on hafnium silicate between terbium and ytterbium was confirmed.

So these properties can make this material an excellent candidate to function both as a biological marker and to increase the efficiency of a solar cell.

[LPM-385] Polarized photoluminescence of one-dimensional nanostructures

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Photonic science requires the precise control of polarization and the direction of light propagation, which has been achieved by using macroscopic elements such as lenses, polarizers and retarders. An alternative way to obtain polarized light is through the use of linear semiconductor nanostructures, which by confinement effects allow to obtain a novel carrier recombination dynamics that generates an angular distribution of their luminiscence intensity and high degree polarization that can be exploited for specific objectives since nanometric scale. In this work, GaN nanocolumns were grown by Molecular Beam Epitaxy (MBE) on Si(111) substrates. Structural characterization of the samples were accomplished by in-situ Reflection High Energy Electron Diffraction (RHEED) and Scanning Electron Microscopy (SEM). Growth kinetics observed by RHEED show a fast lattice relaxation the nanocolumns and the diameter distribution were between 50 and 120 nm with hexagonal transverse geometry. The optical characterization was carried out by linearly polarized photoluminescence (PL), where the polarization of the excitation laser was oriented parallel and perpendicular to the c-axis of nanostructures, and for each orientation the integrated optical emission was measured for parallel and perpendicular polarization respecto to the axis of the nanocolumns. PL peak position in all experimental configurations was centered in 3.41 eV and the polarization ratio reached 0.65 when the excitation electric field was oriented parallel to the nanocolumns axis, and the polarization ratio decreases to 0.15 when the polarization of the source was oriented perpendicular to the *c*-axis. This shows a clear influence on the recombination dynamics of the electron-hole pairs by the polarization of the excitation and its relationship with the one-dimensional confinement effects, which is completely inverse to the radiative behavior of metallic nanowires. An analytical model was developed based on the mechanisms of absorption and emission of light in nanostructured systems and their relationship with the electric field in the radiation-matter interaction. The polarized luminescence can also be observed in systems with anisotropic crystalline stresses or directional dependence of the dielectric function, added to nanostructuring effects of the materials, allows a greater control over the degrees of polarization of the light [1].

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[LPM-463] Electroluminescence detection in solar cells by means of eulerian video magnification and a regular industrial camera

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Electroluminescence (EL) in solar cells is presented when a driving current is passed through them, the light emitted by the cells is in the range of near infrared radiation, the intensity of this phenomenon is directly associated to the quantity of minority carriers, their diffusion length, its lifetime, and hence in the quality of the solar cell to transform radiation energy into electrical energy, too. This is the main reason why EL is one of the most used techniques to verify the quality and defects presented in photovoltaic panels, being also a unique scientific research technique to develop new types of solar cells.

Because of the kind and intensity of the radiation emitted in solar cells EL, highly sensitive and expensive infrared cameras are regularly used. This paper presents a technique in which electroluminescence can be visualized using a low-cost industrial camera with a video algorithm called Eulerian Video Amplification and modulated-current reverse bias.

We demonstrate the feasibility of this new EL experimental set-up, to detect defects in solar cells at a low cost, and perhaps with some modifications, its use to detect the weaker photoluminescence effect, working with less expensive cameras.

[LPM-497] Optical and Electrical Analysis of Heterostructures SiO2/MWCNTs/PSi/c-Si.

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Porous silicon (PSi) has been studied extensively due to its photo luminescence (PL) in the visible range at room temperature. PSi layers are useful for various optical and electrical applications among others. The PSi properties can be enhanced using different materials. In the present work, we have decorated PSi single layers with multiple wall carbon nanotubes (MWCNTs). The thickness of PSi layers was determined by the gravimetric analysis, the surface morphology by scanning electron microscopy (SEM), the optical properties were studied by measuring PL and reflectance spectra and the electrical behavior was analyzed from the experimental obtained I-V curves for which some theoretical transport mechanisms are used to make a study in deep. These materials and structures have potential applications in chemical sensors.

Keywords: Porous Silicon, MWCNTs, Photoluminescence, SEM, Morphology, Electrical characterization.

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[LPM-544] Luminescence analysis of ZnS:Mn nanoparticles

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Zinc sulfide (ZnS) has a band gap of 3.6 eV (in bulk) and presents thermoluminescent properties. These properties are present at micro-scale sizes and can be improved in by changing to an a nano-scale sizes. In addition, property such as luminescence can be increased by adding and impurities such as manganese, which has been chosen for this purpose. Spherical and hexagonal ZnS:Mn nanoparticles with diameters of 30 -50 nm were synthesized by hydrothermal process under different conditions. The samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), and UV/Vis and photoluminescence (PL) spectroscopies techniques. The XRD pattern showed that the ZnS:Mn nanoparticles have a zinc blende structure. The results of UV/Vis absorbance indicate a band gap close to 4 eV, which appears to be related to the nanometric size of the obtained powders.

MICROELECTRONICS AND MEMS (MEM)

Chairmen: Norberto Hernandez Como (Centro de Nanotecnologia, IPN)
Horacio Estrada, (CIDESI)
Wilfrido Calleja Arriaga, (INAOE)

MICROELECTRONICS AND MEMS (MEM) ORAL SESSION

[MEM-105] On the development and characterization of a MOEMS based bidirectional flowmeter

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Current microflowmeters can be used accurately in laminar flow conditions for Reynolds (Re) number greater than 50. However, many applications require accurate bi-directional measurement of very low flow rates using a simple and reliable apparatus at low cost. Design and analysis of an interferometric sensing reading of a MEMS-based element has enabled the successful construction and testing of an accurate flow sensor for both bio-medical and pharmaceutical applications requiring low Reynolds number. The MEMS sensing element was constructed with SOI technology and coupled to an optical fiber for position sensing reading, which position correlates to driven drag forces of sensing flow. Experimental results revealed that the devised microscale flowmeter can perform adequately on bidirectional flow at low Reynolds numbers.

In this work we provide: a) detail description of the MEMS sensing element device including its design parameters, FEA analysis, b) fabrications steps, c) integration into a 3D printed prototyping package and a collecting force part, and d) the optical setup of the interferometric reading of MEMS positioning.

[MEM-290] Graphene contacts laser induced to use in the manufacture of 2D devices OFET´s

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Nowadays, the implementation of electronic devices such as OFET's (Organic Field-Effect Transistor) based on organic semiconductor materials is of great importance; since these are able to possess characteristics comparable to traditional inorganic materials, thus becoming a low-cost alternative and opening the way to a new technology, in addition, the term organic can be extended to nanostructured carbon materials (LIG, rGO). We manufacture OFET's device in a 2D architecture, with MDMO-PPV as semiconductor material and contacts of Laser Induced Graphene (LIG), obtaining a totally organic device. The manufacturing consists in obtaining a three-contact pattern of LIG, which is obtained by irradiating an insulating polyamide with a pulsed CO_2 laser, these contacts work as terminals Source (S), Drain (D) and Gate (G) of the transistor; on the other hand, in the separation between S and D we deposit MDMO-PPV to form the semiconductor channel and, in the separation between Source-Drain and Gate, we deposit an insulating material to obtain an equivalent 2D TFT (MOSFET) architecture. The characterization of the device was performed obtaining the saturation curves, where V_{SD} and V_G are in the range of 0-12 Volts and 0-20 Volts respectively. With these parameters the device shows transistor behavior in its characteristic I-V curves; on the other hand, the currents have an increase of three orders of magnitude, when in the S-D channel there is a heterojunction in bulk of MDMO-LIG, thus obtaining saturation currents of the order of micro-Amperes.

Keywords: LIG, OFET, Semiconducting Polymer

[MEM-294] I-V characteristics of flexible ZnO/PEDOT:PSS Schottky barrier diodes with different bending radius

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The fabrication of Schottky barrier diodes (SBDs) using polyimide substrates is reported in this work. Our fabrication process starts with the deposition and patterning of 100 nm of aluminum as cathode. Then 250nm of ZnO is deposited by Sputtering from a Zn target followed by thermal annealing and patterning. Then, SU-8 photoresist is used to isolate each device and to limit the deposition of PEDOT:PSS by drop-casting. Finally, 100 nm of copper or gold were deposited through a shadow mask as the anode. Current-voltage characteristics were obtained with a Keithley 4200 system with sweeps from -2 to 2 V. The diodes were bent at different bending radius (4, 2 and 1 mm). The extracted parameters as a function of the bending radius were: 4.3 to 2.5 diode ideality factor, 0.83 to 0.78 eV barrier height and 4×10^{-8} to 3.5×10^{-7} A/cm^2 saturation current. Our results indicate that the electrical characteristics actually are improved with the reduction of the bending radius which seems to be related to a variation in the carrier concentration of the ZnO film.

[MEM-434] Improving the performance of the two dimensional electron gas AlGaN/GaN HEMTs by thermal anneal

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The AlGaN/GaN high electron mobility transistor (HEMT) main assets are; its ability to handle high power densities, in the range of MegaWatts/cm^2, high lineal current densities at high frequencies, elevated breakdown voltage (1500 V for a single device) and low electrical noise. Performances that stem from the two dimensional electron gas that constitutes its conduction channel, spontaneously formed at the interface of these materials, and the intrinsic properties of both materials forming its structure as; high breakdown electric field ($\geq$3MV/cm), high free carriers saturation velocity, high thermal stability among others. This electronic device offers strong potential for use in high power solid state applications. Nevertheless, presently, these devices suffer from reliability problems as current collapse which occurs after applications of a high drain-source voltage. This effect has been attributed to trapping of carriers by surface states and by defects in the active layer. In addition, defects are a source of noise generation in field effect transistors [5]. This device is realized utilizing epitaxial layers grown on foreign substrates displaying important mismatch on lattice parameters and thermal coefficient resulting in a material containing a high concentration of dislocations and other point defects. The growth of the HEMT structure can be made by MOCVD or MBE, the first at temperatures around 1000°C and the second at lower temperatures; 800-850°C. The remaining of the HEMT technological processes do not involve high temperature processes but the rapid thermal annealing at 800 °C for just a few minutes to reach the ohmic behavior of the source and drain contacts. In spite of the high temperature at which the structure is grown and the long time the growing process requires it has been found that low temperature thermal treatments improve the charge transport properties of this device, mainly the intrinsic conductance of its channel, the maximal and leakage drain currents, the gate charge transport, among others. The experimental details and results will be given in this presentation.

[MEM-446] CIDESI's mems design and fabrication laboratory

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Microelectromechanical systems (MEMS) represent a technology and devices that impact the life of almost every individual in modern society by enabling the miniaturization of sensors and systems with a wide range of applications in industry and science, from automotive to aerospace, from industrial to scientific developments in medicine, optics, metrology, micro-sensors, entertainment and consumer electronics, cellular telephony and communications, biotechnology, computers, and fundamental physics studies. MEMS are micron-sized devices in which mechanical elements and moving parts, can be defined to develop tiny sensors and actuators, fabricated on silicon wafers, as well as on ceramic and flexible substrates. MEMS technology and devices, nowadays, represent a strong and continuously increasing economic boom to those countries in position to develop them, with annual revenues reaching the 50 billion dollars level. Thus, MEMS are of fundamental importance to any (developed and developing) country to maintain or promote industrial leadership and competitiveness.

In Mexico, the development of MEMS prototypes has been limited and somewhat dispersed among a few of academic institutions. It is clear that based on the importance and the economic and technological benefits that MEMS implies, Mexico should establish and pursue a well-planned strategy to promote and enhance the development of this important technology, with great potential to benefit the Mexican industry to increase its competitiveness.

The main purpose of this presentation is to announce to members of the Mexican academic and scientific communities the creation of CIDESI's MEMS Laboratory; it will be focused on reviewing the laboratory's capabilities for the design, modeling, fabrication, testing and encapsulation of MEMS prototypes, to promote and support collaborations on R&D of microsystems across Mexico.

CIDESI has taken the initiative to establish a relatively complete laboratory where MEMS prototypes will be designed, fabricated, tested and encapsulated for their use in the field, in industry, academic and scientific institutions. A 400m^2 clean room was built at CIDESI, with class 100 and 1,000 areas (ISO 5 and 6), to house the infrastructure that will permit the fabrication of MEMS devices based on surface and bulk micromachining of silicon, ceramic and polymeric materials, to initiate the development of micro-sensors with direct application of industrial, medical and metrological interest and relevance.

CIDESI's MEMS Laboratory became a member of CONACYT's National Laboratory for the technological development and innovation of Embedded Systems, Advanced Electronic Design and Microsystems (SEDEAM), and will be, under collaboration agreements, open to members (researchers, professors and students) of the Mexican institutions that lack this infrastructure, to enable them to carry out projects contemplating the development of MEMS microsensors and microelectronics systems. The MEMS laboratory will start targeting the fabrication of mechanical, electrical and bio-sensors, in close interaction with the private and public sectors, to expand activities to other applications in the near future.

MICROELECTRONICS AND MEMS (MEM) POSTER SESSION

[MEM-93] A full-range wireless capacitive pressure system designed for measuring ventricular pressure

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In clinical practice and medical research, the measurement of blood pressure is a critical issue, since any alteration on it is considered as a public health problem, constituting itself as the main risk factor in suffering cardiovascular, cerebrovascular or renal failure. Currently, the commonly used methods for measuring blood pressure are non-invasive devices and catheter systems, which although they are widely known methods, are plagued by many sources of error or are not suitable for a prolonged recording. The development of an implantable blood pressure sensor could open up new diagnostic and therapeutic possibilities. In the particular case of the left ventricle, once getting the local pressure could allow to obtain a direct, precise and real-time values of the blood pressure at the moment of being irrigated to the body. This work reports the novel design of a capacitive pressure sensor (TMCPS) system with a wireless approach for a full-range continuous monitoring of ventricular pressure. The system consists of two modules: an implantable set and an external reading device. The implantable set, restricted to a 2x2 cm^2 area, consists of a TMCPS array that operate from 5 to 300 mmHg, and are connected with a dual-layer coil, for making a resonant circuit. In this design, the two inductive-coupled modules were calculated considering proper electromagnetically alignment, based on two planar coils, 13.56 MHz frequency to avoid tissue damage and three types of biological tissue as core (skin, fat and muscle). The system was validated with the Comsol Multiphysics and CoventorWare softwares; showing a 90% transmission efficiency, at 3.5 cm distance between coils. The implantable module is composed by aluminum- and polyimide-based devices which allows ergonomic, robust, reproducible, and technologically feasible integrated sensors. In addition, the module is characterized by a simplified and low cost design approach based on PolyMEMS INAOE® technology, featured by low-temperature processing.

[MEM-258] Chemical-resistive behavior evaluation of NiO thin film synthesized by sol-gel method for CO detection inside of commercial aircraft

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Currently, aeronautical safety on combustion gases detection (CO, CO_2) and fuel leaks are of basic interest for semiconductor sensors development. The motivation of this work starts around this fact. The main idea is proposing the use of NiO thin film as sensitive element for CO detection inside of commercial aircraft. Nickel oxide (NiO) is a semiconductor which has a chemical-resistive property that allows atmosphere CO monitoring, its presence in concentrations of up to 35 ppm develop intoxication symptoms for carboxyhemoglobin formation on the blood. NiO phase was synthesized by sol-gel method following the route proposed by Nasrin Talebian and Maryam Kheiribse, using nickel (II) acetate tetra hydrated ($Ni\ (CH_3COO)_2 \cdot 4H_2O$) as precursor and methanol. Sol deposition was carried out by mean of deep coating on glass substrate and the thin film obtained was subjected to a heat treatment at 500 °C during one hour in air atmosphere to oxidize the film.

NiO thin film microstructural characterization was carried out using Scanning Electron Microscopy and X-Ray Diffraction; optical and electrical characterization by mean of UV-VIS (Diffuse Reflectance) and Chemical gas sensor measurements respectively. The results showed homogeneous NiO thin film formed by nodular nanoparticles with size between 9-15 nm and thickness less than 100 nm, which was confirmed with DRX analysis. Band gap value was 3.3 eV, which is in agreement with p-type semiconductors. The NiO thin film chemical-resistive behavior was evaluated with the static environment method, where this film interacts with CO concentrations of 1, 5, 50, 100, 200 y 300 ppm. Serpentine electrodes of Au were deposited on top of NiO to get the best chemical gas sensor measurements and determine its sensitivity, and response time in operating temperatures of 100, 200 y 300 °C.

Keywords: NiO, thin film, sol-gel method, CO detection.

[MEM-282] PVOLED electrical simulations with CdSe quantum dots as active layer

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Photovoltaic Organic Light Emitting Diodes (PVOLEDs) came up from the idea of build devices that would be able to emit light but at the same time absorb part of the solar or ambient light, even from the device itself, and reuse it for electrical current generation. These devices have been of interest for applications in mobile devices such as displays.

Modeling and simulation of Organic Solar Cells (OSCs) and Organic Light Emitting Diodes (OLEDs) have been very helpful for the community since they can reproduce experimental data and they give us a better way to study their behavior and also allow us to optimize some parameters such as mobility, thickness, density of states to avoid spending a lot of resources in making and characterizing physical devices. Simulation of PVOLED devices has not been studied which brings a very good opportunity for working.

In this work, we present an accurate set of parameters for simulating a hybrid solar cell and an OLED individually, successfully reproducing the data reported in the literature with a >96% fitting curves. We used Silvaco-Atlas module to simulate a PVOLED in tandem structure incorporating CdSe quantum dots in a blend with Poly (3-hexylthiophene-2,5-diyl) (P3HT) as active layer for solar cell. We varied mobility, photogenerated current, band gap, thickness, and structure bias to study the electrical behavior of this PVOLED device. We present optimized parameters for this structure and the graphs of *I-V* characterization with their corresponding description.

Keywords: *Modeling, OLED, Organic semiconductor, Quantum dots, Simulation, Solar Cell, Tandem.*

[MEM-315] ZnO/HFO2 Thin Film Transistor fabricated at low temperatures.

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In this work, we fabricated thin film transistors based on Zinc oxide (ZnO) in a Bottom Gate – Top Contact (BGTC) configuration, using hafnium oxide (HfO_2) used as a dielectric deposited by ALD at 100 ° Celsius, the electrical parameters were extracted from the transfer curve.

Using as a substrate (as common gate for all channels) highly doped silicon wafers with an resistivity of 0.001 Ohm/cm, the cleaning of the substrate is done with conventional piranha solution and HF 10%, in the cleaned wafer is deposited the HfO_2 (26-29nm) used as dielectric by ALD at 100 °c, immediately after is deposited the ZnO by RF-Sputtering (-60nm), completed the deposit, the transistor is designed with two masks, the first defines the ZnO channel with conventional photolithography and is attacked with 1% HCl, defined the pattern we proceed to use the second mask defining the aluminum contacts (150nm) by Lift-off.

[MEM-358] Characterization of thin nanostructured TiO2 films as a function of morphology

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A study about the morphology effects on photoluminescence intensity of TiO_2 films is presented. The nanostructured titanium oxide films were obtained by an anodization technique using titanium foils. The morphology is analyzed by means of Scanning Electron Microscopy (SEM). The atomic composition was determined by EDS and Photoluminescence (PL) spectra analysis.

In order to obtain different nanostructured films, several electrolytic compositions are analyzed as precursors. Hence, we demonstrated that the water-$NaSO_4$ ratio could directly influence in the morphology and optical characteristics of the films. Using SEM tools the following morphology films are analyzed: a) highly self-ordered nanotubes with uniformity in diameter, thickness and density distribution, b) amorphous films with varied nanoporous and other types of nanoparticules. The PL intensity, as a tool, showed that the self-ordered nanotubes have better intensity than the nanoporous and nanoparticle films.

[MEM-371] Characterization of inter-metallic Mobius connection in resonant oscillators using nanoscale CMOS technologies

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The Rotary Traveling Wave Oscillator (RTWO) has two ring-shaped differential transmission lines as resonator and it is connected at their ends or terminations by a Mobius connection. Due to the characteristics of the advanced Complementary Metal-Oxide-Semiconductor (CMOS) manufacturing processes, the resonator ring cannot be implementd as a medium with a constant characteristic impedance, and due to the sequence of the CMOS manufacturing steps, the transmission lines forming the resonator contains corners, overlaps and bends that alter the transverse area of the resonator. The most complex discontinuity of the RTWO resonator is the Mobius connection; this discontinuity is generally implemented using angles of 90° or 45°, different metal (aluminum and/or copper) levels and arrays or stacks of intermetallic connections (vias). In this work we characterize the 45° Mobius connection commonly used in the RTWOs and ROAs (Rotary oscillator arrays) for different geometrical configurations in three CMOS technologies. The results show that the Mobius connection commonly implementd using the last two top metal levels is not the most optimal and using lower metal levels it is possible to reduce the inductance and capacitance parasitic in these connections up to 24%, 45% and 35% for the technologies of 180nm, 130nm and 90nm, respectively.

[MEM-386] UV detector fabrication employing ZnO self-assembled nanostructures

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There a great interest in to develop UV detectors to strategic applications such as secure communications or monitoring UV spectrum. There are several approaches to the production of p-n junctions to that purpose using ZnO or GaN nanostructures. Here the results of the characterization of detectors fabricated employing ZnO self-assembled nanostructures deposited by RF reactive sputtering are presented. The procedure developed by M. Avila-Meza et al. [1] was employed to deposit ZnO nanostructures on 4 inches p-type silicon substrates. Substrates were processed at CICTA-UACJ using a mask with circular 1 mm diameter Cr. Squared samples 2 mm side were diced and then bonded using Al wire on a rectangular 8 pin frame. Transport properties (I*vs*V and C*vs*V) of selected samples were characterized using an Agilent commercial equipment. The spectral response of the measured samples was obtained and correlated with electrical characteristics.

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[MEM-562] Synthesis and characterization of thin layers of Ga2O3 by spin coating method

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The nanostructured semiconductor oxides are being investigated intensively during the last years. There is great interest in its optical and electronic properties due their wide band gap, like the Indium oxide, Titanium oxide and the Zinc oxide. These materials exhibit optical transparency in the visible light spectrum and an electrical conductivity close to the typical of semiconductors. The Gallium oxide (Ga_2O_3) is an oxide semiconductor that presents different optical, electrical and structural properties that makes it a very interesting material for use in the manufacture of new devices and technological advance. The cost of producing semiconducting materials has always been a disadvantage for its development, which is why we seek to reduce the cost of production while the quality of this is maintained. The Spin Coating method reduces the cost of its production, as it is a low-cost equipment compared to other methods of synthesis and deposit. This allows to create thin films with different thickness and little material. For this reason in this work our main objective is the obtaining of the nanostructured material by spin coating. To achieve this, several experiments were carried out with substances at different molarities and deposit speeds, varying the times and obtaining nanostructured Ga_2O_3 on Si and GaAs substrates.

All this in order to characterize it and analyze the results with favorable electrical and optical properties for use in integrated circuits, electronic equipment such as transistors as well as its use in solar cells. The nanostructured films of gallium oxide obtained are characterized using the techniques of X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM). This allows knowing and reporting its physicochemical and electrical properties. Finally, we can mention that knowing the properties of the films we will be able to give an application to the films obtained.

Keywords: gallium oxide, nanostructure, semiconductors, spin coating.

NANOSTRUCTURES (NSN)

Chairmen: Yenny Casallas (UPIITA-IPN)
Esteban Cruz Hernández (CIACYT -UASLP)

NANOSTRUCTURES (NSN)
ORAL SESSIONS

[NSN-21] Photoluminescence of Multi-Quantum Well AlGaAs/GaAs(631) heterostructures: confinement/ dimensionality effects.

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In the last decades a new field of research called wave engineering has opened a vast range of quantum applications in the field of high performance optoelectronics and transistors using ultrathin (nano) heteroestructures. The fabrication of superlattices (SL) it's a matter of special importance regarding the design of optoelectronics (e.g. lasers) in behalf the ability to handily design the electron's wave function and energy nested in these heterostructures. This work deals with the growth an optical characterization of AlGaAs/GaAs MQW over the surface of (631) GaAs type A substrates. The intrinsic anisotropic properties of this crystallographic plane is optimal to achieve nanocorrugation that for instance conduces to the self-assembling of quantum wires (QWRs) or one-dimensional (1D) confinement. Previous work demonstrated the nanocorrugation of the surface strongly depends on the beam equivalent pressure of As (P_{As}) and Ga (P_{Ga}), then as well the pressures ratio $P_r = P_{As}/P_{Ga}$. In this work the optical properties AlGaAs/GaAs MQW heterostructures grown as a function of P_r and with different QW widths Lw are studied. The MQW heterostructures consists of five periods of 10 nm AlGaAs barriers. For the GaAs wells we used Lw = 2, 3 and 4.5 nm. Furthermore, for each L_w the P_{As}/P_{Ga} ratio was diversified to achieve distinct corrugation order. 14K PL spectroscopy of the samples showed the transitions (A^0,C) and (B,B) located at 1.494 eV and 1.512, respectively.[2] In addition, the QW-related transitions are observed above 1.55 eV, whose position depends on the growth conditions and the sample structure. As it can be expected the energy of the QW emission blueshifts as the QW width is decreased from 4 nm to 2 nm, at constant P_r. On the other hand, for L_w =3 nm and P_r =22 the QW emission is located at E_w= 1.598, while for the sample grown with the L_w=3 and P_r =10, the QW transition is observed at Ew=1.638. The shift has been associated to changes on the dimensionality of the electron confinement, i.e. the quantum confinement transition from 2D to 1D. Finally, through AFM characterization the corrugation of the samples surface was verified even on the last of the grown layers.

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[NSN-47] Electronic distribution in a nanowire Y-junction under an external electric field

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One-dimensional systems (1D) are those in which charge carriers can move along a spatial direction, while they are quantum confined in the other two directions. Due to the strong interaction between electrons, excitons, phonons and photons, these systems have unique properties that have made them one of the nanostructures with high application potential in nanotechnology.

Recently, new nanoelectronic elements such as 1D system junctions are being proposed to form bifurcated (or Y-type) wire structures. These systems consist of three terminals that make up the structure Y of lengths of a few micrometers and radii of tens of nanometers. The Y junctions present an unique switching behavior and great potential to be used as a new type of logical device in nano-electronics.

In this work, we present a theoretical study, based on experimental parameters, by developing a model which is able to calculate the electronic and transport properties in the Y-junctions. We also report different behaviors of an 1D electron gas when it is transported by different terminals and the electron gas density and the external electric field values are varied. Finally, our results are compared with available experimental data showing a good agreement.

[NSN-66] Chitosan nanoparticles and propolis extract coating for strawberry quality preservation

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Nowadays, the use of coatings to preserve horticultural products is of great interest. Also, application of Nanotechnology as an emerging science due to the more effective surface area-to-volume ratio, is a good way to potentiate the effect of new materials. In this work, chitosan nanoparticles were synthesized using the nanoprecipitation method, in which 2.5 mL of the diffusion phase (acetic acid and chitosan) were added to 40 mL of the dispersed phase (ethanol and propolis extract) using a peristaltic pump and kept under stirring. Once the nanoparticles were formed, the obtained solution was placed on a rotary evaporator to eliminate the solvent and stored under refrigeration (4 °C). Propolis extract was obtained by maceration with ethanol (90%) and ultrasonication technique (1 h). After that, the solvent was removed (1 week) and the different propolis extract concentrations were elaborated: 10, 20 and 30%. Six formulations including chitosan, glycerol, chitosan nanoparticles and propolis extract were elaborated. The coatings were characterized by Transmission Electron Microscopy (TEM) and dynamic light scattering (DLS). Also, the sensory properties on strawberries were evaluated after 8 days storage at 4 ±1 ^{o}C. The results showed that the best formulation was composed of 33% chitosan nanoparticles and for the extract concentration of 10%. From TEM micrographs spherical in shape and well dispersed nanoparticles inside the coating were observed. Size particle was 291 ± 6 nm and Zeta potential value was 21 ± 1 mV demonstrating a good stability of the coating. Related to sensory properties of the strawberries after 8 days storage, weight loss was 9%, a lower value compared to the control (17%). Firmness, color, soluble solids and antioxidant capacity were kept for the fruits. In the near future, the coating will be tested *in vitro* to assess the antimicrobial activity in different bacteria and fungi.

[NSN-76] Electrical, structural, and optical behavior of graphene/ ZnO layers

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Nowadays, ZnO/G has attracted interest as a highly efficient means of manufacturing photovoltaic cells for energy production. ZnO based nanostructures have attracted a great interest because of their scientific and technological applications, due to its wide bandgap (3.37 eV) and large exciton binding energy (60 meV) [1-2]. On the other hand, graphene is the most fascinating nanomaterial because of its unique structure of carbon atoms arranged in hexagonal honeycomb lattice, and with fascinating mechanical, thermal, optical and electrical properties [3-4].

Graphene was synthesized via the liquid phase exfoliation method and ZnO solution was prepared in DI water and methanol. The graphene is mixed with ZnO solution to form of graphene/ZnO nanocomposite. Finally, the mixture is used to produce thin films by Ultrasonic Spray Pyrolysis at 450 °C. Their composition, morphology, structure, transmittance and electrical performance were characterized by scanning electron microscopy, transmission electron microscopy (TEM), x-ray diffraction, uv-vis spectroscopy, Raman Spectroscopy, I-V curves. The results showed that graphene composited presents ZnO nanoparticles and its behavior could be used to fabricate optoelectronics devices.

Furthermore, spray pyrolysis is a simple method to deposit a thin oxide layer by direct spray of precursor on hot substrate and it can be a good candidate of a costless method compared with another expensive technique to produce graphene, like: CVD, PECVD and Epitaxy.

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[NSN-96] The Secret Life of Nanoparticles: often ignored characteristics that impact interactions in chemical, biological and environmental systems

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There is an increasing awareness of reproducibility issues in many areas of science including those associated with materials, biological, computational and chemical research. Engineered nanoparticles can be designed to have behaviors and properties that are helping to advance treatment of diseases, improve water quality, enable advanced electronics and produce sustainable energy at low costs. However, nano-objects, present fundamental synthesis, characterization and handling challenges that are often ignored or unrecognized by parts of the scientific and technical community. The frequent tendency of such particles to interact with surrounding media and to respond to environmental changes complicates understanding their properties as a function of time in different environments but also presents interesting opportunities. These behaviors impact research reliability, impact product lifetimes and cause inconsistencies and conflicts in the literature. Important issues include knowing about the rate at which they change after synthesis, during storage and processing, and in different media. This presentation will highlight some of the general behaviors of nanoparticles using research on Fe oxide-shell metal-core, ceria, and Ag nanoparticles.

[NSN-119] Synthesis and characterization of carbon nanospheres/polymethylmethacrylate composites

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In recent years a variety of carbon nanomaterials including nanospheres, nanotubes, nanosheets and nanofibers have been studied due to their unique mechanical properties, electrical and thermal conductivity, making them a suitable material for many applies in electronics, aeronautics, astronautics industries and many others. It is common the carbon nanotubes (CNTs) use as reinforcement in advanced composites developing. Nevertheless the problem is the CNTs agglomeration due Van der Waals forces which causes a poor dispersion in the polymer matrices.

Carbon Spheres (CSs) is another material which is ideal and promising in substantial enhancing the mechanical and electrical properties of composites due to their high specific surface area and electrical conductivity. In this study CSs, previously obtained by chemical vapor deposition, were incorporated in polymethylmethacrylate (PMMA) matrices. Nanocomposites with 5, 7 and 9 wt % CSs concentration were synthetized through mixing solution at 250 rpm during 2 hours, after they were kept at room temperature until complete solvent evaporation (toluene). The CSs/PMMA were characterized by different techniques. Scanning electron microscopy showed the CSs embedded in PMMA. The characteristics CSs peaks were observed at 1382.24 cm^{-1} corresponding to D-band, G-band at 1587.09 cm^{-1} and G´ at 2738.89 cm^{-1}, identified through Raman spectroscopy. Fourier transformed infrared analysis determined the main functional groups corresponding to C=O, CH, CH_2 and CO stretching. The nanocomposites were evaluated by Vickers Microhardness (HV) and the electrical conductivity measurement. The electrical conductivity and hardness increased according to the CSs concentration. The composites with 9% CSs content showed the double microhardness improvement respect to the pristine polymer, reaching conductivity values up to 7.76 x 10^{-2} S/m.

In summary, carbon spheres were incorporated in polymethylmethacrylate matrices using an inexpensive, simple and effective method. CSs/PMMA composites with improved properties in comparison to the pristine PMMA were synthetized. These composites can be used for multiple future applications in several areas.

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[NSN-135] Magneto-transport characteristics of nanosheets of graphene in different microstructures and morphologies

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Two semiconductor carbon nanowalls (CNWs) samples with different morphologies (such as length and edges) and internal microstructures (presence of defects, interfaces and interlayer space of graphene) reveal differences in the electrical and magnetotransport MT properties. The quasi-2D wall is formed by few graphene layers in a vertical deposition. The two CNWs (called Sample 1 and Sample 2) were grown by a Plasma Enhanced Chemical Vapor Deposition (PECVD) process varying deposition temperature and Ar flux. Scanning electron microscopy, transmission electron microscopy and Raman spectroscopy were used to substantiate the structural and morphological differences. Sample 1 showed a prominent magnetoresistance (presence of weak localization and antilocalization) and higher conductivity with respect the Sample 2. These behaviour is explained in terms of the effect of electron scattering at reactive edges, more number of defects and boundaries and dense crystalline regions separated by interfaces. Also, this last characteristic leads to a neglected landau level in the Quantum Hall Effect, suggesting that the internal microstructure is important. Our results propitiate a way towards the use of vertical graphene or CNWs in magnetoelectronic nanodevices with magnetic properties tuneable through their morphology and microstructure.

[NSN-246] Characterization of bifenthrin nanoparticles produced by Laser Ablation of Solids in Liquids.

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In the present work colloidal organic nanoparticles were synthesized by laser ablation of solids in liquids, using deionized water and PVA solution as liquid medium. The ablated material was a commercial bulk target of bifenthrin insecticide. The UV-Vis spectroscopy allowed obtaining the characteristic absorbance spectrum which on one side confirmed the presence of the nanoparticles and on the other, by the level of absorbance their concentration. Structural and size characterization was carried out by TEM. The crystal structure of the nanoparticles was studied by comparing the interplanar distance of the nanoparticles determined by TEM with the interplanar distances of the bulk material observed in XRD. The nanoparticles sizes varied between 3 and 20 nm, with a narrow size distribution. Males and females of *Drosophila melanogaster* were used in order to test the toxicity of the obtained colloids. The results showed that the lethal dose can be achieved at short times with lower concentrations in comparison with doses commonly applied when bulk material is used.

[NSN-286] Inorganic nanotubes by the template based ALD method.

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Dimensionality is a crucial factor determining the properties of nanomaterials. The 1D structure has properties such as high aspect ratio and large surface to volume ratio which play an important role in applications like optoelectronics, nanoelectronics and photocatalysis.

Here we present a very suitable approach to obtain inorganic nanotubes (NTs). The method is based in the usage of carbon nanotubes (CNTs) as templates when coated by atomic layer deposition (ALD). Different type of templates have been explored to favor the template-ALD precursors interaction at the initial stage, resulting the nitrogen-doped CNTs (CNx) as the more efficient templates. The method allows the control on the wall thickness of the inorganic NTs down to the nanometer level. Moreover, the NTs composition can be modified or even radial heterostructures can be designed. Once the ALD coating has been achieved on the CNTs templates, the template can be removed by oxidation either in dry air or in an ozone-rich atmosphere. The template-based ALD method has shown versatility to generate free standing nanotubes with yields of milligrams per batch.

The different stages of the template based ALD method for NTs have been developed and characterized in detail by techniques such as: TEM, high resolution EDXS line scans, SAED, Raman spectroscopy, TGA and XRD.

Finally, the potential of the method for the design of 1D nanostructured building blocks for applications is shown with two illustrative cases in the photo-catalysis and nanoelectronics fields.

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[NSN-320] Single ZnO nanowire-based gas sensors

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Nanostructure-based devices (carbon nanotubes, superconducting wires, inorganic nanotubes, etc.) are promising participants of the next sensor generation.

Nowadays, rigorous safety and environmental regulations requires high-performance monitor and sensor systems; improved and high sensitive sensors are the key components. In the case of chemical management, either in industry, research labs or home, low concentrations of hazardous gases are difficult to detect with common gas sensors. Semiconductor nanostructures as sensor elements are proposed to meet the high-sensitivity requirement.

In this work, we studied the conductometric response (electrical resistance) of single ZnO nanowires tested as gas sensor elements and explore their capability to detect very low concentrations of H_2.

Single ZnO nanowire gas sensor devices were fabricated by manipulation and electrical connection of single nanowires into a four-electrode aluminum probe. Device fabrication was *in situ* carried-out in a dual-system scanning electron microscope-focused ion beam with a manipulator and a gas injection system in/column. Gas sensors were operated in a gas concentration-controlled chamber. The electrical response of single-wire devices shows response times up to 29 s for a 121 ppm of H_2 pulses, with a variation in the nanowire resistance appreciable at room temperature and at 373.15 K of approximately 8% and 14% respectively; ZnO nanowires are good candidates to detect low concentrations of H_2.

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[NSN-373] Biomimetic Sol-Gel TiO2 Synthesis

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TiO_2 is a semiconductor used in photocatalysis, solar cells, self-cleaning coatings, etc. These broad applications depend on its crystallinity and size, which implies a precise control in its synthesis.[1] The synthesis of materials with high level of precision in size, shape, and composition has been achieved by nature, where living organisms are formed of biomineralized inorganic structures.[2,3] However, achieve this ideal synthesis in the laboratory is still a challenge for scientists, is for this reason that we are interested in mimic nature.

In this work, we explored the biomineralization process in vitro of TiO_2. We used a heptapeptide to synthesize TiO_2 nanoparticles of anatase at room temperature. The peptide act as a hetero-ligand that control the growth and crystallinity of the nanoparticles. If a residue in the peptide sequence is modified, the control in biomineralization is diminished, indicating that the overall sequence is necessary to achieve the adequate material.[4] On the other hand, to increase the complexity of the TiO_2 structure, we used a bacteriophage as a biotemplate for the synthesis of mesoporous TiO_2. This template allowed to obtain a narrow pore size distribution as well as low microporosity due to the highly stable filamentous structure.[5] Thus, biological templates can be used to get novel nanostructures of inorganic materials employing greener synthesis routes.

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[NSN-409] Preparation of metallic nanostructured substrates by pulsed laser deposition for Surface-Enhanced Raman spectroscopy (SERS).

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The nanostuctures are synthesized by laser ablation using a Nd: YAG laser emitting at a wavelength of 355 nm with a pulse duration of 10 ns. The target is placed inside a vacuum chamber at a pressure of $2.5x10^{-5}$ Torr. Nanostuctures are made by varying the number of pulses and the laser energy density. The nanostructrres are characterized in some cases by high resolution electron microscopy HRTEM and TEM. UV- Vis spectroscopy is also reported. The influence of the morphology and distribution of nano-structured gold, silver, cooper and aluminum substrates on the localized surface plasmon resonance wavelength and surface enhanced Raman signal (SERS) is investigated. The SERS studies were performed using methylene blue as test molecule at different concentrations. It is found that the SERS signal increases monotonically with the size of the Ag, Au, Cu, Al nanoparticles and exhibits a máximum for a particular morphology. An analysis of the SERS spectra is performed employing a derivative procedure. We have analyzed a characteristic peak of the test molecule: MB in (1627cm-1) characteristic of a carbon ring v(C-C) by computing the corresponding derivative against wavelength. A jump between derivatives was found. The surface plasmon wavelength shows a strong dependence on the nanostuctures morphology which evolves progressively from nanospheres to more complex shapes.

[NSN-467] Interface understanding of nanomaterials' surface functionalization

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Development and design of new materials with surfaces that present an organized arrangement of organic and inorganic functional groups, has gained research importance. Surface modification by chemical or morphological alteration, has been widely used in order to achieve functionality of Nanomaterials. When modified, the surface gets different characteristics in comparison to the initial material. Changes are possible through functionalization, bringing new features and properties to a material by changing its surface chemistry, generating novel materials. In this work we describe the functionalization of nanoparticles with different coupling agents. For the different applications of those modified nanomaterials, the understanding of the interface and chemical modification is of prime importance for the optimized use and correct application of those nanomaterials. The nanoparticles and nanomaterials were characterized by different techniques including XPS, SEM and EDS among others. The results obtained shown the effect of the functionalization on the surface of the nanomaterials and the functionality gained by its chemical modification.

[NSN-535] Quantitative Chemical Measurements of Core-Shell Nanoparticles

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Nanoparticles are increasingly employed in a variety of areas ranging from healthcare to photovoltaics. Their utility depends upon the manner in which they interact with their surroundings, for example, whether they are well dispersed, or can chemically bond to other species. These properties are a function of the chemistry at the interface between the particle and their medium. Whether intentional or not, the surface, or shell, of a nanoparticle is almost invariably different to the bulk, or core.[1] Characterisation of such shells is extremely important to understand the performance of nanoparticles in applications where consistency in behaviour is demanded. Organic coatings, in particular, are challenging to study by traditional approaches, such as electron microscopy and X-ray scattering. This coatings are vitally important for example in biomedically relevant particles, which often have delicate organic coatings consisting of polymers and biomolecules.

In this talk, methods which are capable of measuring the amount of material in the shell such as centrifugation, light scattering and optical spectroscopy will be considered, since these may be applied to particles in colloidal suspension with minimal preparation.[2-4] However, these methods are confounded by a number of artefacts and assumptions as well as an inability to measure the chemical composition of the shell. In contrast, XPS provides a quantitative analysis of both the amount of material in a shell and its composition. There are two main challenges to this approach: sample preparation and data interpretation. A simple method for measuring shell thickness from XPS data is available,[5] and this has now been validated[6,7] and extended[8,9]. An Excel spreadsheet to perform the calculations is freely available on the NPL website[10]. This talk provides an overview of the challenges of nanoparticle characterisation and describes the practical use of XPS in this context.

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[NSN-543] Study of the nanostructure catalyst by XAFS technique at SSRF

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In this talk the XAFS beamline and related techniques at Shanghai Synchrotron Radiation Facility (SSRF) will be first described. Then some typical applications in the field of nanostructure catalyst will be given. In the last several new beamlines for surface science at SSRF will be introduced, especially the energy materials beamline, combined with the two techniques of XAFS and XPS, which will become a powerful tool to study the nanostructure catalyst materials in the near future at SSRF.

[NSN-546] International standardisation of terminology and measurement for graphene and nano-objects

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In this talk I'll discuss the why, what, when, how of international standardisation of nanotechnologies and in particular graphene and related 2D materials and nano-objects. Valid measurement methods and standardisation are vital for industrial confidence. Potential end-users of innovative materials such as graphene and highly designed nanoparticles must be able to rely on the advertised properties in order to instil trust in this emerging industry. To help, international experts are developing measurement standards in ISO TC229 (nanotechnologies) and ISO TC201 (surface chemical analysis) amongst other committees. This includes a key set of standards to determine the properties of graphene in both powder, liquid dispersion and CVD sheet form led by NPL.

In order to validate these and other draft standards, VAMAS interlaboratory studies are undertaken. NPL led studies in nanoparticle shell thickness, nanoparticles concentration and graphene characterisation will be discussed.

Those interested in this field come from different backgrounds, for example, physicists and biologists and can be scientists, regulators or NGOs, for example. To avoid any misunderstandings, and to facilitate both comparability and the reliable exchange of information, it is essential to clarify the concepts, to establish the terms for use and to establish their definitions. The ISO standard on terminology for 2D materials has recently been published and the terminology for nano-object characterisation is being revised. The standards mentioned here will be outlined along with other standardisation and prestandardisation projects.

NANOSTRUCTURES (NSN)
POSTER SESSIONS

[NSN-5] Study on the application of Raman Spectroscopy for early detection of cervical cancer

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Cancer is a disease in which cells in the body multiply without control. When this starts in the neck of the uterus, is called cervical cancer, or cancer of the cervix. Cancer can spread to the other parts of the body later. Cervical cancer is one of the leading causes of death from cancer among women around the world. Most of these deaths occur in low and middle-income countries. The primary cause of precancerous lesions and cervical cancer is persistent or chronic infection with one or more of the “elevated risk” (or oncogenic) types of human papillomavirus (HPV). In these patients a tumor marker system could be an additional tool to derive the status of the tumor. Subsequently, these markers may be useful to correlate with response to anti-cancer treatment and recurrence of the disease. Increases in the levels of sialic acid can be considered as potential inflammatory marker which would serve to aid in the diagnosis, prognosis and monitoring cancer therapy. Thus, using spectroscopy Raman with silver nanoparticles (NPsAg) is seeks to determine the concentrations of sialic acid in patients with cancer women with benign and precursor lesions and invasive cervical to determine the stadium of the people about development of cancer. Already existing previous tests with this technique which has already measured the concentration of sialic acid in women with other types of conditions which have provided saliva samples, and which found them the concentration of sialic acid.

[NSN-6] Nanocatalyst of CuNiPt alloy, supported on reduced graphene oxide

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Controllable synthesis of non-noble alloys remains a significant challenge. Among core-shell nanoparticles of various combinations, those made of an inexpensive metal core and a noble metal shell has received particular attention.

The cores obtained with phases (111) which facilitate coverage at the same stage by the platinum which greatly favors the oxygen reduction reaction.

Nano-catalyst of NiCu is synthesized by two steps; reduction of non-noble metals as nuclei and decoration of platinum (shell) by galvanic displacement. New synthesis of catalysts for the reduction reaction of oxygen by the adequate amount of oleylamine and oleic acid and precursor salts of non-noble metals, Cu (acac)2 and Ni(acac)2 , and using morpholine borane as a reducing agent, and supported on a reduced graphene oxide matrix which confers electronic density to the catalyst. The prepared NiCu@Pt octahedral core-shell were characterized by TEM, octahedral nanoparticles have narrow size distribution, with a measured average edge length of 30 ±5 nm. The EDX analysis by elemental mapping show that three elements were found homogeneously distributed throughout nanoparticles. The XRD pattern shows characteristic peaks, it suggests that CuNi is decorated whit Pt. The metallic core inherits the crystal structure of its composing elements, i.e., the face-centered-cubic (FCC) structure. The diffraction peaks at can be assigned to (1 1 1), (2 0 0), (2 2 0) and (311) crystallographic planes, respectively, which correspond to FCC phase. The electrochemical performance of NiCu decorate with Pt/C was evaluated by cyclic voltammetry, CO stripping and rotating disk electrode in HClO4 as electrolyte. NiCu@Pt/C shows better catalytic activity in terms of mass activity 311mA/cm2 and specific activity, which is 246 mA/cm2 , respect to commercially available 20-wt% Pt/C-Etek® with mass activity of 105 mA/cm2 and specific activity of 184 mA/cm2 .

[NSN-17] Study of the effect of spherical gold nanoparticles in PNIPAM bulk hydrogel and chlorophyll solutions

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This work is mainly focus to analyze the effect of spherical gold nanoparticles (Au-NPs) in two systems: PNIPAM thermosensitive bulk hydrogel and aqueous chlorophyll solutions. In order to insight the effect in both systems, spherical gold nanoparticles of around 20 nm diameter were chemically synthesized and analyzed by absorbance spectroscopy, which allowed to identify its characteristic surface plasmon resonance (SPR) peak at 534 nm. To analyze the effect of the presence of the nanoparticles in the first system, the thermosensitive PNIPAM hydrogel was chemically obtained in bulk form, and then 5 different concentrations of Au-NPs were placed in a 1X1X1 cm piece of the hydrogel. After that, the hydrogel+Au-NPs system was illuminated with a 532 nm continuum laser, wavelength which is very close to the SPR. It was founded that the hydrogel with larger concentration of Au-NPs experiment a faster volumetric phase transition, characterizing the thermosensitive hydrogel, than the other concentrations. The observed behavior is explained due to the SPR induce vibrations in the water molecules contained in the hydrogel, which allowed the necessary heating process for the phase transition. The effect in the second system was analyzed by extracting chlorophyll from spinach leaves in water and then including different concentrations of Au-NPs. The effect of the nanoparticles was corroborated by monitoring the photoluminescence (PL) of the chlorophyll+Au-NPs system under different excitation wavelengths. The PL intensity was observed to decrease when increasing the concentration of Au-NPs. In the last system, the correlation between the PL intensity and the presence of Au-NPs could be useful for bio-sensing proposes, for example changing the nanoparticles by ions or molecules of interest.

[NSN-19] Analysis of the 2D-3D transition during the MBE growth of stacked InAs/GaAs quantum dots.

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In(Ga)As semiconductor quantum dots (QDs) as low dimensional materials have been continuously studied due their interest in their optical and optoelectronic properties, which have improved significantly the performance in nano-devices.[1] However, there are still some challenges to be overcome in order to reach the successful implementation of the QDs structures in common devices, that is the case of the vertical alignment in multilayer heterostructures. The QDs by MBE are synthesized employing the Stransky-Krastanov growth mode, which is based on the InAs/GaAs lattice mismatch, hence the heterostructure is intuitively strained.

In this work, the insitu analysis of the growth of stacked InAs QDs was studied, with the purpose to obtain the parameters involved in the process of diffusion and nucleation. Five periods of InAs/GaAs were deposited for the structure. In each period, 2.1 ML InAs was grown followed by 20 nm of a GaAs capping layer. Finally, the structures were ended with 200 nm of GaAs. The 2D-3D transition of InAs was studied by monitoring the RHEED 002 diffraction spot intensity during the InAs nucleation. It was implemented an analytical model to analyze insitu the nucleation and diffusion parameters of the QDs growth, which was recently proposed by Eugenio et al.[2] Fitting procedures of the model to the RHEED QDs nucleation curves for each one of the stacking layers, indicated that the critical thickness (H_c) decreases as the number of deposited QDs layers increased. This is due to the accumulated strain for successive layers.

Conversely, despite the successive growth of multilayers of QDs the adatoms diffusion length remained almost constant, which means that the density of the QDs is the same in each of the stacked layers. Regarding this observation, it is worth to comment that the vertical alignment of the QDs is a well-known process, promoted by the creation of low-strain nucleation centers above each one of the capped dots. Numerical simulation of the strain tensor $\in_{xx}$ calculated along a vertical slice that cuts the center of the QDs showed that its highest value is reached just at the QDs apex ($\in_{xx} = 1.2$) and it steadily decreased down to $\in_{xx} = 0.34$ once the QDs are capped with 20nm of GaAs, but it never returns to zero. Therefore, the InAs of the forthcoming layer is grown on a locally tensile strained layer of GaAs, allowing for the vertical alignment of QDs.

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[NSN-24] A DFT study of the magnetic and electronic properties of FePtx (x = 10, 11, 12) clusters

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Due to their magnetic properties such as, great values in the magnetization and high magnetic anisotropy and high values in reactivity index, FePt binary clusters are candidates for ultra-high magnetic recording media and thet are good candidates for catalysis. In these nanosystems the mixing of atoms is favored and the magnetic order is ferromagnetic-like, which can be contrasted to pure Pt and Fe clusters. In this work, we present DFT results for electronic properties such as chemical hardness and the value of the local magnetic moments. The calculations were made with the VASP (Vienna ab-initio Simulation Program) code with the Perdew-Burke-Ernzerhoff approximation for the exchange-correlation potential. VASP solves the Khon-Sham equations in the augmented plane wave basis set, taking account the core electrons within the projector augmented wave method. Our results show that the mixing of atoms is favorable and all the clusters pure and nanoalloys present magnetic behavior preferently with ferromagnetic-like order. In FePt clusters, the value of the total magnetization is greater than the corresponding magnetization of the respective pure Pt clusters; the Fe impurity gives the main contribution to the total magnetization.

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[NSN-33] Hydroxyapatite-Au nanostructures as drug delivery system for Doxorubicin

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Doxorubicin, an anthracycline antibiotic, is one of the most effective cytotoxic drugs for the treatment of several neoplastic conditions, such as leukemia, soft tissue and bone sarcomas, breast and ovarian cancer, among others. However, the clinical utility of this drug is limited for its side effects especially, cardiotoxicity. An approach to reduce these side-effects is the use of nanoparticles-based drug carriers. Nanoparticles and nanostructures have gained ground in drug delivery systems because they possess unique physical, electrical, magnetic and optical properties due to the effects of quantum mechanics in a nanometer scale. Besides, they offer a lower exposure of healthy tissues to the cytotoxic drug; thanks to the enhanced permeability and retention effect. Composites systems are attractive because they can group the properties of each of the species into a single entity to obtain a material with superior properties to any of the species present separately. Hydroxyapatite (HA) has excellent biocompatibility due to its similar structure to human bone, as well as its good capacity of drug adsorption. On the other hand, the Au nanorods possess practically no toxicity to the human body due to their high chemical stability, they also possess the property of Localized Surface Plasmon Resonance (LSPR), which has made the Au a widely proposed material for drug delivery and photothermal therapy (PhTh). The gold nanorods can be used in PhTh in a range of electromagnetic radiation called the water window (700-1200 nm), so the LSPR have to be between these limits to damage in the minor way the healthy cells. In this project, hollow $CaCO_3$ nanostructures were obtained by a precipitation of $Ca(NO_3)_2$ with Na_2CO_3 using SDS as a stabilizer. The hollow $CaCO_3$ nanostructures were transformed in HA without affecting the morphology of the material using Na_3PO_4 solution via microwave. In the other hand, the synthesis of Au nanorods was made by the typical seed-mediated growth method. The HA-Au nanocomposites were synthesized by an immersion method of the HA nanostructures in a diluted solution of Au nanorods. The precursor and transformed materials were characterized by FTIR, XRD and SEM. The gold nanorods were characterized by UV-Vis and SEM. The HA-Au nanocomposites were characterized by UV-Vis DRS and SEM. The resulting hollow HA-Au microspheres nanocomposites were explored to study the drug loading and release properties of doxorubicin (DOX) under absence and presence of infrared radiation. The experimental results show that the HA-Au material is promising for drug delivery and control dosage applications.

Keywords: Hydroxyapatite-Au, Hollow microspheres, Drug delivery system

[NSN-45] Derivation of an effective potential for many-electron interacting into doped nanostructures

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Strong confinement in nanostructures of electrical carriers, photons, and phonons makes it very attractive laboratory systems for probing new physics phenomena. Electron-electron (e-e) interactions in one-dimensional (1D) quantum wires (QWRs) or zero-dimensional quantum dots (QDs) shows unique and interesting properties of great interest both experimentally and theoretically. Even so, the problem of many electrons interacting in nanostructures is a very challenging problem.

In general, existent approaches involve large computational times and complex mathematical calculations when many-body forces are explicitly included in large structures such as QWRs. In this work, we present the derivation of an effective potential that describe the interaction of many electrons (as large as 10^{24} e/cm^3) in a simple way. Such derivation is generated by considering of the e-e interacting by a Yukawa like potential.

We report that the derived effective potential is able to describe the effects of the electronic confinement in all the three dimensions, which is not the case of the Yukawa potential. We also present electronic density distributions as a function of the screening parameter and the size and geometry of QWRs and QDs.

[NSN-46] Effects of an external electric field on the effective potential of many-electron interaction applied to nanoestructures

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Recent advances in nanofabrication and technology of semiconductor quantum wires (QWRs) and quantum dots (QDs) promises a wide spectrum of potential applications. The latter is due to the modification of the nanostructure properties, such as density of states, electronic transport or optical properties which are quite different to those of the bulk material.

In particular, due to the one-dimensional quantum confinement, QWRs have a high potential to be applied in the next generation of optoelectronics and electronic devices. For these reasons the QWRs has been subject of extensive experimental an theoretical studies in the recent years.

One of the subjects of considerable interest is the effect of an applied electric field to the QWR. When the electric field is applied in the confined plane (x-y), the well know Stark effect is observed. However, due to the inherent complexity in modeling the e-e interaction along the QWR, very few studies regarding the effects of an electric field, applied along the z-direction, are reported.

In this work, we present the derivation of an effective potential, which is able to describe the interaction of many electrons confined in low-dimensional structures under the effect of an external electric field. Our model contains the material parameters, the substrate, the dopant level, the cross section geometry of the QWR and the magnitude of the external electric field. We also report the calculated electronic density distributions into QWRs for different electronic concentration and external electric field strength.

[NSN-50] Synthesis, reduction and simultaneous doping of graphene oxide for electrostatic repulsion

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In the present work a synthesis and simultaneous process of reduction / doping of graphene oxide with nitrogen (N-rGO) for applications in repulsion of negative electric charged low density lipoproteins (LDL) wich are carriers of cholesterol,is shown, by means of XPS a 9.57% at, doping with nitrogen is demonstrated and it is verified that the pyrrole type nitrogen is predominant, due to nitrogen doping the surface of the N-rGO reaches high levels of negative electric charge, which is verified by wettability tests between LDL and the synthesized N-rGO, contact angles between 95.7 ° and 130.4 ° were obtained which indicates repulsion between both materials. The N-rGO was also characterized by SEM and TEM where a wrinkled morphology typical of this type of material is observed and the hexagonal atomic arrangement of GO is distinguished. Characterization was also carried out using AFM where thicknesses of up to 2 nm were found, indicating the presence of few layers, in addition by means of FTIR it is demonstrated that the material does not undergo significant structural changes in contact with the LDL. In addition, characterizations are shown by DRX and RAMAN, which also show evidence of the presence of nitrogen and finally, cell viability tests using 3-(4,5-dimethylthiazolyl)-2,5-diphenyltetrazolium bromide (MTT) assay were carried out on human umbilical cord endothelial cells (HUVEC) to analyze the cellular response at different concentrations of N-rGO, obtaining favorable behavior up to concentrations of 100 (μgmL).

[NSN-55] Photocatalytic evaluation of TiO2-MoS2/TiO2 heterostructure film on degradation of Rhodamine B under visible light

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Titanium dioxide (TiO_2) is the semiconductor most used as photocatalyst, for their excellent photocatalytic properties for degradation of organic pollutants in air and waste water, additionally titania is a material chemical stable, inert, nontoxicity, and low cost. Titania has an optical absorption edge between 380 to 415 nm for anatase and rutile respectively absorbing only the 5% of total sunlight. To extend the optical absorption edge toward the visible spectrum, the researches have modificated TiO_2 with several strategies as doping with rare earth ions, CdS/TiO_2, and composites as WO_3/TiO_2 [1-3], among others. Molybdenum disulfide (MoS_2) is an indirect band gap semiconductor with an energy gap of 1.2 eV in the bulk form, the band gap of MoS_2 increases with decreasing crystal thickness due to quantum confinement, Matthew D. J. Quinn et al, report a band gap of 1.97 eV for MoS_2 exfoliated particles and the efficient photocatalytic activity under visible light for degradation of methylene blue [4]. On the other hand the recovery of powder photocatalyst after the reaction is a problem that need be resolved. In this work we report for the first time a methodology of assembled the TiO_2-MoS_2/TiO_2 heterostructure films with excellent photocatalytic activity under visible light. The heterostructure films were assembled by combination of electrospinning, hydrothermal and spin coating techniques. The morphology, elemental composition, crystalline structure, and optical properties were analyzed by SEM, TEM, EDS, XRD and DRS techniques respectively. The absorption edge of TiO_2-MoS_2/TiO_2 heterostructure films was shifted to visible. Photocatalytic behavior of all films was monitored for decoloration rate of Rhodamine B solution under visible light irradiation, the 100% of dye solution was decolored after 5 hours of irradiation, and the adsorption effect of MoS_2 was eliminated.

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[NSN-72] Capsicum Annuum var. Annuum Green Synthesis of silver nanoparticles: Evaluation of morphology, kinetics and thermal properties

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Silver nanoparticles (AgNPs) were synthesized using green extract from *Capsicum Annuum var. Annuum* as a reducing agent. The reduction kinetics was followed by UV-vis spectroscopy and Fourier-Transform Infrared Spectroscopy (FTIR). Formation and growth of AgNPs were confirmed with the UV-vis spectra due to the increase in the band intensity of the surface plasmon resonance (SPR) characteristic for AgNPs around 460 nm. The kinetics of the synthesis was followed by slight changes for the characteristic infrared bands observed for the extract, which decreased, as the reaction proceeded. Formation, growth, shape and size of AgNPs were confirmed by Transmission Electronic microscopy and UV-vis spectra. AgNPs were elaborated for different concentrations, temperatures and pHs. The thermal properties were measured using photothermal techniques. Additional complementary analyzes to evaluate the crystal structure and composition of the AgNPs by Scanning Electron Microscopy (SEM) and X-ray Diffraction (XRD), respectively, were used. This study was the initial step in order to investigate the kinetics AgNPs nanoparticles elaborated by green synthesis, with improved characteristics to be used in applications such as antimicrobials.

[NSN-83] Morphological and Optical Characterization of Gold Nanoparticles Decorated Porous silicon

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In this article some of the main physical characteristics of porous silicon (PS) obtained by electro chemical etching using $HAuCl_4$ in the electrolyte are described. The morphological and optical features of PS decorated with gold-nanoparticles (AuNPs) were analyzed in function of the chemical etching time. The insertion of AuNPs inside the PS were performed simultaneously with the formation of the porous silicon layer. Scanning electron microscopy (SEM) analysis showed the formation and incorporation of AuNPs with an average size of 20 nm in the PS structure, which has a pore size of 1.5 µm. Also, it was possible to observe the loss of Si in function of the etching time. Photoluminescence spectroscopy analysis shows a decreasing of the PL intensity, which can be related to the presence of oxygen in the samples. Raman spectroscopy was used to estimate the size of the Si nanocrystals in the PS structure, which suffers a reduction in size due to the presence of $HAuCl_4$ in the electrolyte.

[NSN-91] Plasmons in graphene finite superlattices

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In recent years, graphene plasmonics, has attracted significant interest motivated by graphene´s unique high carrier mobility, electrically or chemically tunable carrier density, long-lived and strong plasmon excitation confinement. In the context of optoelectronics and nanophotonics, graphene is considered as promising plasmonic material working in the mid-infrared and terahertz spectral windows. However, in a single layer graphene, the electromagnetic energy has a limited capability to plasmon excitations. To obtain a more powerful capacity of excite plasmon resonance, one can employ multilayer graphene structures as possible solution. In this work, we investigate the propagation of plasmon waves in a finite superlattice structure composed of alternating graphene layers spatially separated a distance *d* embedded in a dielectric medium and surrounded by a substrate with different dielectric properties. To find the dispersion relation for bulk and surface plasmons, a general dielectric function can be obtained by solving the recurrence relations for the coefficients of the electric potential in different regions of the finite graphene layered structure.

[NSN-97] Bimetallic nano-structures of Au-Ag: Preparation and optical properties

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The synthesis of bimetallic nanomaterials has been increasing in the last decade due to its unique physic-chemical properties and its nanotechnological applications in catalytic activity, optoelectronics, chemical sensors and treatments against tumor diseases. We present in this report a novel "bottom-up" synthesis method for obtaining bimetallic nanoalloys (random, nanowire-networks and hollow nanospheres) of Au-Ag at room temperature. The nanostructures were characterized using TEM, EDS and UV-Vis. TEM images corroborated the presence of random nanoparticles with a uniform quasi spherical geometry with sizes between 10-20 nm. In the case of nanowire-networks and hollow nanospheres, it had showed a diameter of approximately 11 nm and 70-130 nm respectively. The interplanar distances found at 0.24 nm and 0.23 nm correspond to the values reported in the literature for a crystal lattice for gold (1 0 1) and for silver in the bulk (1 1 1). The EDS spectrum showed the coexistence of gold and silver in the nanostructures. The UV-Vis spectra showed evidence that the alloys had been formed, due to the shift of the surface resonance plasmon (SPR) bands, which showed absorption peaks centered at 480 nm, 385 nm, and 643 nm for the random alloys, nanowire-networks and hollow nanospheres respectively.

[NSN-101] TiO2 inverse opals with gold nanoparticles inclusions as active film in chemical sensors

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The TiO_2 opals were functionalized with gold nanoparticles and were used in the fabrication of chemical sensors for the detection of hydrogen (H_2) and ammonia (NH_3) using hydrogen concentrations in the order of parts per million (ppm) at moderate temperatures (200-500°C). The results showed that the inclusion of gold nanoparticles on the surface of TiO_2 opals improves the sensing performance. Particularly the sensor response increased two-fold and the time constants were reduced to seconds, in comparison with the sensor without gold nanoparticles at the optimal sensor operating temperature. These results show that the TiO_2 inverse opals are an excellent option in the development of third-generation gas sensors.

[NSN-102] Photocatalytic H2 evolution using the ZnO nanowires grown by VLS technique

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ZnO nanowires were grown using the vapor liquid solid (VLS) technique on same kind of seed layer aluminum doped zinc oxide (AZO) grown by two different techniques. The first kind of seed layer were synthetized by sputtering technique, while the second kind were developed by ultrasonic spray pyrolysis (USP). Results shows that the morphology of the obtained nanowires is dependent on the deposition technique of the seed layer. Highly vertical orientated nanowires were obtained on the sputtering deposited films and random orientated nanowires for the USP deposited films. The H_2 production capacity of the nanowires were measured under broadband illumination using a 300W Xe lamp. It was found that the morphology of the nanowires plays an important role on the production of hydrogen. Also, it was found that the addition of co-catalyst did not provoked any increase in the production of hydrogen which shows that the nanowires grown in the present work are defect free and shows good potential for energy applications.

[NSN-112] Pyrene as precursor to synthesis of carbon beads by chemical vapor deposition

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The diversity of Carbon Nanostructures (CNS) such as fullerenes, carbon nanotubes, carbon beads, etc., has become a continuous interesting research object. Due their unique properties CNS can be applying in nanodevices, energy storage, separation technologies, and lubricants. Carbon beads possess intrinsic properties which can be finely tuned by changing parameters such as diameter, chemical composition, bulk structure and crystallinity. Some CNS synthesis methods have been developed. The Chemical Vapor Deposition (CVD) compared to other synthesis methods has some advantages: lower synthesis temperature, lower cost, process control and is easy to use, etc.

The aim of this research was the carbon nanostructures synthesis by CVD method using pyrene as carbon source. The carbon beads were grown on stainless steel core in to a tubular quartz reactor. The synthesis temperatures were 800, 850 and 875 °C. Reaction time was 30 and 40 minutes. Argon was used as carrier gas at 10 ml/min. After cooling down, the samples were analyzed by Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Fourier Transform Infrared Spectroscopy (FTIR), and Raman Spectroscopy.

SEM micrographs showed a spherical morphology with 0.2 - 1 micrometer diameters, called carbon beads for several authors. Beads were the unique kind of found morphology. The carbon contain is the 100% for all samples. FTIR spectra showed a pick around 3400 cm^{-1} corresponds to OH vibrations and showed the presence of C=O in a range among 1590 and 1706 cm^{-1}. The D and G bands were observed around 1300 and 1600 cm^{-1} respectively by Raman spectroscopy.

In conclusion the characterization techniques shown the carbon beads produced from pyrene contain 100% carbon. The diameter of carbon beads was influence by synthesis temperature, the smallest diameters were found in sample corresponding to 875 °C.

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[NSN-118] Effect of silver-dopant on the optical, structural and morphological properties of Ga2O3 thin films

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Gallium oxide (Ga_2O_3) is a metal oxide material with α, γ, δ, ε and β polymorphs; among these polymorphs, the compound β-Ga_2O_3 with monoclinic structure is the only thermodynamically stable whit relevant technological applications in electronic devices for example. There are many reports on the effect on the surface structure β-Ga_2O_3 films with different elements as Si, Sn and Cu. In this work a reliable procedure to control the surface morphology of Ga_2O_3 nanometric films is reported consisting in the formation of nanometric bilayers Ga2O3/metal by RF sputtering at room temperature conditions. The surface structure modification explained by the evolution of the initial amorphous character of the as-grown films towards the nanocrystalline phase driven by a post-grown annealing stage and metal couple.

In this work the optical, Structural and morphological properties of the Ga_2O_3: Ag arrays were evaluated using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy. Silver (Ag) films were chosen considering its chemical reductive property A relationship between the growth procedure and the resultant microstructure and optical properties is proposed.

[NSN-141] Synthesis of Gold Nanoshells with Plasmon Resonance tuned to the Infrared Region of the Electromagnetic Spectrum

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Gold nanoshells, consisting of a silica core surrounded by a gold shell, present a shift on their surface plasmon resonance to the near infrared part of the electromagnetic spectrum, when synthesized on specific dimensions. This paper presents a simple method to prepare the nanoshells, a step by step characterization, as well as their absorbance spectrum. The silica spheres (130±5 nm) were obtained using the well-known Stöber method, and were functionalized with 3-aminopropyltriethoxysilane to create open links to attach gold nanoparticles. The gold nanoparticles (8±3 nm) were synthesized by the reduction of chloroauric acid in the presence of tri-sodium citrate and sodium borohydride as capping and reducing agents respectively. Then, the silica cores were seeded with the gold nanoparticles. The gold shell was grown from the gold seeds with the help of $Au(OH)4^-$ and formaldehyde. The gold hydroxide was prepared with a solution of potassium carbonate and chloroauric acid. UV-Vis spectroscopy results showed a progressive shift on the absorbance peak to the near infrared throughout the synthesis. Transmission electron microscopy images suggest that the absorption peak movement coincided with the completion of the shell.

[NSN-142] Synthesis of graphene oxide with zinc oxide nanoparticles

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Graphene oxide (GO), which is an oxidized form of graphene, has carbon atoms with sp2 and sp3 hybridization and can be considered as an insulating material compared to graphene. GO exhibits various carboxyl and hydroxyl functional groups and is soluble in water. The electrical properties of GO can be changed by varying the oxygen content, water molecules and impurities and efficient hole transport material for organic solar cells. Due to the presence of oxygen based on functional networks in the GO basal plane, it can make bonds with a variety of organic and inorganic materials. Recently, many efforts have been dedicated to the design and manufacture of composite materials or hybrid materials that integrate GO or reduced with polymers, nanoparticles, or even controlled nanotubes and fullerenes. The functionalization of graphene with different molecules is a powerful chemical route to adapt its properties. In this work, the graphene oxide compound is prepared with zinc oxide nanoparticles with the help of a simple ultrasonic cuvette. The GO-ZnO hybrid composite formation was due to the adsorption of ZnO nanoparticles in the leaves of GO surface at 90 ° C. The reaction product was characterized by X-Ray Diffraction (XRD) of the powdered samples and the Electronic Transmission Microscope (TEM) was used to investigate the morphology.

[NSN-153] Synthesis and Characterization of Pt3Ni doped with Co Alloy Nanoparticles for the Oxygen Reduction Reaction

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With the industrial revolution began the development of transport. In the middle of the 18th century, the use of fuels increased the carbon dioxide emissions in the atmosphere, although at that time electric batteries had been an alternative, irreversibility was a limiting factor. Currently, fuel cells offer a potentially more efficient and cleaner source of energy due to their high efficiency as a result of the chemical energy converted directly to electrical energy with low emissions, compared with internal combustion engines. However, two significant technical gaps limit their commercialization: cost and reliability. The primary challenge in the widespread of fuel cell technology is to decrease the content of Pt in catalysts without losing their performance. The synthesis of Pt_3Ni doped with Co nanocatalyst for oxygen reduction reaction (ORR) in acid media presented.The catalyst prepared through chemical reduction with $Pt(acac)_2$ (0.051 mmol), $Ni(acac)_2$ (0.039 mmol), oleylamine (9.0 mL),and oleic acid (1.0 mL) were loaded into a three-neck flask and heated to 130 °C under an N_2 stream. Cobalt hexacarbonyl $Co_2(CO)_8$ and/or tungsten hexacarbonyl $W(CO)_6$ were then added into the vigorously stirred solution, and the temperature was subsequently raised to 230 °C and allowed to remain there for 20 min with vigorous agitation, for subsequent dispersion in a carbon matrix (Vulcan Carbon) previously thermally treated. XRD proved the presence of the alloy Pt_3Ni doped with Co in the catalyst.TEM micrographs showed the morphology of the nanoparticles. Cyclic voltammetry evaluated the electrochemical performance of Pt_3Ni doped Co/C, CO stripping and rotating disk electrode in $HClO_4$ as the electrolyte. Pt_3Ni doped with Co/C nanocatalyst showed the best catalytic activity concerning mass activity and specific activity than commercially available 20 wt% Pt/C-Etek® catalyst. Therefore, this finding suggests a methodology for producing a carbon supported nanocatalyst which could use as a cathode electrode in a PEM fuel cell.

[NSN-160] Fabrication of simple Polyethylene oxide/Chitosan fibers doped with hexahydrate Cerium III

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Nanofibers oscillate in diameter from a few nanometers to some microns. They are fabricated from several materials such as polymers or composites finding a broand range of applications in several industries such as textil, medical, sensing, among others. This work was focused in the fabrication and characterization of single nanofibers base on polyethylene oxide (PEO, 3.5% w/v) and Chitosan (Cs, 1.5% w/v) polymers, and doped with hexahydrate cerium III (CeIII) for bioremediation porpouses. The injection rate (0.1 and 0.5 mL/hr), relative humidity (30 and 35%), linear distance (5 and 15 cm), voltaje (10 and 25 kV) and CeIII concentration (1.5, 2.5 and 3.5 %w/v) were controlled during the fabrication process. We found that is posible to fabricate six fiber samples at 25 kV, 5 and 15 cm, 10 and 25 kV, 0.1 and 0.5 mL/hr for 1.5, 3.5 and 3.5 %w/v of CeIII. SEM, AFM, and XRD studies were carried out for the fabricated samples, which will be presented here.

[NSN-164] Study of the magnetic susceptibility of nanostructured magnetite with a biopolymer obtained by different synthesis methods

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Different synthesis methods were performed to obtain pure magnetite and functionalized with a biopolymer, the particle size has a great dependence on the synthesis method, as well as a relationship with the response to magnetization. obtaining as a result a variation in the morphology depending on the method and conditions of synthesis. The Mycroscopic Scanning Electron (SEM) resultedin spherical morphologies and particles sizes in the range of 50 at 150 nm. The magnetization test and hysteresis curves show that the magnetite nanoparticles have superparamagnetism properties. FTIR spectra show the magnetite-gum arabic characteristic peaks of the biopolymer in 1050 cm^{-1} (C-O), 1150 cm^{-1} approximately 1600 cm^{-1}(C=O) , the peak that is apprimately 1300 cm^{-1} corresponds to O-H and peak near 570 cm^{-1} is characteristic of masgnetite (F-O). With potential for applications of cancer treatment due to magnetic hyperthermia. The synthesis method that gave the best results of magnetic susceptibility was that of chemical co-precipitation.

[NSN-165] PbS nanocrystals anchored on nitrogen-doped carbon nanotubes as active film in chemical sensors

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In this work we present the fabrication PbS nanocrystals anchored on nitrogen-doped carbon nanotubes as active film in chemical sensors. This active layer was characterized by STEM, RAMAN and X-ray (XDR). From the characterization results, it was obtained from the STEM micrographs that the grain size of the PbS samples was found to be ~15 nm and on the surface carbon nanotubes doped with nitrogen were anchored uniformly. From the XRD spectra, peaks located in the following angular positions are shown: 2θ = (26.00, 30.20, 43.20, 50.10 and 61.70) that correspond to the PbS and the peaks of the nanotubes overlap with similar positions. From the RAMAN spectra the wave numbers were obtained in the peaks 136, 194, 435 and 483 cm^{-1} corresponding to the fundamental longitudinal optical (LO) phonon mode of rock-salt structure, first overtone (2LO) and second overtone (3LO) respectively. The strong band in ~133-140 cm-1 is attributed to a combination of longitudinal and transversal acoustic modes. PbS nanocrystals anchored on nitrogen-doped carbon nanotubes were used in fabrication of chemical sensors for detection of humidity, isopropanol and acetone. The times of response and recovery of the sensor when it detects dampness were of 6s and 16s respectively, in case of the isopropanol they were of 8s and 10s and for the acetone they were of 10s and 20s.

[NSN-166] Hydrophobization of Kraft-type cellulose and microfiber cellulose obtained from soybean husk in ultrasonic field

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Soybean husk is obtained as a byproduct of soybean processing to obtain oil. In this work, an alkaline-based process was carried out to obtain cellulose from soybean husk for use in the production of soybean paper. An average of 60% of cellulose content can be recovered. The obtained cellulose fibers were subjected to a sonication process by means of ultrasound for 3, 6 and 12 hours, after which the fibers were filtered and dried at 30 °C to produce Kraft paper. The tensile strength test for this paper is found to reveal fiber reinforcement up to 19%. Also, it is known that the addition of nanoparticles to cellulose paper can improve its mechanical strength, chemical stability, biocompatibility and hydrophobic properties. Here, 20-nm size SiO_2 nanoparticles were used for hydrophobization of paper based on Kraft cellulose and on cellulose obtained from soybean. To study hydrophobicity, morphology and topography of the prepared Kraft paper and SiO_2 coatings on cellulose fibers, the obtained composites were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), FTIR-spectroscopy and contact angle measurements. Fibrous particles of irregular shape were observed, similarly to the cellulose morphology of secondary fibers used in the production of recycled paper. The cellulose morphology is found to be very similar to cellulose from wood. Findings in this research can be used to develop alternatives to obtain cellulose from organic wastes with applications in the paper industry with potential to replace cellulose from trees and reducing their use, thus contributing to the impact on the environment by reducing the felling of trees.

[NSN-167] Non-standard ROS-generating combination “theraphthal – ascorbic acid” in low-temperature transformations of carbon allotropes.

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Multi-wall carbon nanotubes and graphite are relatively stable carbon allotropes, which could be solubilized and/or unfolded by a series of physical and chemical methods. Here, we present a low-temperature formation of several nanocarbons starting from these precursors, such as nano-onions, graphene sheets, and carbon nanoribbons. The experiments were carried out under ultrasonic treatment of aqueous systems “carbon allotrope – theraphthal – ascorbic acid” at various ratios and concentrations. Resulting nanocarbons were studied by scanning electron miscroscopy, transmission electron miscroscopy, XPS, FTIR and Raman spectroscopy. Based on the experimental results, the mechanisms for carbon nanotube unfolding and separation of graphite layers were proposed. These reactions are based on the formation of Reactive Oxygen Species (ROS) by theraphthal in ultrasonic conditions and their further interaction with carbon precursors. These transformations can be considered as greener methods for obtaining nanocarbons.

Keywords: nanoonions, nanoribbons, graphene, MWCNTs, theraphthal, electron microscopy.

[NSN-194] Optimization of the synthetic route for scandium metal-organic frameworks MIL-88B(Sc) and its amino derivative

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Global climate change due to greenhouse gas emission (CO_2) is drawing attention world widely. CO_2 is emitted into the atmosphere from some industrial processes such as automobile engines. Adsorbents which have been applied to CO_2 capture include, porous silicates, activated carbons, zeolites, metal oxides and metal-organic frameworks (MOFs) [1, 2]. MOFs, have been the subject of CO2 capture studies and their functionalization is one such category with promising applicability. Functionalization of MOFs is desirable because in this way it is possible to make them more selective toward CO_2, CH_4, and H_2 [3]. For example the functionalization by amino groups has demonstrated to increase the affinity of these materials toward CO_2. Herein, we report the functionalization of scandium carboxylate MOF, MIL-88B, in particular with amino groups, by using a novel optimized low temperature/mixed solvent route of synthesis and their used as CO_2 adsorbents. The improved synthetic method yielded crystalline materials with different morphology under reflux, mixed solvents and solvothermal methodologies.Three routes to synthesize NH_2-MIL-88(Sc) were found at a temperature range between 65-90, with reaction times 12 or 24 h. Characterization methods included powder X-ray diffraction, scanning electron microscopy, energy dispersive X-ray spectroscopy, gas adsorption and thermogravimetric analysis. Characterization by SEM microscopy was performed on the materials, one of the samples exhibited morphology like bipyramidal hexagonal prism-like single crystals ~30-50 μm in length and ~5 μm in width. The adsorption properties of the amino functionalized material was compared with the unfunctionalized form MIL-88B(Sc). The obtained materials show no uptake at -196 for N_2 so at that temperature no pore opening occurs, however, at -77 it does adsorb CO_2. The CO_2 adsorption behaviour of NH_2-MIL-88B(Sc) material shows gradual opening structure and demonstrates that the amino-functionalization enhances CO_2 adsorption with uptakes of 3 mmol g^{-1}, in contrast to the unfunctionalised MIL-88B(Sc), which has no uptake at the same temperature.

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[NSN-201] Microencapsulation of colloidal gold nanoparticles with alginate using the gelation process

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Using the process of gelation, microcapsules with colloidal gold nanoparticles core and alginate shell were prepared with different metallic concentrations (0.010 - 0.030 mg / ml). Metal nanoparticles were synthesized using the colloidal chemistry reduction method. $HAuCl_4$ solution was reduced with sodium borohydride in the presence of sodium citrate as a stabilizing agent at room temperature. Spherical and stable particles with average size in the nanometer scale (15.1 nm) were obtained. Homogeneous immobilization of colloidal dispersion of Au nanoparticles in microcapsules of alginate was obtained. The optical properties of the colloidal dispersion and the formation of the microcapsules were evaluated using UV-Vis spectroscopy and optical microscopy. The properties of thermal diffusivity as function of the concentration of the gold nanoparticles were studied using thermal lens spectrometry. Higher values of thermal diffusivity of the microcapsules were obtained with the increase in the concentration of metal nanoparticles in the core. The behavior of the thermal diffusivity was corroborated using a theoretical model.

[NSN-213] Quantification of ketorolac in blood serum using Surface-Enhanced Raman Spectroscopy

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Nowadays, for a spectroscopic analytical method with potential clinical applications, such as serum analysis, the capability of performing a quantification of the substance of interest is as important as detecting it. In Surface-Enhanced Raman Spectroscopy (SERS) the substance quantification is based on an intensity rise of the analyte characteristic SERS peaks. This intensity rise is directly proportional to the amount of substance in the sample within a certain range of concentrations, thus making possible the plotting of a calibration curve and a later interpolation using SERS peak intensity [1]. In this work we present the identification of ketorolac in blood serum and its corresponding quantification. First of all, spherical silver nanoparticles with a diameter of 60 nm were synthesized to be used as SERS substrate, these were made through an $AgNO_3$ reduction. Afterwards, six different ketorolac solutions at different concentrations were prepared from a commercial ketorolac injectable solution (30 mg/mL). Later on, two blood samples were obtained from a female Wistar rat, one prior to ketorolac administration and the other one 30 min after it. The serum was obtained by natural blood coagulation and one centrifugation cycle. The SERS spectrum acquisition time of every solution and sample was of 1 s.

After all spectra were acquired, two calibration curves of the intensities of ketorolac SERS peaks as a function of concentration were plotted, using the ketorolac solutions spectra at different concentrations. One calibration curve was done with the peaks appearing at 1600 and 1560 cm^{-1} which correspond to phenyl group, whereas the second one was done with the peaks appearing at 1520 and 1270 cm^{-1} corresponding to the pyrrolizidine. Prior to making the interpolation, the natural intensity contribution of serum for each peak was subtracted from the post-administration spectrum using the data from the pre-administration one. Once this was done, the intensities for each peak of interest were interpolated with its corresponding calibration curve. We found that the amount of ketorolac in serum is quantifiable by any of both calibration curves plotted, which means it can be quantifiable by measuring concentrations of phenyl groups or pyrrolizidine ones. These quantifications prove that SERS can be a reliable analytical method either for detection or quantification of drugs in blood serum.

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[NSN-228] Effect of lithium on the electronic properties of porous silicon for energy storage applications

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Theoretical studies on the effect of Li on the electronic properties of porous silicon are still scarce; these studies could help us in the development of Li-ion batteries of this material which overcomes some limitations that bulk silicon has. In this work the effect of interstitial and surface Li on the electronic properties of porous Si is studied using the first-principles density functional theory approach and the generalized gradient approximation [1, 2]. The pores are modeled by removing columns of atoms of an otherwise perfect Si crystal, dangling bonds of all surfaces are passivated with H atoms, and then Li is inserted on interstitial positions on the pore wall and compared with the replacement of H atoms with Li. The results show that interstitial Li creates effects similar to n-type doping where the Fermi level is shifted toward the conduction band with band crossings of the said level thus acquiring metallic characteristics. The surface Li introduces trap-like states in the electronic band structures which increase as the number of Li atom increases with a tendency to become metallic. These results could be important for the application of porous Si nanostructure in Li-ion batteries technology.

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[NSN-229] In situ study of laser fragmentation of gold microparticles in water: effect of the laser wavelength

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The laser synthesis and processing of colloids encompasses a variety of methodologies which allow for the production and tuning of nanoparticle size distributions in liquids. The use of nanosecond pulsed lasers has been a common tool for such tasks, whether through the fragmentation of microparticles suspensions or the melting and fusing of nanoparticle colloids.

The goal of this inquiry was to study, in situ, the influence of the fundamental, second and third harmonic wavelengths of a Nd:YAG pulsed laser on the fragmentation of gold microparticles suspended in triple distilled water. Such wavelengths involve the IR, visible and UV regions of the electromagnetic spectrum, which have been previously reported to result in distinct nanoparticle size distributions and production efficiencies because of their different absorption by gold. Our study comprises the in situ periodic capture of the sample´s UV-Vis-NIR spectra along with the fragmentation laser pulse's absorbance and its associated photoacoustic signal, as well as SEM/TEM analysis. Given that the amplitude of the photoacoustic signal is proportional to the absorption of the laser pulse, it may indicate changes in the efficiency of the fragmentation as the mean particle size decreases.

Our results show that particle fragmentation, as well as melting or agglomeration, is dependent upon the wavelength being used. This might indicate that different mechanisms are at play for each wavelength or that, given the same mechanisms, they may differ in their influence. Nanoparticles in the samples synthesized by visible and UV pulses exhibited grouping, which can be accounted for by the sample´s greater absorbance in those regions of the electromagnetic spectrum. This may result in a greater heating of the fragmented particles, leading to their melting and further grouping. At the same time, the amplitudes of the photoacoustic signals decreased for all wavelengths as the number of fragmentation pulses increased, which suggests a lower fragmentation efficiency due to an increase in the absorption and scattering by the media that reduces the fluence of the laser pulses on their focus position. Such behavior can also be inferred from the absorbance of the fragmentation pulses, as it increased and saturated with the number of pulses.

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[NSN-232] Ti-Ta alloy produced in solid state for prospective hard coating applications

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The Ti-based alloys implants have shown a high biocompatibility and resistance to corrosion, however in sliding and friction functions, titanium suffers a significant wear. With the aim of extending the life cycle of prostheses, biomedical coatings have been developed to improve the biological and mechanical interaction of implant-bone through combine the properties of substrate and coating. In addition, surface modification techniques are applied to substrate-coating systems in order to improve the device performance in terms of mechanical and chemical wear. On the other hand, the requirement in joint replacements to promote implant-bone interactions and reduce the risk of infections have motivated the synthesis of porous coatings capable of carrying specific bioactive on the titanium-based medical devices. Tantalum has excellent biocompatibility, favors osseointegration due to its high degree of porosity and its excellent stability during shearing between the porous surface implant and the surrounding bone. Hence, recent investigations have focused on the synthesis of Ti-Ta system with excellent anticorrosive and oxidation performance due to the formation of a protective layer of tantalum oxide.

Therefore, the aim of this work was to synthesize a Ti-25Ta alloy by mechanically alloying varying the milling time. Through x-ray diffraction analysis it was determined that the mechanical alloying process favors the formation of solid solutions ($\alpha + \beta$) with nanometric crystal size since 5 h of high energy milling. In order to evaluate porosity and hardness, the nanocrystalline powders were sintered under vacuum. The hardness values range between 26 and 38 GPa, while modulus is between 270 and 380 GPa. Subsequent heat treatments from 800 to 1000°C were performed to analyze the oxidation behavior of the sintered alloy. According to scanning electron microscopy analyses, the sample exposed to 1000°C for 30 min under vacuum exhibited the formation of a tantalum oxide layer. The obtained results suggest the possible use of his material for hard coating applications in biomedical alloys.

[NSN-237] Fabrication of core-shell nanofibers of PVA/EtG doped with Eu

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Rare earths are well known for increasing the chemical reactivity of positive functional groups when they are combined with other materials. Among them, europium is the most reactive of all. In this work we present the fabrication and characterization of core-shell fibers of polyvinyl alcohol (PVA) and ethylene glicol (EtG), doped with Europium (Eu), by using electrospinning. The core was made of PVA:EtG/Eu (9.5:0.5, 9:1, 7:3 M) while PVA was used as shell at 6 %v/v. Injection rates (v_{in} = 0.10ml/h and v_{out} = 0.18ml/h), relative humidity (28-31% and 40-45%), linear distance (12 cm), and voltage (18-23 kV) were controlled during the fabrication process. XRD, FTIR, SEM, DSC and TGA were carried out to study the morhopolgical, compositional and thermal properties of fibers. Particularly, sample fabricated at 9.5/0.5 M of PVA:EtG/Eu and 28-31 %RH presented bilayer nanofibers with Eu^{3+} related emission at 620 upon 393 nm excitation.

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[NSN-263] Synthesis of zerovalent nickel nanoparticles for chromium adsorption

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Nowadays, the implementation and widespread of nanotechnology sciences in the market for environmental applications has been obtaining greater interest especially in recovery processes, water treatment, ecological packaging and oil absorbers. Including the study, design, synthesis, manipulation and application of such materials, devices and functional systems through the careful control at the nanoscale. The metallic nanoparticles have taken great relevance at present, given that they have diverse applications in different areas of knowledge, this is due to their optical, magnetic, catalytic and electrical properties.

In this study we present the synthesis, characterization and chemical evaluation of zerovalent (ZV) nickel (Ni^0) nanoparticles. The as-synthesized metallic nanoparticles range in sizes of 30-50 nm, after a thermal treatment in a reducing ambient of argon we obtained the zerovalent nanoparticles with sizes of 100-200 nm with a fcc crystalline structure of Ni. The adsorption was carried out by studying the interaction of Ni^0 with potassium dichromate solutions, Cr(VI), at different concentrations from 10 to 100 ppm and pH values from 3 to 9. The results yield removal efficiencies of up to 96 % for 10 ppm and 66 % for 100 ppm. The global outcome of the test proves the potential of zerovalent nanoparticles, specifically ZV-Ni^0, for cleansing of contaminated drinking and/or potable water with heavy metal ions. The expectation in the future is to be able to carry out water purification on a large scale for the benefit of society.

[NSN-265] Anchoring Au Nanoparticles on Carbon Nanotubes

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Metallic nanoparticles (NPs) produce a significant electromagnetic field enhancement near their surface due to localized surface plasmon (LSPR) resonance excitation by the incident light. When an analyte molecule is located near them, a substantial increase in its Raman signal occurs, the basis for surface enhanced Raman spectroscopy (SERS) detection [1].

The design of hybrid materials capable of supporting macromolecules over optically active NPs is required [2]. One promising idea is to build a substrate made of carbon nanotubes (CNTs) with plasmonic NPs anchored on them, to exploit their great physical properties and the possibility to access the optical properties of the metallic NPs.

The work herein presented exploits the ‘‘*Polymer wrapping*’’ technique to anchor gold NPs over CNTs. This is achieved by creating a homogeneous net charge on the CNTs surface opposite to the charge of the NPs to be anchored [3]. The first step was to synthesize the nanostructures and prepare aqueous dispersions. Next, the carbon nanotubes were coated with poly(sodium 4-styrenesulfonate) in a single step. Subsequently, two different approaches were explored for the NPs coating with poly(allylamine hydrochloride) on their surface. Finally, the CNTs and AuNPs solutions were mixed for the NPs anchoring on the CNTs to obtain the desired composite.

Each stage was carefully characterized by: UV-Vis Spectroscopy to verify the plasmon resonance band of the AuNPs; Zeta Potential to measure the net surface charge of the nanostructures once coated; and TEM to evaluate the polymer coatings, as well as the attachment of AuNPs to the CNTs surface.

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[NSN-269] Parameters affecting the crystalline quality of Au seeds and its influence in the Au concave nanocubes yield

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Great attention has turned into the Au seeds needed for the *"seed-mediated methods"*used to grow Au NPs by colloidal synthesis techniques. The Au seeds correspond to small nanoparticles (NPs) between ~2-4 nm in diameter. The crystalline quality of the seeds has been proposed as an important factor to increase the yield of specific morphologies in this type of synthesis [1-3]. A crucial factor for tuning the plasmonic response of the colloidal samples.

Here in, the influence of the seeds quality on the yield of *Au concave nanocubes* is evaluated. We explored the main parameters that affect the crystalline quality of the seeds, such as temperature and ripening time of the seeds sample. Moreover, we present experiments to decrease the population of seeds with crystalline defects by an oxidative approach. The samples obtained were characterized by ultraviolet-visible spectroscopy and transmission electron microscopy.

The main results indicate an influence of the synthesis temperature for the seeds and the time left for ripening on the crystalline quality of the seeds. Moreover, the evidence obtained indicate a trend favoring the oxidation of seeds with crystalline defects over the oxidation of monocrystalline seeds. We present evidence demonstrating that the seeds play a main role when trying to increase the yield of of Au concave nanocubes by colloidal techniques.

Acknowledgments: We would like to thank to UNAM DGAPA-PAPIIT through IA103117 project as well as CONACYT through the Fordecyt project 272894. We are also thankful to Israel Gradilla, Francisco Ruiz, Eloisa Aparicio, Jaime Mendoza, Eduardo Murillo and David Dominguez for technical support.

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[NSN-270] ORR by Nitrogen-doped Carbon Nanotubes together with Fe304 catalytic activity for wastewater treatment

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An invaluable tool to develop functional material corresponds to the assembly of nanostructures from the bottom-up, which can be used to improve conventional water cleaning treatments, taking advantage of properties such as adsorption, filtration, and catalysis [1].

The oxygen reduction reaction (ORR) produces either hydrogen peroxide (two-electron pathway) or water (four-electron pathway) [2-3]. Nitrogen-doped carbon nanotubes (CNx) have gained attention due to its ability for ORR becoming a potential replacement for metallic catalysts. On the other hand, an important advanced oxidation process (AOP) is the Fenton reaction which combines iron cations and hydrogen peroxide to produce free radicals highly reactive to organic species [4].

On this line, we aimed for the ORR two-electron pathway to produce hydrogen peroxide in-situ by CNx to be used as a precursor source for Fenton reaction using anchored-magnetite nanoparticles as a source of iron cations for the above mentioned AOP.

We have worked modifying the change of nitrogen doping concentration by the synthesis temperature to explore how the ORR is affected. X-ray photoelectron spectroscopy (XPS) showed the contribution of four different nitrogen species. A tendency in the amount of graphitic Nitrogen is related to a decrease in the onset potential measured by electrochemical characterizations.

We have also worked on the dispersion and stabilization of magnetite nanoparticles with different surfactants to obtain an anchoring route on CNx for the AOP. Applying UV-vis spectroscopy, we have observed a decrease in organic dyes concentration due to the Fenton reaction using the stabilized magnetite nanoparticles.

These results point towards the anchoring of these nanoparticles in a CNx membrane (buckypaper) looking forward for a functional material which could enhance the electrochemical promotion of the Fenton reaction, a key reaction for wastewater treatment.

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[NSN-287] Synthesis and characterization of self-assembled silicon nanoparticles embedded in a ZnO matrix produced by reactive RF sputtering.

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Self-assembled silicon and germanium nanoparticles embedded within a SiO2 matrix have been successfully produced taking advantage of the roughness associated with the sputtering deposition process[1,2].

In this work the same approach has been employed to explore the possibility to produce silicon nanoparticles embedded within a zinc oxide matrix on soda-lime glass and p-silicon substrates. A sequential deposit of ZnO/Si/ZnO layers was carried out employing three different thicknesses of silicon interlayer and three different temperatures of deposit. Oxygen content of the working plasma was modulated through argon partial pressure. We present the results of the optical and structural characterization of the samples using X-ray diffraction, UV-Vis, Raman and photoluminescence spectroscopies. Results of SEM and AFM microscopy are presented.

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[NSN-307] Biosensor for phosphorus detection

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The "phytate" or also called "phytic acid" is the main storage form of phosphate and inositol in seeds of plants and grains. Phosphorus, present in phosphate, in this form, is not could used by humans, dogs, pigs, birds,etc, because they lack intestinal digestive enzyme phytase. It must to make a reaction of phytate with phytase to be able to make phosphorus available for assimilation of the organism.
To determine phosphorus availability of different foods, standardized methods are required, which must allow an accurate phosphorus feed to save feeding costs.

There are currently spectrophotometric methods to measure the amount of phosphorus available in solution using a chromophore, but this type of method is very slow and involves many conditions. In present work, the enzyme phytase from yeast Pichia Pastoris and sensing system, using carbon nanotubes functionalized will be used to determine the concentration of phosphorus present.

[NSN-310] Synthesis of graphene quantum dots (GQDs) and determination of thermal diffusivity of nanofluids containing GQDs.

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Abstract

Using the Hummers method and graphite as a precursor, it was synthesized Graphite Oxide (GO) and Graphene Oxide (GpO). These materials are dispersed in Dimethylformamide at 200 ° C for 8 hours. The remaining solution is filtered with water and ethanol until a neutral Ph is obtained, the powders recovered from the filtrate are dried at 65 ° C to obtain the Graphene Quantum Dots (GQDs). These GQDs are dispersed in water and ethylene glycol to obtain nanofluids. Cuasiespheric forms characteristic of GQDs are observed by means of electronic transmission microscopy with average sizes between 20 and 30 nm. The IR spectra of the GQDs show the vibrational modes of the C = O at 1699 cm^{-1}, C = C at 1578 cm^{-1} and C-O at 980 cm^{-1} bonds. The Raman spectra show the G band at 1580 cm^{-1} which is attributed to the graphitic order, the D band at 1350 cm^{-1} attributed to the presence of disorder in the graphitic lattice and the 2D band at 2682 cm^{-1} which is an overtone of band D. In the Uv-vis spectra, absorption bands at 230 nm are observed in the GO samples and at 271 nm in the GQDs samples associated with the C-C and C = C bonds respectively. On the other hand, thermal diffusivities of water-based nanofluids (1.42 x 10-7m2 / s) and ethylene glycol (0.94 x 10-7m2 / s) were determined by means of a thermal wave resonator.

[NSN-319] Size Dependence of the Optical and Thermal Properties of InP Quantum Dots

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The synthesis of semiconductor nanocrystals, also known as quantum dots (QD's), has generated a great interest in recent years due to the unique physical properties of these nanostructured materials, arising from quantum confinement effects. A series of indium phosphide (InP)-based QDs of different sizes were synthesized using the one-pot method without precursor injection by varying the concentration of tris(trimethylsilyl)phosphine [P(TMS)$_3$] and indium myristate [In(MA)$_x$] as well as the reaction time. The optical absorption and emission features shift to higher energies as the QD size decreases. From the UV-Vis absorption spectra, optical properties such as band gap energy can be calculated, obtaining values between 2.0 and 2.87 eV, and a shift in absorption edge can be seen from 230 to 300 nm as the concentration of [P(TMS)$_3$] increases. Photoluminescence spectra present a wide emission band in the visible spectrum region with the maximum peak located between 2.1 to 2.9 eV for the different samples. On the other hand, the thermal diffusivity of InP QDs was measured by using the thermal-wave resonator cavity (TWRC) technique; obtaining thermal diffusivity values in the range from 8.060 x 10^{-4} to 9.588 x 10^{-4} cm^{2}s^{-1}. These results show that the thermal diffusivity decreases as the nanoparticle size is smaller. We discuss the effect of the QD size on these optical and thermal properties.

[NSN-341] Synthesis and characterization of magnetite nanoparticles

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Magnetic materials have unique properties in the nanoscale size that can be tuned by controlling their size and morphology. In particular magnetite particles having size less than 40 nm displays superparamagnetic behavior, it is zero net magnetization at room temperature when no magnetic field is applied, instead its bulk counterpart that has a ferromagnetic character. These properties make them suitable for biomedical applications, water treatment. This work presents the advances on the synthesis and characterization of magnetite by using urea and iron salt in aqueous solution. Proceeded samples were characterized by TEM, XRD, FTIR and VSM, to obtain their morphology, structural chemical and magnetic nature. TEM revealed well-crystallized 20 nm size nanoparticles, the magnetite phase was corroborated by XRD and FTIR, hysteresis loop revealed the superparamagnetic behavior of the product. This nanomaterial has potential applications in magnetic hyperthermia and water remediation.

[NSN-348] Characterization of lectin-conjugated gold nanoparticles by spectroscopic methods.

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The spectroscopy techniques are based on the light-matter interaction, thus allowing the obtaining of structural information of a molecule, among the techniques widely used for this purpose are Ultraviolet-visible spectroscopy (UV-vis) and Fourier-transform infrared spectroscopy (FTIR). In this work these techniques were used to characterize the assembly of a nanostructured device consisting on gold nanoparticles (AuNPs) as a platform and four lectins; Maackia amurensis (MAA), Sambucus nigra (SBA), Ulex europaeus (UEA) and Glycine max (Gmax). The assembly was performed by mixing 400 µl of a solution of biosynthesized gold nanoparticles with chitosan (medium molecular weight) and different concentrations of lectins: 1ug, 3ug and 5ug, the solution was kept at 4 ° C under stirring at 450 rpm for a period of 12 hr. When analyzing the UV-Vis spectrum corresponding to the assembly, the coating of the lectins to the gold nanoparticles produced a displacement of the maximum peak of absorption of 21,7,10 and 13 nm for the nanostructured devices (MAA, SBA, UEA and Gmax) respectively, this bathochromic displacement is consistent with a coating of the AuNPs and a change in the refractive index by the union with the biological element. On the other hand, the coating was also characterized by FTIR, the spectrum corresponding to the couplings showed displacements at high and low frequencies as observed in other works when this type of interaction is achieved (Álvarez et al., 2014), this displacement corresponds to an electrostatic union between the gold nanoparticles and the biological element. The spectrum of the conjugate (nanoparticle-lectin) showed the characteristic bands of chitosan (1078, 1645, 3334 cm-1) as well as the bands related to the presence of the biological element (1359cm-1), this was evidence enough to confirm the coupling, therefore both techniques are useful and complementary each other to demonstrate and confirm this type of interaction.

[NSN-352] Multiwalled carbon nanotubes esterification effect during functionalization process

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The carbon nanotubes synthesized by different techniques present inevitably carbonaceous impurities and metal catalyst particles reducing the mechanical or electrical properties. A purification technique is applied to eliminate foreign particles and improve the dispersion of CNTs by means of functionalization leading to -OH and -COOH on the surface to generate a chemical compatibility with a solvent or polymer solution for different applications. Nevertheless, the chemical method with a strong acid can degrade the nanotubes, including the metal catalyst solvation, inducing the suspended form of CNT. One alternative to solve this fact is to add a solvent less polar as an alcohol. In this study, MWCNT synthesized by CVD were functionalized by chemical treatment with a mixture of concentrate acids of H_2SO_4/HNO_3, the mixture was sonicated by 3 hours and 24 h of contact, the solvation appeared, and ethanol was adding. The CNTs settle, and Raman spectroscopy showed a big fluorescence, and SEM demonstrate the settle and adhesion of salts forming bundling with the CNTs. On the other hand, an esterification of Fischer was present during the mixture of the carboxylic acids and alcohol, reducing the signal of carboxylic acids in 1750 cm-1 and showing a new signal in 1632 cm-1 in the FTIR test. This solution can offer the settle of CNT after functionalization, but the esterification can modify its applications during combination with other techniques.

Keywords:

Carbon nanotubes, functionalization, carboxylic acid, esterification.

[NSN-356] Graphene electrode for unmanned aircraft

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Energy problem in aeronautical sector is one of the most important issues facing aeronautical industry due to the scarcity and exhaustibility of fossil fuel reserves. Therefore, it is important to study and implement alternative fuel supply for this sector. Development of new technologies to meet the high energy demand has led to research of new materials for applications in photovoltaic devices that result more efficient and economical, such as graphene. This nanomaterial possesses excellent electrical properties for applications in photovoltaic devices, since its electrical conductivity is 0.96×108 $(\Omega m)^{-1}$. In this work, a methodology was developed to design and build an electrode using graphene. A spin coater was constructed for the deposition of graphene on conductive substrates (ITO). The graphene was synthesized from the modified Hummer method and characterized by scanning electron microscopy (SEM) and by X-ray diffraction. We considered that this device is a good candidate for applications in the aeronautical sector since its characteristics make it a material capable of revolutionizing the aeronautical industry because organic graphene base solar cells can be implemented in unmanned aircraft (UAV).

Keywords: graphene, solar cell, aeronautical.

[NSN-365] Synthesis and characterization of carbon nanopearls obtained by CVD process

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Carbon Nanopearls (CNPs) are define as monodisperse nanospheres of nanocrystalline carbon. CNPs have been of interest to nanoscience due to their high potential as proteins carriers, nucleic acids and drugs molecules, and as potential field emission cathodes, etc. The most common growth method used for these nanomaterials is a Chemical Vapor Deposition (CVD), using different pure metallic particles as a catalyst.

In this research, CNPs were synthetized using silica sol-gel films as supporter and using nickel oxide as catalyst. The reduction of nickel oxide for producing nickel carbide was carried out using three percentages of acrylic resin. Acetylene and nitrogen were used as precursors by CVD, instead of methane and argon with three different growth times at 700°C.

Morphology of the CNPs was analyzed using environmental scanning electron microscopy. Raman spectroscopy and X-ray diffraction were also used to characterized nanoparticles. Heat Transmission coefficient of the nanoparticles was determined using photothermal method.

Keywords: CVD carbon nanopearls, Carbon nanospheres, Carbon nanomaterials.

[NSN-366] Effect of the incorporation of carbon nanostructures in films of ldpe/lldpe on its properties and its photodegradation

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The incorporation of carbon nanotubes (MWCNT) multi wall and Graphene to different concentration in a mixture of polyethylene of low density/linear low density polyethylene (LDPE/LLDPE), for blown film extrusion. Ultrasound was used for the dispersion of nano structures of carbon in molten polymer was studied. It was determined the resistance to artificial weathering accelerated with UV radiation of films nano structured. Films with or without degradation were characterized by FTIR, X ray and the fall of tension and elongation properties and CPG distribution Division and branching of chain by Chain Scission Distribution Function (CSDF) function was used to determine which population of weights Molecular are involved in the degradation of the polymer. Molecular weight of the films studied by GPC, turned out to be from 100,000 to 115,000 g/mol before being irradiated, and the decrease in molecular weight high averages after his accelerated aging was observed. Analyses of mechanical traction of the films revealed a decrease in the tensile strength after being irradiated. The differential scanning calorimetry (DSC) and diffraction of X rays (XRD) analysis showed a change in the Crystal structure of the films before and after being irradiated, with the crystalline region, approximately a 20% increase. Films that showed the best performance to UV radiation were those with the highest concentration of MWCNT (2%).

[NSN-368] Physical properties of carbon nanotubes deposited on "p" type semiconductor materials for photovoltaic devices.

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In recent years, nanotechnology research has focused special attention on carbon nanotubes (CNT) due to their extraordinary electrical properties for promising applications in photovoltaic devices. Previously, carbon nanotubes have been used as posterior contacts of cadmium telluride (CdTe) solar cells obtaining improvements in their conductivity, filling factor and efficiency [1]. In this work, single-walled carbon nanotubes were obtained by a microwave method and afterward were deposited by spray-painting technique as the top layer over an aluminum doped zinc oxide (ZnO: Al, AZO) substrate, with the following structure: non-conductive glass/ZnO: Al/CNT [2]. AZO transparent conducting thin films were deposited by a radio-frequency (RF) magnetron sputtering system at room temperature in pure argon ambient and a high vacuum level [3]. Eight zinc oxide samples in different conditions were processed with a thickness between 99 and 284 nm. The films with carbon nanotubes were examined by scanning electron microscopy (SEM). The influence of sputter power, deposition time, film thickness and electrical properties (electrical resistivity, laminar resistance, and conductivity) of layered films was investigated. The optimization of the growth parameters (RF power, sputtering pressure, thickness) was also carried out.

Keywords: Carbon nanotubes, thin films, sputtering.

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[NSN-375] Analytical model proposal for the 2D-3D growth mode transition in the synthesis of InAs/GaAs quantum dots.

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Since the past decade, the synthesis and properties of zero-dimensional materials like quantum dots (QDs) have been studied to improve significantly the performance of new generation electronic and optoelectronic devices. Thus, the development of analytical tools that could assist in describing the QDs growth is crucial. In the present work, an analytical model to study the diffusion of the adatoms related with the nucleation of the QDs is reported. Along the 2D-3D transition the QDs self-assembling process is controlled with adatoms diffusion mechanisms, and so the surface density *r* of diffusing species evolves according to $\partial\rho/\partial t = D\nabla^2\rho$, where *D* is the diffusion coefficient. Considering an in-plane isotropic media the equation can be solved in cylindrical coordinates, ρ can be expressed as $\rho(r, \varphi, t) = \sum X_j(r, \varphi)e^{-K_m t}$, where $X_j(r, \varphi)$ is the 2D diffusion coordinate and K_m is termed as the rate constant which is proportional to *D* [1]. By considering a uniform hexagonal distribution of QDs separated by λ, in the low-density limit the boundary condition $X_j(r, \varphi)=0$ must be reached for $r = m\lambda$ and $j = n\pi/3$ (m∈Z:m∈[1,∞] and n∈Z:n∈[1,6]). According to the kinematics theory, the diffraction intensity can be written as: $I(t) \propto |A(\boldsymbol{q})|^2|(1-e^{i\boldsymbol{q}d})^{-1} + \sum\theta_j(t)e^{-ij\boldsymbol{q}d}|^2$ where ***q*** is the scattering vector, *d* is the layer spacing, $\theta(t)$ is the time-dependent coverage of the nth layer and *A*(***q***) is the scattering amplitude. These terms are related to $\rho(r,\varphi,t)$. Now, considering the first order of scattered intensity equation as a solution for the adatoms diffusion, reaching an equilibrium 2D state *I*(*t*) can be expressed as $I(t) = \Delta I[1-e^{-K_m t}]$ [1]. Since the QDs nucleation process takes place not before the critical thickness H_c has been reached, and *I*(*t*) must be rewritten as follows:

$$I(t) = \Delta I[1 - e^{(-K_m(t-H_c))}]$$

The model was proven during the MBE growth of InAs QDs on GaAs (100) substrates. The RHEED 002 diffraction spot accounts for the scattered intensity related to the islands nucleation; so it was monitored along the relaxation of the InAs/GaAs strained system. By fitting *I*(*t*) to the 2D-3D transition curves it was found that H_c did not present a significant dependence on the buffer layer growth temperature (T_{BL}). Conversely, the K_m parameter decreased from 6.01 to 5.35 as T_{BL} increased. Since K_m is proportional to the surface adatoms diffusion, it means that QDs density increased as T_{BL} increased. Atomic force microscopy measurements corroborated such information and consequently validated our theoretical model.

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[NSN-379] Dopamine and caffeine encapsulation within boron nitride (14,0) nanotubes: classical molecular dynamics and first principles calculations

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Classical molecular dynamics (MD) simulations and first principles density functional theory (DFT) calculations are developed to investigate the dopamine (DA) and caffeine (CA) encapsulation within boron nitride (BN) zigzag nanotubes (NT) with (14,0) chirality. Classical molecular dynamics studies are done at canonical and isobaric-isothermal conditions at 298 K and 1 bar in explicit water. The MD simulations reveal that both dopamine and caffeine are attracted by the nanotube, however only dopamine is able to enter the nanotube while the caffeine moves at the vicinity of it, suggesting that both species can be transported: the first by encapsulation in the nanotube and the second by drag. These findings are analyzed in terms of the dielectric behavior of the system, pair correlation functions, the diffusion of the species and the energy contributions. The DFT calculations are performed according to the BLYP approach and applying the atomic base of the divided valence 6-31g (d) orbitals. The geometry optimization is achieved using the minimum energy criterion, accounting for total charge neutrality and multiplicity of one. Geometry optimizations results indicate that the DA encapsulation takes place under physorption interactions. The encapsulation induces the HOMO-LUMO gap reduction yielding a semiconductor behavior. The charge redistribution produces polarizations in the BNNT-DA and BNNT-CA atomic structures. Calculations of the adsorption energies indicate physorption interactions. The work function decrease and the chemical potential values suggest the proper transport properties in these systems, which may allow their use in biomedicine.

[NSN-400] Fabrication and characterization of PVC/GO Membranes for water filtration

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In this project, polyvinyl chloride (PVC) composites with graphene oxide (GO) will be studied for the manufacture of membranes for water filtration. GO has been applied with satisfactory results in investigations of wastewater filtration and water desalination, however, combinations of GO with other polymers or the use of 100% GO for this application is not very suitable due to its high cost. By using PVC in combination with GO, the mechanical properties of PVC with GO are enhanced and improved, as well as reducing the cost of GO membranes. In this work, membranes with different proportions of GO @ PVC will be manufactured by a dry mixing method, to study the effect on the mechanical properties (tension, elongation, Young's modulus) permeability and retention of solids / suspended / dissolved salts. The morphology and distribution of GO in the PVC matrix will be studied by scanning electron microscopy and energy dispersive X-ray spectroscopy. The molecular structure and microstructure will be studied by infrared and Raman spectroscopy, which will allow to know the interaction that exists between the 2 materials. The thermal properties, as well as the abrasion, fluidity and aging of the mixtures will be studied. The retention of salts will be studied by gravimetry, X-ray fluorescence and ion chromatography. The formulation to be proposed will be the one with the combination of better mechanical properties, solid retention and stability, also proposing the filtration range (nanofiltration, ultrafiltration or reverse osmosis) in which the membranes would be applied.

Financial support from SIP-IPN 21081187 is granted as well as to Mexichem for the use of facilites and commercial GO acquisition. SEM-EDS were measured at LANBIO (Cinvestav Mérida) supported by FOMIX and CONACYT. Dra. P. Quintana and MSc. D. Huerta are acknowledged for LANBIO access and SEM-EDS measurements.

[NSN-401] Synthesis of CuO-ZnO/carbon nanoparticles using discharge arc immersed in liquid

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The synthesis of metallic nanoparticles is a growing research field in chemical science. The particles in size of 1 to 100nm are characterized by properties greatly different form those of the bulk materials with same chemical composition. As the metallic particles are reduced in size, the bulk properties of the particles disappear to be substituted by those of a “quantum dot”, following quantum mechanical rules. Because of the size reduction, the high specific Surface área to volumen ratio leads to enhanced nanoparticle catalytic activity.

Among the various metallic nanoparticles, CuO-ZnO nanoparticles have attracted considerable attention since they important metallic materials in modern technologies. The significant interest has been focused on these nanoparticles due to their unusual optic, catalytic, mechanical and electric properties. Several ways of protecting the nanoparticles from oxidation have been proposed, besides being used in carbon matrices for different applications.

In this work we present the creation of nanoparticles of CuO-ZnO/carbon using the technique of discharge arc immersed in distilled wáter. We sought to determine the optimum conditions for the growth of nanoparticles varying system parameters such as current (50-300A).

[NSN-403] Synthesis of Fe2O3-Co3O4 nanoparticles to be used as flame retardant additives in PVC

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Since the last century and with accelerated human development, there are increasingly more combustible materials (disposable containers, packaging and construction materials) in homes, industries and businesses, often surrounded by a dense population. In addition, new materials are generated every day with potential fire risk; however, there is no complete knowledge about what kind of combustion mechanism is carried out and how to reduce the firing risk these materials may have. Poly(vynil chloride), PVC, is a versatile and economic polymer used in several applications such as construction industry and in the medical, electronic and automotive sectors. The use of flame retardant additives in PVC formulations enhances their self-extinguishing ability and helps to inhibit smoke generation, making them useful mainly in wire and cable coating manufacturing. Nanoscale additives have the advantage to boost their properties due to their higher surface area compared to bulk material; there are some studies done with nanoscale metallic oxides (MO) of iron and cobalt into polymeric matrix which improvement in flame retardant, mechanical and thermal properties are reported. In this work, synthesis of nanometric metallic oxides (Fe_2O_3, Co_3O_4) by Wet Chemical Method was made to use them as additives for PVC composites manufacturing in order to improve their fire retardancy properties. X-ray diffraction patterns (XRD) of metal oxides nanoparticles obtained separately and in the core-shell arrangement shows the presence of Fe_2O_3 and Co_3O_4, hexagonal and cubic respectively, with crystallite size less than 50 nm calculated with Scherrer equation. Thermogravimetric analysis (TGA) shows that the presence of the synthetized metal oxides into the PVC matrix diminish the weight loss at 400 °C compared to PVC without MO and to PVC with antimony trioxide, commercially used as flame retardant additive, this is attributed to the ability of MO to form larger amount of char from the composite degradation, this char acts as an insulation between the front of flame and the polymeric material, which diminishes heat release flow and polymer pyrolysis rate and so the burning rate. Further characterization include Infrared Spectroscopy (FTIR) to determine interactions between MO and PVC composite and Differential Scanning Calorimetry (DSC) to determine thermal transitions changes due to the MO addition; and Cone Calorimeter to study the fire behavior.

[NSN-414] Preparation of Graphite and Carbon nanoparticles by laser ablation in distilled water with and without ultrasonic excitation.

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In this work we report the synthesis of Graphite and Carbon nanoparticles by laser ablation of a graphite and Carbon target immersed in distilled water. The laser used is a Nd: YAG emitting at 1064 nm with a pulsed length of 10 ns. The effect of an ultrasonic excitation and the laser energy density on the size and shape of the nanoparticles is investigated. The nanoparticles size and shape are determined from transmission electron microscopy (TEM) micrographs. The samples were characterized also by Raman spectroscopy. Photoluminescence measurements were also performed. The UV-Vis measurements show a typical plasmonic absorption at 265 nm approximately this band is characteristic of Graphite. In general samples fabricated under ultrasonic excitation are composed on nanoparticles and plane like structures. Without the presence of the ultrasonic field individual nanostructures having spherical shapes are observe. Furthermore different experimental conditions were studied such as height of water above the target and the spot size effect. The main results are presented.

[NSN-416] Preparation with and without ultrasónico excitation of gold nanoparticles by laser ablation in distilled water

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The objective of this work is to report the synthesis of gold nanoparticles by laser ablation of a Au target immersed in distilled water. The laser used is a Nd: YAG emitting at 1064 nm with a pulsed length of 10ns. The effect of an ultrasonic excitation and the laser energy density on the size and shape of the nanoparticles is investigated. The nanoparticles size and shape is determined from transmission electron microscopy (TEM) micrographs and in some cases energy dispersive spectroscopy (EDS) is presented. The gold nanoparticles, as synthesized, are highly crystalline in nature. The UV-Vis measurements shows a typical plasmonic absorption at 650 nm approximately band characteristic of Au metallic spherical particles of nanometric size. Furthermore different experimental conditions were studied such as height of water above the target and the spot size effect. In general nanoparticles prepared under ultrasonic conditions are smaller than does obtain without the ultrasonic field. The cleaning procedure and the water quality and purity are essential for obtaining satisfactory results.

[NSN-428] Cubic InxGa1-xN Quantum Wells by Conventional Molecular Beam Epitaxy (MBE) and Migration Enhanced Epitaxy (MEE)

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Nitrides are promising semiconductor materials for optoelectronic applications such as Light Emitting Diodes (LEDs) and Laser Diodes (LDs). This is mainly due to their outstanding properties, some of which are the direct energy gap, which covers a large part of the solar spectrum, from the infrared with Indium Nitride (InN) to the ultraviolet with Gallium Nitride (GaN) and Aluminum Nitride (AlN) [1,2]. The nitride family can be crystallized in two structures: a stable phase with hexagonal structure and a metastable phase with cubic structure, each structure present different physical properties due to the accommodation of the atoms. In the present work, we present the growth of cubic $In_xGa_{1-x}N$ quantum wells (QWs) with c-GaN barriers by two methods: the first one is Molecular Beam Epitaxy (MBE) and the second ones is Migration Enhanced Epitaxy (MEE), with the purpose of comparing the segregation of the Indium (In) atoms from the well to the barrier and their surface diffusion in the cubic structure of the wells. The $In_xGa_{1-x}N$/GaN QWs with thickness of 10 nm and the GaN barriers with 30 nm were grown on GaAs (001) substrates to induce the cubic phase. For the first growth method of the QWs, the growth temperature (T_g) was from 600 to 680 °C with the same flow of In (BEP_{In} = $1.8x10^{-7}$ Torr), and the growth surface was exposed simultaneously to three elements In, Ga and N. For the second, T_g was from 480 to 530 °C with the same flow of In (BEP_{In} = $1.8x10^{-7}$ Torr); in this case, the growth surface was exposed to alternate periods of N, Ga and In of 4 s each one. The SIMS depth profile allowed to identify the formation of c-$In_xGa_{1-x}N$ in the quantum wells by the two methods, and the corresponding incorporation and segregation of In. We found a lower desorption and segregation of In in the QWs by the MEE method, this could be due to the low growth temperature that are used in this method. For the MBE method we obtained emissions at room temperature from 2.23 to 2.99 eV, and for the MEE method the emissions were from 2.17 to 3.10 eV, which corresponding to visible spectrum (violet, blue, green and yellow). In this way, the transitions of energy in the visible spectrum were adjusted by modifying the In concentration in InxGa1-xN alloy. Likewise, numerical simulations were carried out to understand electronic transport in the heterostructures, and the possible energy levels for the recombination hollow-electron were determined.

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[NSN-435] Adsorption of gas molecules on Cu atom-decorated siligene

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Two-dimensional (2D) nanostructures in the honeycomb lattice are currently materials of interest due to their unique electronic properties as compared to their bulk counterparts. In the present work, the structural and electronic properties of mono and bilayer of the lateral hybrid structures of silicene and germanene named as siligene are systematically investigated. Research on the adsorption of some gas molecules (O_2, N_2, CO, NO) [1,2] on the surface of pristine siligene and decorated siligene is presented, using a transition metal: Cu atom. Geometries and partial density of states are calculated through density-functional-theory (DFT) calculations. The most stable site for copper the sites over the centre of the hexagons of the honeycomb lattice are the more stable sites. The most stable adsorption geometry, the adsorption energy and the charge transfer of the gas molecules on the siligene surface are presented. We calculated from first principles the adsorption of molecular gas in Cu in a siligene supercell of 1 × 4 × 4. The siligene without Cu presented adsorption energies below 1 eV, however the molecules adsorbed in Cu presented energies around 1 eV with the exception of the O_2 molecule that showed an energy of 1.4838 eV. In the densities of states, the Cu has a contribution in the valence band, the O is found by the Fermi level and the N in the conduction band. Our calculations showed that metal element can significantly improve the interaction of gas molecules and Cu-decorated siligene. The metal Cu may be the best options among all the metallic elements used.

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[NSN-436] Sol-Gel Synthesis of Strontium Titanate Nanofibers by Electrospinning

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Strontium titanate ceramic fibers were obtained using sol-gel and electrospinning methods, giving an alternative for preparing ceramics in the form of fibrillar membranes. The electrospun strontium titanate nanofibers fibers were characterized by X-ray diffraction, Scanning Electron Microscopy, and Infrared and Raman spectroscopies. The green fibers obtained from the ceramic precursors had a diameter of 140±35 nm. Based on the thermal analysis, the phase transition from tetragonal titanium oxide to the perovskite structure of strontium titanate was determined to take place at 800°C. At 1000°C the shape of fibers was preserved, with mean diameter of 103±39 nm. By infrared spectroscopy, Raman spectroscopy and X-ray diffraction analysis, it was determined that ceramic fibers at 1200°C had a perovskite-like structure characteristic of strontium titanate.

[NSN-444] Optical and structural properties of InGaAsSb on GaSb(100) substrates grown by liquid phase epitaxy

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The $In_{x}Ga_{1-x}As_{y}Sb_{1-y}$ quaternary alloy is one of the most important materials for a broad range of infrared optoelectronic applications [1], since its direct band gap can be extended from 0.73 to 0.29 eV, which corresponding to a wavelength from 1.7 to 4.3 µm [2]. This alloy exhibit a zinc-blende structure and a considerable variation of its properties with the composition (*x,y*). In this work, we present the study of the variation of the structural and optical properties of $In_{x}Ga_{1-x}As_{y}Sb_{1-y}$ alloy as a function of As composition (*y*). The quaternary alloy on GaSb(100) substrates was grown by Liquid Phase Epitaxy (LPE), under palladium-purified hydrogen atmosphere inside a horizontal reactor in a conventional sliding boat. In order to eliminate the oxides of the GaSb substrate, after the charge of the GaSb substrate in the boat, the temperature was raised at 640 °C. Then, the temperature was decreased at 529 °C to grow the $In_{x}Ga_{1-x}As_{y}Sb_{1-y}$ alloy for 1 min. High resolution X-ray diffraction (HR-XRD) allowed us to determine the structural properties of the epitaxial alloy. In the diffraction patterns from the (004) planes we found two peaks: the first one corresponding to the GaSb substrate (to the right of the pattern) at 30.3624° with a narrow linewidth (FWHM=16"), and the second one corresponding to the $In_{x}Ga_{1-x}As_{y}Sb_{1-y}$ quaternary alloy (to the left of the pattern). As the As concentration increases, the peak diffraction of the alloy gradually shifts from 30.4003 to 30.3807°, approaching the GaSb substrate signal. The lattice mismatch obtained from these patterns were from $1.1\text{x}10^{-3}$ to $5.4\ \text{x}10^{-4}$, respectively, indicating a greater lattice match of the alloy with the substrate as the As concentration increases. Additionally, we have obtained the band gap energy (E_g) of the alloys from the photoluminescence (PL) spectra at low temperature 23 K. As the As concentration increases, the E_g decreases from 1.98 to 1.92 eV.

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[NSN-455] Preparation and characterization of MCM-48 mesoporous silica grafted with Poly(N-vinylimidazole)

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The development of hybrid materials based on mesoporous silicas and polymers have received much attention due to they combine the properties of their components giving as result composite materials with unique properties. Specifically, amine-containing polymers have attracted attention due to its capacity to adsorb CO_2 and H_2S from natural/shale gas, and complex with heavy metal. Poly(N-vinylimidazole) (PVIm) is an interesting material which contains aromatic-type amine groups in its backbone which make it suitable for the applications above mentioned. In the present work, the covalent grafting of PVIm onto MCM-48 mesoporous silica via free radical polymerization was developed. The synthesis of the mesoporous MCM-48 silica was carried out through sol-gel method at room temperature. In order to perform the grafting of PVIm, the surface of MCM 48 silica was functionalized previously with vinyltrimethoxysilane (VTMS). This gives as a result the incorporation of functional vinyl groups onto silica surface that allow the covalent grafting of PVIm via free radical polymerization. The MCM-48-PVIm hybrid materials were characterized by X-ray diffraction (XRD), infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), and transmission electron microscopy (TEM).

[NSN-464] Effect evaluation of reaction time on the composition and structural, optical and morphological properties of WO3/rGO nanocomposites

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Tungsten oxide (WO_3) is an n-type semiconductor metal oxide, with a band gap of 2.6 to 3.3 eV, excellent electrical, optical and structural properties; however, depending on the synthesis method, its morphology and properties change, leading to different applications. On the other hand, it has been proposed that the incorporation of reduced graphene oxide improves the electrochromic properties of WO_3. Therefore, in this work, WO_3/rGO nanocomposites were synthesized by means of a simple chemical method, the reaction time was varied (5, 7.5 and 10 h) to evaluate its effect on the composition, structure, morphology and optical properties of the materials. XRD patterns show the orthorhombic structure of tungsten oxide. In the Raman spectroscopy, the bands 1344 cm^{-1} and 1588 cm^{-1} corresponding to modes D and G are observed, in addition to the 713 cm^{-1} and 807 cm^{-1} corresponding to GO and WO_3 respectively. The band gap calculated from the Diffuse Reflectance spectra is in the 2.2 - 2.4 eV range. The morphology and elemental composition of the synthesized samples were evaluated with SEM/EDS.

[NSN-477] Study of the electrical conductivity of bimetallic Cu/Ni particles for solar cells

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The conjugation of properties between two metals improves the electrical properties. In the case of Cu/Ni it is of particular interest, since both have a wide absorption band in the visible region of the electromagnetic spectrum. However, the structure of the particles depends fundamentally on the method and the synthesis conditions.

In this work, the conjugation of Copper and Nickel is presented by sol-gel synthesis in acidic conditions. The morphological characterization was performed by scanning electron microscopy. To analyze the electrical conductivity, measurements were made of the resistance of the materials with respect to temperature increases in the range of 25 to 100 ° C. A spherical morphology was observed with diameters of 100, 85 and 30 nm for Cu, Ni and Cu/Ni, respectively.

The results showed that the Cu/Ni compound had a greater contact area due to the fact that it had a smaller diameter compared to the individual materials and that it also favored the electrical conductivity of the compound since it increased up to three orders of magnitude compared with the individual materials of Cu and Ni that was only an order of magnitude.

[NSN-480] Synthesis and characterization of BiFeO3/ZnO heterojunction for photocatalysis applications

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Bismuth ferrite (BFO) is a multiferroic material with a rhombohedrally distorted perovskite structure that exhibits the coexistence of G-type antiferromagnetic (AFM) spins with a Néel temperature of 643 K and ferroelectric (FE) polarization with a Curie temperature of 1103 K.[1] This material has received noticeable attention due to its potential applications (as spintronics, data storage, microelectronics, and magnetic sensors).[2] Recently, this perovskite has shown an photovoltaic effect, which makes it a promising candidate for the design of optoelectronic devices. On the other hand, ZnO is a semiconductor used widely due to that it presents properties of great interest for optoelectronic, photovoltaic and photocatalytic applications. This material is a n-type semiconductor with a band gap of 3.2 eV.[3] There are reports that use both BiFeO3 and ZnO for photocatalytic applications. In this work, we present the synthesis and characterization of $BifeO_3$/ZnO heterojunction in order to find suitable properties for the photocatalytic degradation of organic dye. First, BFO powder was synthesized via molten salts method.[4] The salts employed were NaCl and KCl (1:1). For preparing BFO/ZnO heterojunction, the BFO power obtained was added to a chemical solution containing zinc nitrate. Ammonium hydroxide was used as an precipitating agent.[5] The structural, morphological and optical properties were analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and UV-vis spectroscopy (UV-Vis).

Keywords: BFO/ZnO heterojunction, molten salts, co-precipitate.

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[NSN-483] Effect on thermal conductivity of magnetorheological fluids due to loads of carbon nanofibers

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Amongst the great challenges of the science of materials is to obtain compounds whose physical properties can be controlled. The development of new flexible and versatile composites with controlled thermal properties is a growing demand in the smart materials area. An example of these materials is magnetorheological (MR) fluid, a dispersion of highly magnetizable microparticles in a non-magnetic carrier fluid. In the presence of an external magnetic field, these materials can be changed from a fluid-like state to a solid-like state. This is due to the preferential aggregation of the microparticles that leads to the formation of chain-like structures in the direction of the applied field. The thermal properties of these materials can be enhanced by loading the MR fluid with nanostructures and applying an external magnetic field. In recent years, several studies have been carried out in order to understand how the inclusion of carbonaceous nanostructures into different matrix change their properties. Carbon nanofibers (CNF) represents a novel nanometric material and has been shown that its incorporation in a matrix can improve its physical properties. In particular, the thermal properties of the carbonaceous nanostructured materials, as CNF, are of interest for basic science as well as for technological applications.

In this work, the thermal properties of MR fluids based carbonyl iron powder (CIP) with the inclusion of carbon nanofibers under the influence of low intensity and homogeneous magnetic field were studied. The thermal diffusivity of the samples was determined by a photopyroelectric technique with a sample thickness scan. The thermal conductivity was calculated and studied as a function of the CNF a CIP volume concentration and the intensity of the applied magnetic field. The results show that the heat transport depends strongly on volume fraction of CNF. Due to the high thermal conductivity of the CNF, a low loading percentage is needed to obtain significant growth in the thermal conductivity of each sample. In the absence of a magnetic field, the MR fluid at 5% of CIP shows an outstanding increase in thermal conductivity respect to the matrix due to the presence of CNF, achieving an increase up to 3 times with 2 % of CNF volume concentration. However, when the magnetic field was applied, the improvement in thermal conductivity decreases for all cases. The analysis of the thermal conductivity was analyzed through the Lewis-Nielsen model that considers the maximum concentration and a form factor relative to structures formed in the sample. These materials might find practical applications in systems in which the CNF improve the spreading of heat away like devices for storage and generation of energy, among others technological applications that require the precise control of dissipation.

[NSN-485] Effective thermal conductivity of graphene nanoplatelets based thermal compounds

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This research is focused on the thermal improvement of compounds loaded with graphene nanoplatelets in relation to its diameter, specific surface and volume fraction. The thermal diffusivity of samples was measured by a photopyroelectrical technique with sample thickness scan. The results show that heat transport on these compounds strongly depends on the graphene nanoplatelets volume fraction, due to the high thermal conductivity of nanoplatelets compared to the matrix. The thermal conductivity of the samples was calculated, and its enhancement was analyzed using a modified Lewis–Nielsen model, taking into account the dependence of the maximum packing fraction and the form factor of the graphene loads. These materials might find applications in systems in which the graphene compounds improve the extraction of heat away from selected zones.

[NSN-487] A magneto-optical characterization technique to determine the magnetic functionalization of carbon nanostructures

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The development of new technologies based on carbonaceous nanostructure materials is an area of great development in recent years. These materials have shown extraordinary physical properties, however one of the great challenges is to control the orientation of these in a matrix. The magnetization of carbon nanostructures offers a means for the manipulation of these and their effectiveness depends on the method with which the magnetization is carried out. A physical technique to magnetize carbon nanotubes is using magnetic fluids, intelligent materials composed of magnetic nanoparticles dispersed in carrier fluid. Evidences of the manipulation of these functionalized nanostructures of carbon through magnetic fields is in the study of magneto-optical effects related to the exposure of ferrofluids with under the influence of a magnetic field.

In this work, carbon nanofibers were magnetically functionalized, and the amount of magnetic material adsorbed by these nanostructures was calculated through an optical technique based on the Beer-Lambert law. Carbon nanofibers (CNF) were added at different volumetric concentrations inn ferrofluid (FF) matrices, varying the concentration of magnetite (Fe_3O_4). After a mechanical agitation of 24 hours, the materials were allowed to settle for several days until no changes were observed in the color of the remaining fluid. Finally, the concentration of the remnant fluid was analyzed. The results allow determining the optimum volumetric concentration for a ferrofluid such that the amount of magnetite absorbed by the CNF is the maximum possible. In such a way that for a volumetric concentration of 0.15% of CNF an adsorption of 76% of magnetite is achieved for a FF at 0.03%, of 58% for a FF at 0.05% and for a FF at 0.5% the adsorption decreases to 42%. This allows optimizing the magnetization process for a good response of these materials to low intensity magnetic fields.

[NSN-488] Functionalization routes for GO and TiO2 and its applications in coatings

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Nowadays, the need for functional materials has grown substantially, due to the search for a better quality of life. Nanotechnology has been considered an enabler to achieve this goal, through nanomaterial and nanostructures. The surface modification of nanomaterials plays a key role. The main goal of this work was to achieve hydrophobic coatings through nanomaterials' functionalization, using as precursors GO nanostructures and TiO_2 nanoparticles. These nanomaterials were functionalized separately with two functionalization agents as octadecylamine and octadecylphosphonic acid. The main purpose to use these molecules was to enhance the hydrophobic properties of the nanomaterials and thus of its coatings. After functionalization, the four new systems of TiO_2-ODA, TiO_2-ODPA, GO-ODA, GO-ODPA nanoparticles were characterized by XPS, FTIR and water contact angle, the results showed the successful functionalization of the nanomaterials.

[NSN-492] Activation and magnetic functionalization of carbon nanofibers

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In the last years, materials that can be magnetically manipulated have generated a large number of investigations due to a structural control of the materials is translated into the modulation of its thermal, optical, electrical and mechanical properties. The "modulated properties" make a material very useful and are tools for technological development. Some of the materials with which we can perform this technological development are carbonaceous nanostructure materials, such as carbon nanofibers (CNF). These materials have shown remarkable physical properties, however, one of the great challenges is to control the orientation of these in a matrix. The magnetization of carbon nanostructures allows its manipulation, thus the method with which the magnetization is achieved has a transcendental importance.

In this work, a carbon nanostructures magnetization technique is presented through a chemical process. After activation of CNF by hydrochloric acid (HCl), a coprecipitation is realized in an inert atmosphere chamber using ferric chloride and ferrous chloride solutions, in mechanical agitation for several hours. Following, the nanostructures are collected and are added to a solution of sodium hydroxide (NaOH) under stirring. Afterward, the material is washed using distilled water and decanted once achieving a neutral solution. Finally, the magnetic CNF are dried at a temperature of 70 ºC. The magnetized CNFs are analyzed through the characterization techniques BET, XRD, XPS, RAMAN, SEM, TGA, FT-IR and obtaining their magnetic response. The results show the formation and adherence of magnetic particles on the surface of the CNF, this by activating the surface of the nanostructures and controlling the oxidation of the iron nanoparticles. These materials have excellent applications as additives for heat sinks, filaments, and compounds, in addition to their great application in the medical area.

[NSN-496] Evaluation of oxide layer formation in equiatomic AlCoNi alloy with minor additions of carbon

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For structural and high temperature applications, the development of structural alloys with enhanced mechanical properties and good oxidation and corrosion resistance is required. The chromia (Cr_2O_3), alumina (Al_2O_3) and silica (SiO_2) are the preferred oxide scales to protect the high-temperature alloys against oxidation due to their inherent slow growth rates at elevated temperatures. Commercial superalloys for aerospace applications usually contain chromium and aluminum, but high content of these elements could increase the brittleness of the alloy. Under the definition of low, medium and high entropy alloys, the formation of solid solution instead of brittle intermetallic compounds is achieved. Hence, the aim of this investigation is the synthesis and evaluation of oxide scale formation in an equiatomic AlCoNi alloy with additions of carbon as minor alloying element.

The AlCoNi alloy with minor additions of carbon was fabricated by mechanical alloying and sintering. The effect of carbon was investigated through additions of graphite and carbon nanotubes. Subsequent thermal treatments in air at relative high temperature were performed in order to evaluate the formation of protective oxide layer in the surface of the material. The oxide scales were characterized by x-ray diffraction, scanning electron microscopy and nanoindentation analyses. The formation of an aluminum oxide layer was detected after heat treatment at 1000 °C. The carbon additions promote less porosity and increase grain boundaries in the nanostructured material, the last effect can helps to mitigate the Al depletion at the metal-layer interface. Graphite content reduces the growth rate of oxide layer.

[NSN-498] Phase transitions and stability of the as-milled reaction products: high temperature X-ray diffraction analysis

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In this work, it has been designed a study with the aim to understand the relative stability or metastability of the as-milled reaction products. It is to say, the sluggish step associated to the mechanochemical synthesis of PbSe via the high-energy milling process. A detailed discussion of phase transition pathway from $PbSeO_3$ –or even $PbSeO_4$– to PbSe nanostructures, or vice versa, via coordination polyhedra is proposed. The main interest is in detecting the stability or metastability of the as-milled reaction products through the bond parameters distortion. Those results are associated with the thermal decomposition behavior of $PbSeO_3$ –or even $PbSeO_4$– studied by in situ high temperature X-ray diffraction.

[NSN-505] Immobilization of enzymatic extract in carbon nanostructures (NTC and nano-spheres)

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Conventional materials such as metals, ceramics and polymers can not meet all the requirements that new technologies seek to solve the most immediate problems in the world related to energy and the environment. Carbon nanostructures have emerged as a material of considerable interest because of their structure exhibit extraordinary mechanical, electrical, thermal and chemical stability properties; as well as a large specific surface area. These nanostructures have been recognized as promising supports for peptides, proteins and enzymes. Biocatalysis is one of the main fields that can benefit from this type of supports, which is making it one of the most powerful tools in biotechnology. The objective of this work was to immobilize enzymatic extract in two different carbon nanostructures (NTC and nano-spheres) for later use as a biocatalyst. The NTC and the nano-spheres were synthesized by the vapor deposition method, later they were characterized by means of XRD, Raman and SEM to know their structure, later the enzyme extract was immobilized by means of the covalent bonding method with glutaraldehyde to carry out the union , this was characterized by SEM and electrochemical techniques (EIS and VC). The obtained results showed that both nano-structures can be obtained by the same synthesis method, by means of Raman spectroscopy it was observed that multiple wall NTC were obtained, SEM micrographs showed the morphological structures of both nano-structures, in which He appreciated the shape of carbon nano-spheres and NTC. The composites obtained were tested by cyclic voltmetry and electrochemical impedance spectroscopy, which showed a good electrochemical performance to be used as biocatalysts.

Keywords: NTC, nano-spheres, enzymatic extract, biocatalysts

[NSN-530] Synthesis of mesostructured titanium dioxide by a simple and novel method and it's characterization: Optimization of the process

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Titania is one kind of important materials, which has been extensively investigated because of its unique electronic and optical properties. A large number of efforts have been made to synthesize mesoporous TiO_2 materials with high surface area and uniform pore size, for their applications in many fields. The present work demonstrates the usefulness of the combination of sol-gel method and soft hydrothermal method in preparing mesostructured titanium dioxide materials. Synthesis of mesoporous of titania involved titanium butoxide, triethanolamine (TEAOH), hexadecyltrimethyl ammonium bromide (CTAB), sodium hydroxide as Ti-source, hydrolysis stabilizer, template and alkaline material, respectively. Also optimization of the synthesis protocol was carried by using different temperature for hydrothermal treatment and also by varying the amount of water addition during the synthesis. BET analysis showed a higher surface area of 186.215 m_2/g at 100^0C as compared to other hydrothermal temperature. The sample retained its structure even after the calcination at 500^0C. SEM images displayed a well-defined homogenous pores all over material. XRD data reveals a peak approx. 1nm which corresponds to mesoporous nature of the titania material. The synthesis procedure that we are concluding could be used for the synthesis of other difficult-to-obtain mesoporous materials and can offer applications in medicine, biology, environmental engineering, etc.

KEYWORDS TiO_2, Mesostructured, synthesis, optimization.

[NSN-539] Tuning optical properties of ITO thin films with tilted nanocolumnar structures grown by rf-sputtering in oblique angle deposition

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The optical properties of tilted nanocolumnar indium tin oxide (ITO) thin films on glass substrates through the sputtering technique without and with annealing temperature to 250°C in the air are reported. The influence of the flux incident angle on the optical properties is investigated. The samples were prepared under different flux incident angles (α) of 0°, 40°, 60° and 80° respectively. Scanning electron microscopy images showed nanocolumnar inclination shaped structures and presence of porosity. The inclination respect to a vertical line increased whit increase the flux incident angle. The deposited films with annealing temperature showed a cubic structure with preferential (222) plane orientation and crystallites sizes between ~46 nm and ~67 nm. The transmittance values for all samples (without and with annealing) are in the range of 70-90% in the 450-1050 nm wavelength region. The band gap energy had values of ~3.48 to ~3.62 eV and values of ~3.74 to ~3.92 eV to films without and with a temperature of annealing respectively. When the flux incident angle is increased, the refractive index of the films is decreased between ~1.4 to ~1.8 and ~2 to ~2.2 for without and with annealing temperature effect respectively. Thus, the band gap energy and the refractive index properties of the film can be modified over a wide range by adjusting the flux incident angle and the temperature of annealing. It is suggested that the oblique angle deposition technique provides ITO films with more application possibilities by allowing their optical properties to be tailored.

PLASMA AND VACUUM
(PLV)

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Miguel Ángel Santana-Aranda, (CUCEI, UdeG)

PLASMA AND VACUUM (PLV) ORAL SESSIONS

[PLV-81] Influence of mean kinetic energy of the plasma on the properties of si and ge thin films grown by pulsed laser deposition

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Silicon and Germanium thin films are of particular interest because their high mobility of charge carriers and compatibility with actual technology and devices such as solar cells and sensors. These films have been grown mainly by chemical vapor deposition, but this method require toxic gases as precursors and can become very expensive.

Physical vapor deposition techniques such as sputtering or pulsed laser deposition (PLD) have not been extensively studied for these materials due to the difficults for achieving a good control on the deposition process. PLD offers the possibility of producing high quality thin films. When pulsed laser produced plasmas are studied in PLD experiments, higher control and reproducibility can be achieved. The Langmuir probe is a device used to determine several plasma parameters, such as mean kinetic energy and density of the plasma which have a direct influence on the films properties.

Silicon and Germanium thin films were grown by ablating targets of 99.99% purity of silicon and germanium individually using a 1064 nm Nd:YAG laser with 6 ns pulses and output energy of 600 mJ under vacuum conditions. Silicon films were grown on glass sustrates and germanium films were deposited on silicon sustrates. The goal of the study is to analyze the influence of plasma parameters in physical properties of the films. The samples were characterizated by Raman spectroscopy, X-Ray diffraction, scanning electron microscopy and X-ray photoelectron spectroscopy.

[PLV-158] Implementation of Ion Pump, NEG and Bakeable BNNT Cryopump System to Reach Extreme High Vacuum

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New accelerator initiatives require spin polarized electron photoinjectors which can be produced by gallium arsenide (GaAs) photocathodes . The GaAs photoguns must provide high average current (>>1mA) and a long operating lifetime. Its performance depends on our ability to improve vacuum inside the chamber. The Center of Injectors and Sources (CIS) at Thomas Jefferson National Accelerator Facility has nearly reached extreme high vacuum (XHV) P=1x 10^{-12} Torr by combining Non-Evaporable Getter (NEG) pumps and ion pumps(IP) in the Continuous Electron Beam Accelerator Facility (CEBAF) polarized source. Obtaining XHV pressure requires careful material selection and preparation, and appreciation for pump characteristics, capability and limitations. Measuring pressure at XHV is also a challenge so gauges must be used that have low x-ray limits, and the x-ray contribution to the pressure must be measured. In this project we investigated cryopump technology to reach and maintain an XHV regime on the electron gun to achieve P<1x 10^{-12} Torr, using a bakeable cryopump with mechanically attached Boron Nitride Nanotubes (BNNT), and the NEG-ion pump system. We also measured the x-ray limit of the extractor and bent belt-beam (3BG) gauge that we used to measure the pressure. Additionally we used the Monte Carlo simulation software MolFlow+ to model the pressure distribution in the chamber, using the expected outgassing rates, measured temperatures, and expected pump speeds for the NEG, ion and cryopumps.

[PLV-170] Study of reactive magnetron sputtering via plasma emission spectroscopy: correlation to thin film characteristics

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In this work we present a detailed study on the relation between the plasma spectroscopy and different deposition parameters of reactive magnetron DC sputtering (MS). Silicon and titanium targets while being sputtered with Ar at constant mass flow ratio, were exposed to O_2 or N_2 which were gradually introduced into the deposition chamber and then removed to obtain a hysteresis behavior. This behavior was interrogated in real time by means of optical emission spectroscopy (OES) observing at the vicinity of the target and a connection between the emission lines ratio (using neutral and/or ionized species) and the reactive sputtering mode (either metallic or dielectric) is stablished. Several emission lines from Ar, reactive gas and the target material were employed to make this study. Some of the deposition conditions were chosen to deposit an actual film and then characterize it via ellipsometric spectroscopy and X-ray photoemission spectroscopy (XPS). The aim of this work is to eventually be able to foresee the outcome of reactive magnetron sputtering and correlate the plasma emission to the thin film characteristics with a high degree of repeatability.

[PLV-245] SYNTHESIS OF SiGe ALLOYS BY THE SIMULTANEOUS LASER ABLATION OF Si AND Ge TARGETS

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Ge rich SiGe alloys have been deposited by the simultaneous laser ablation technique. The individual laser produced plasmas were diagnosed by means of TOF technique based on Langmuir planar probe measurements. Mean kinetic energy and density of the ions were estimated from TOF curves. In order to grow SiGe alloys, Si and Ge plasmas were combined, the plasma parameters of Si were fixed while varying the parameters for the Ge to get different compositions. Films were grown at room temperature on glass and Si substrates. The as grown samples were thermally annealed from 400 to 700°C and Raman spectroscopy measurements were carried out in situ while heating in order to observe structural changes with temperature. The as grown and annealed films (700°C) were structurally characterized by X-ray diffraction. Results show a dependence of structural properties of the film on plasma parameters.

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[PLV-295] More studies of Hollow Cathode Discharges: electrode geometry and material

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Hollow Cathode discharges have been known since the paper by F. Paschen in 1916 where he demonstrated that such a system could produce a high electron flux and plasma density. The term "hollow cathode" is used to describe almost any cathode with a cavity-like geometry, cylindrical, planar or spherical, such that the plasma is confined within conductive walls which are at the cathode potential. In the same way that magnetic trapping of the electrons in a magnetron gives an increased plasma density, in the hollow cathode the geometry produces a high density plasma, partly, by reducing the loss of electrons. Three types of discharge can exist in a hollow cathode, at low power and/or a low gas pressures the plasma is a typical low-current high-voltage glow discharge. However, for certain combinations of gas pressures, P, and hollow cathode diameter, d, at relatively large applied powers, the negative glow of the plasma almost completely occupies the interior volume of the electrode. In this case the plasma current can be 100 to 1000 times that for the typical discharge and the plasma density is correspondingly larger. Finally, if the cathode is not cooled the discharge can transform into a dispersed arc, and as the electrode temperature increases thermal-field electron emission becomes an important additional source of electrons, and this in turn, increases even further the plasma density and current.

The conventional explanation for the high plasma density involves the existence of high energy “pendulum” electrons which are reflected from the opposing sheaths on either side of the inside of the cathode; the long trajectory of these electron is considered to be able to produce an increased number of secondary electrons, with this resulting in the higher plasma density and current. We will discuss some of the problems associated with the well-accepted model and describe a new explanation based on the formation of doubly charged ions. We will also present recent studies of the dependence of the I-V characteristics of the discharge on the geometry of the cylindrical cathode (internal diameter and length), and the ion-induced secondary electron emission of the material used to make the cathode.

[PLV-306] Modification of the structural and mechanical properties of TaN film with Zr inclusion produced by DC Magnetron Sputtering on Si.

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The inclusion of the M material in the TNx or TCx matrix modify its morphology, structural and chemical composition that affect its mechanical, electrical, optical and tribological performance that improve their application field. The TaN has been investigated such as diffusion barrier but nowadays has been studied by its mechanical properties that could improve the wear resistance of parts that work under high demand operation like the hip prosthesis.

This work presented the study of the morphology, structural and chemical composition modification and their effects in the mechanical properties of TaN film with Zr inclusion with the variation of applied DC power to Zr target (P_{Zr}) produced by CD magnetron co-sputtering. The P_{Zr} application produced the film with columnar morphology at low values that change to dense morphology at higher. This kind of effects was observed in the film structure with the change from a C-TaN to H-TaN and the modification in the Ta-Metallic phase and smaller TaN crystal size. These differences affected the film hardness, obtaining lower values on the film with Zr inclusion.

[PLV-387] Temperature effects in synthesis of nanostructured films by pulsed laser deposition: Comparison of substrate heating and post-annealing

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Pulsed laser deposition (PLD) is a well-established technique for producing nanostructured films and the growth temperature is a key process parameter to control the film morphology. On the other hand, post-annealing of thin films is an efficient method for surface engineering allowing to change the particle size, shape and structure. However, the temperature effects during and after PLD are still poorly understood, a direct correlation between the two methods of nanostructure formation is missing, and the control of sizes of PLD-produced nanoparticles remains a challenge. In this work, we report experimental results on comparison of morphology of nanostructured metal films produced in two PLD regimes, (a) a substrate kept at an enhanced temperature T_s (in the range 300-800 °C) during PLD and (b) post-annealing at the same temperature for films deposited at room temperature. Gold and silver films were deposited with the mass thickness h in the range 3-8 nm. We demonstrate that the final film morphology, for both synthesis ways, is mainly governed by a combination of the two parameters, T_s and h. Various mechanisms underlying film structuring in different PLD regimes such as nucleation, particle surface diffusion and evaporation, island coalescence, assembling of preformed small clusters, solid-state dewetting, and Ostwald ripening are discussed. Ways to control the particle size distributions under PLD conditions are also discussed.

[PLV-445] Characteristics of Various Pulsed Plasmas for Nanoscale Etching

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As the device dimension continues to shrink to sub-10 nm as well as for 3D memory, precise etching technology is required. In recent years, pulsed plasmas using fluorocarbon (FC) containing gases with different fluorine/carbon ratios have been introduced for the etching of fine patterns which requires tight feature control for a small trench or a slit with a high aspect ratio in semiconductor industry [1]. Especially, due to various advantages such as selective etching, less charging effect, and increased plasma uniformity, pulsed plasmas have been more actively investigated for deep nanoscale pattering [2]. For the pulsed plasmas, not only the source power but also the bias power is pulsed together and the synchronized pulsing, where the source power is pulsed on and off at the same time with the bias power, is generally used [3]. For the semiconductor etch processes, pulsed plasmas are also investigated not only for capacitively coupled plasmas but also for inductively coupled plasmas because different (conductor/dielectric) materials are etched repeatedly for a multi-layer etching and the etching requires high selectivity with tighter CD control. However, in pulse plasma, the plasma chemistry which involves gas recombination during the pulse-off time is more complex, therefore, the plasma chemistry of some molecular gas mixtures and their surface reactions in the pulse gas phase is poorly understood.

In this study, the effect of various pulsed plasma chacteristics on gas dissociation and etch characteristics has been investigated using 27.12 MHz ICP source power and 13.56 MHz bias power. The characteristics of plasmas for synchronized pulsing and asynchronized pulsing will be compared while varying the duty percentages and pulse on/off time between the source power and bias power. For better control of the critical pulse plasma parameters, we investigated the pulse phase diagnostics and elucidated how these plasmas may affect processing and optimizing etch processes.

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PLASMA AND VACUUM (PLV) POSTER SESSIONS

[PLV-80] Bismuth telluride thin films via crossed beams PLD

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Bismuth telluride thin films were grown by pulsed laser deposition (PLD). The interest for this work came from the search for a feasible and reproducible method for synthetizing stoichiometric Bi_2Te_3 films, this due to its excellent thermoelectric properties, in addition, the material exhibits exotic states of matter that make it a topological insulator, one of the building blocks for the electronics of the future.

For the films synthesis, a pulsed Nd:YAG laser with 1064 nm wavelength, 5 ns pulse duration an 10 Hz of frequency was used. In this study two independent targets of bismuth and tellurium were simultaneously ablated looking for a combination of Bi and Te plasmas, thus providing flexibility on the laser energy and focus deposition conditions, in contrast to alloyed targets where congruent transfer of stoichiometry is not always possible; the deposition was done at a pressure of 3.8×10^{-6} Torr for 20 minutes, three glass substrates at room temperature were introduced into the chamber, allowing characterization of the films to be done over a wider area in order to account for plume-substrate interaction at different places of the deposited samples.

The obtained films have a metallic mirrorlike appearance, and present good adhesion to the substrate. Samples composition was characterized by Raman spectroscopy, EDS and XPS since full structural characterization by Raman is not possible considering the coexistence of similar hexagonal structures of different Bi-Te phases on the films, leading to uncertainties, that information must be correlated with EDS and XPS data; on the other hand, crystallinity measurements were performed with XRD for each sample, plus the target analysis. Film morphology was analyzed by SEM and AFM profiles for thickness.

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[PLV-95] Synthesis of TiO2/CuOx thin film composites by the simultaneous ablation of Ti and Cu metallic targets

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Titanium Dioxide (TiO_2) is an n-type semiconductor material that has been used for different applications such as photo-catalysis, hydrogen separation and dye sensitized solar-cells. The band gap for TiO_2 anatase phase is 3.2 eV, which means that UV light is needed to generate a photo-catalytic reaction. In this work, we proposed to generate a combined system of TiO_2 with Copper Oxide (CuO_x) to reduce the TiO_2 band gap so that the photo-catalytic process can be induced under UV and Visible light.

We present the results obtained for the synthesis of a combined system of TiO_2 and CuO_x thin films deposited on glass substrates. We used a reactive Pulsed Laser Deposition (PLD) technique with a mixture of argon/oxygen. The produced plasma was diagnosed by means of the time of flight technique using a Langmuir planar probe; the voltage drop across a 20 Ohm resistance was measured and the current was calculated in order to estimate the ion density and its mean kinetic energy, with the aim of having a control on the deposition process.

A Nd:YAG pulsed laser with a wavelength of 1064nm was divided into two equal beams using a beam splitter. Each individual beam was focused on the surface of Titanium (Ti) and Copper (Cu) solid targets respectively for 15 minutes under an argon/oxygen pressure of 20 mTorr. Primarily we obtained an amorphous TiO_2 thin film and a CuO thin film, afterwards we deposited a multilayered thin film of TiO_2/CuO/TiO_2 and finally a combined system of TiO_2 and CuO_x by ablating both Ti and Cu targets simultaneously.

The obtained thin films were characterized by X-Ray Photoelectron Spectroscopy (XPS), X-Ray Diffraction (XRD), Raman Spectroscopy, Ultraviolet-Visible spectroscopy (UV-Vis) in order to know the stoichiometry and oxidation phases and Transmission Electron Microscopy (TEM) was used to define the morphology.

Characterization reveals that a TiO_2 amorphous phase was deposited in any of the different experiments but Cu reacts in different ways depending on the plasma characteristics, it is shown that we can obtain different Cu oxidation states an even synthesize metallic Cu nanoparticles in a TiO_2 matrix.

[PLV-132] Synthesis of Paramelaconite via Laser Ablation in Liquids

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Chemical methods for producing nanoparticles, metallic in particular, are well known. However, application prospects might be restricted due to possible impurities. Laser ablation of solids in liquids is basically free from this limitation, because nanoparticles in this case are produced owing to the mechanical interaction of dense vapor of the liquid with the molten layer on the target surface. Due to the abaltion of the solid surface, a plasma plume from the target is generated, which unlike PLA on vaccum, is confined by the surround liquid. This confinement effect induce an extra pressure and, therfore, extra temperature, favoring the formation of metastable phases. In this work, paramelaconite nanoparticles have been obtained under pulsed high power Nd: YAG laser ablation of a copper target in propanol while varying time, power and wavelength. Copper oxide nanoparticles were characterized by UV-visible, high resolution transmission electron microscopy (HRTEM), TEM and X-ray diffraction. Transmission electron microscopy (TEM) demonstrated particle size in the range 10-100 nm. The interplanar distance was calculated from the electron diffraction pattern and HRTEM. It was observed that nanoparticle size depends of the wavelength and intensity of the laser, resulting into smaller size using 532 nm laser light. In our study, is found that laser wavelength of 1064 nm produces a better defined shape than 532 nm. The results show that stability of paramelaconite is affected by the high temperatures and oxidizing atmosphere, leading to a mixed phase of tenorite and paramelaconite. The obtained nanoparticles are spherical according to TEM images.

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[PLV-171] Optimizing deposition parameters for reactive magnetron sputtering by monitoring the plasma optical emission spectroscopy

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Thin films technology has grown during the last years due to its many applications. Extensive research has been focused on silicon oxides and nitride, and titanium oxide films for its excellent properties. Although the wide variety techniques for thin film deposition, reactive magnetron sputtering is one of the preferred. However, one of the major drawbacks of this technique is the lack of repeatability of the film properties under the same deposition parameters as a result of the so called target poisoning.

The aim of this work is to obtain the optimal deposition conditions for SiO_2, Si_3N_4 and TiO_2 thin films grown by reactive magnetron sputtering in order to guarantee specific film properties, especially refractive index for optical filters applications. Optical emission spectroscopy was used to monitor the deposition process in real time and to observe the species contained within the plasma. Information of the emission intensity was employed to obtain intensity ratios between certain emission transitions, which were then correlated with the film optical properties analyzed by spectroscopic-ellipsometry. Relation between these parameters can give valuable knowledge about the deposition rate and refractive index, which will allow to fabricate thin films with variable refractive index and with a high degree of repeatability.

[PLV-172] Classification of aluminum alloys by an inexpensive Laser Induced Breakdown Spectroscopy system

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Laser induced breakdown spectroscopy (LIBS) has been widely used for elemental analysis of solid, liquid and gaseous samples due to its portability and the practical null sample preparation. Due to the changing nature of the induced plasma the necessity of using a time-resolved spectroscopy system, consisting of a Czerny-turner spectrograph and an ICCD camera, is usually mandatory; however, these systems are delicate and the portability could be difficult. Although field spectrometers with a CCD detector could have relatively high spectral resolution, their main drawback is the trouble to synchronize the laser beam trigger to the beginning of the spectral acquisition. If the trigger issue is resolved with a relatively low jitter, these spectrometers could be an attractive alternative for characterization of material composition via LIBS.

In this work, a CCD spectrometer (Avantes, AvaSpec) is tested to determine the composition of several aluminum alloys by applying statistical tools such as Principal Component analysis of the ratio of the emission lines from emitting species within the induced plasma. Different experimental parameters were studied and results are discussed in terms of the correct identification of the Al alloy.

[PLV-202] Fabrication of semi-transparent CdS/CdTe thin film solar cells by magnetron sputtering

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In this work, thin films were deposited using the magnetron sputtering technique to obtain the CdS/CdTe heterostructure grown on SnO_2:F coated soda-lime glass substrates. Two different methods of $CdCl_2$ treatment were used; the first consisted in the use of $CdCl_2$ solution and the second, was carried out by evaporated $CdCl_2$. The influence the treatment on the properties of the CdS/CdTe structure was studied. In addition, sputtering parameters were set to reduce the thickness of the CdTe film since they have a great potential in the manufacture of semi-transparent PV windows, which can be deposited on different substrates.

X-Ray Diffraction (XRD) was used to identify the preferential orientation and crystallite size. The optical characterization was studied by photoluminescence (PL) and UV-VIS spectroscopies; through which it was possible to determine the bandgap of the material. The morphology of the material, surface and grain size was studied with the scanning electron microscope (SEM) and the atomic force microscope (AFM).

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[PLV-240] Development and characterization of thin films of Bi2Sr2Can-1CunOx by RF Sputtering method

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The development and obtaining thin films from superconducting materials has been one of the current objectives of solid state physics in order to increase its possible applications in the electrical field by means of electric current transport without resistance or "supercurrents". In the case of the bismuth base superconducting system $Bi_2Sr_2Ca_2Cu_3O_{10}$ or Bi-2223 phase, a great effort has been made to stabilize it due to its electrical properties and its high critical temperature (T_c~ 100-110 K). In this work, films were obtained from a superconducting $Bi_2Sr_2Ca_2Cu_3O_{10}$ target on quartz substrates using the RF Sputtering technique. The films were obtained at a pressure and temperature of $1.4x10^{-3}$ Torr and 300 °C, respectively. Once the superconducting films were obtained, thermal treatments were carried out by varying the time and temperature of the treatment. The targets and films of $Bi_2Sr_2Ca_2Cu_3O_{10}$ were characterized by X-ray diffraction, Raman spectroscopy, EDS and Meissner effect. The results obtained are discussed in terms of growth parameters

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[PLV-241] Development and characterization of YBa2Cu3O7-X Superconductor thin films by pulsed laser deposition

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The study and application of superconducting materials has had a remarkable growth since its discovery. Applying these materials in electrical devices such as generators, motors and electrical transformers, as well as electric power transmission lines. This in order to increase energy efficiency mainly in the electricity generation sector through sustainable resources; implementing these advanced materials in wind and hydraulic turbines. In this work a $YBa_2Cu_3O_{7-X}$ superconducting target was obtained by the solid state reaction technique using the following precursors: Y_2O_3, $BaCO_3$, and CuO. Once the superconducting target was obtained, $YBa_2Cu_3O_{7-X}$ thin films were obtained by pulsed laser deposition technique. The target and the films were characterized by X-ray diffraction, Raman spectroscopy, EDS and resistance measurements as a function of temperature. The results are discussed in terms of the growth parameters.

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[PLV-248] Mechanical characterization of nanocrystaline ZrN thin films under forming gas influence

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In this work, the mechanical properties of reactively sputtered ZrN thin films deposited on (100) silicon wafers are reported. These films were grown by a DC-Sputtering system under the influence of forming gas (NH_3) and Argon to encourage the reduction of oxide impurities in the films, and they were synthetized using different deposition power. that varied from 60 W to 90 W on the Zr target. The different samples were studied in this work by EDX measurements to obtain the chemical composition. X-ray diffraction measurements showed that the thin films are indeed crystalline. As a consequence, the XRD analysis also confirmed the cubic structure of ZrN. The mechanical properties were measured by nanoindentation and they showed that the films hardness had an average of 14 GPa under different weights on the films.

[PLV-275] CdS and CdTe ultrathin films grown by RF sputtering

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Currently the use of fossil fuels, is the main source of energy used globally, and coupled with the great global population growth, energy demand grows, this brings about the depletion of these fossil resources at a dizzying pace, which already begin to be depleted in different parts of the planet. To delay this situation or if it is possible to find a solution, the use of so-called "alternative sources of energy" has been proposed, which can be the key point to solve the world's energy problems. Solar energy comes in large quantities to almost all parts of the planet and also has a great advantage: it is free. For this reason, it is proposed to use it through photovoltaic devices, which transform this energy into electricity. The present research project proposes the use of thin film solar cells to build photovoltaic panels; that can be used as photovoltaic windows, taking advantage of the characteristics of the ultrathin films of cadmium telluride (CdTe) whose main feature is that it produces cells that have a natural polarized, taking advantage of this to produce these windows. The deposition of the thin films will be done by means magnetron sputtering, since this physical process generates very uniform films, which is a great advantage to be used as photovoltaic windows. The heterostructure of the solar cell to be developed corresponds to the following: SnO_2/CdS/CdTe where SnO_2 is a TCO, and CdS and CdTe, are n-type and p-type semiconductors, respectively. In this work, we report the influence of growth parameters on physical properties of CdS and CdTe films grown by RF sputtering. The crystalline structure was characterized by X-ray diffraction. Film thicknesses were measured directly by profilometry. The results are discussed in terms of growth parameters.

[PLV-334] Elemental composition of ZnO:Al thin films by laser induced breakdown spectroscopy

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In the present work, Laser Induced Breakdown Spectroscopy (LIBS) is used to investigate elemental composition of the synthesized ZnO:Al thin films. ZnO:Al thin films were deposited by ultrasonic spray pyrolysis onto glass substrates with 0, 0.5, 1.0, 2.0, 3.0, 4.0, 5.0 and 10.0% [Al^{3+}/Zn^{2+}] ratios in the deposition solution. We have investigated LIBS spectrum of ZnO:Al thin film in air atmosphere using Nd:Yag laser. The Al, Zn and O lines were found in LIBS emission spectrum. The Zn/Al intensity ratio was identified as a representative parameter of the thin film material properties. It was demonstrated that Al intensity increased as the percentage of aluminum was incorporated in the ZnO matrix increased.

Acknowledgements

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[PLV-363] CdS thin films grown by RF sputtering: Influence of the growth parameters on photovoltaic response

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Cadmium sulfide (CdS) is an n type semiconductor material, with a bandgap oscillating between 2.4 to 2.6 eV. It presents two characteristic crystalline structures, cubic, Zinc-Blenda type, and hexagonal-wurtzite type. Its optical transmittance in the near ultraviolet-visible spectrum is high (greater than 70%), this property makes it very attractive for being applied as window layer in solar cells based on thin films. However, until now, the electrical resistivity decreasing in CdS films is a challenge in the field of research. In this work, a chacarterization of the optical, structural and electrical properties of CdS thin films deposited by RF sputtering is presented. The films were optically characterized by their optical transmission measured by spectrophotometry in the ultraviolet-visible range of 200 to 1100 nm and the bandgaps were determined from these spectra by using the Tauc´s method. Additionally, Raman spectroscopy and photoluminescence analyzes were performed. The crystalline structure was characterized by X-ray diffraction. The electrical characterization was developed by means of the 4-point probe, Van der Pauw and Hall effect, thus determining the electrical resistivity, conductivity type, carrier concentration and electron mobility. Film thicknesses were measured directly by profilometry and confirmed by the Manifacier´s method. Both deposited films (by chemical bath and sputtering) were separately applied for manufacturing a glass/TCO/CdS /CdTe heterostructure to evaluate its performance as solar cell by determining its characteristic current-voltage (IV) curve under an 1.5 AM illumination.

Keywords: Thin films; Sputtering; Solar cellsTransparent electrodes.

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[PLV-399] Textured surface by reactive ion etching for the formation of black silicon as an alternative of anti-reflective layers for use in solar cells

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Black silicon (b-Si) has surface structures with a very low reflectance. It possesses light trapping properties, due to its high absorption rates in a relatively wide range of wavelengths making it a perfect candidate for the development of more efficient silicon solar cells; The principal characteristics of the b-Si are high surface density and light reflection between the structures formed in it.

The texturing method chosen was the reactive ion etching system (RIE) with Sulfur Hexafluoride and Argon, which eliminates the wet etching process disadvantages. Furthermore, the surface reflectance is reduced with a very slight loss of superficial silicon. This technique can be applied to different silicon structures (-mono or -polycrystalline), i.e. for multiple crystalline orientations. RIE uses chemically reactive plasma for the formation of black silicon. The plasma is generated under low pressure (vacuum) by an electromagnetic field. The high-energy ions in the plasma attack the surface of the wafer and react with it.

The tests in RIE were carried out on 15 pairs of samples of polished silicon type P and silicon type N with a previous chemical treatment in KOH. While varying the time, the electric potency and the gas flow we obtained the optimal conditions. Furthermore, we continued carrying out tests in 20 pairs of a sample, looking forward to, reproducibility and different improvements with chemical treatments before etching in RIE. The engraved surface of b-Si shows a reflectance close to 1% for the wavelength of 550 nm and no more than 5% in the range of 200 to 1200 nm, pickling at a thickness of 600 nm on average.

The I-V measurements by means of a solar simulator, were performed on both sides of the solar cell, obtaining good results in both cases; However, it was necessary to optimize the RIE parameters, the annealing times, the polishing of the wafer and the thickness of the evaporation material for the ohmic contacts, so that when the IV curve of our cells is obtained, the benefit is clearly observed.

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[PLV-413] Polyallylamine matrixes with multimodal size distribution of embedded silver nanoparticles synthesized by DC plasma

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Polyallylamine-Ag (PAl-Ag) thin films composites containing Ag nanoparticles were prepared by DC glow discharges and characterized by SEM, EDS analysis, TEM, XRD, FT-IR, UV-VIS spectroscopy, and DC conductivity measurements. The synthesis by plasma made possible the one-step formation of layered materials of PAl and PAl-Ag composites for possible applications as coatings on medical products and wound dressings. The metal content in the films composites was controlled as a function of the monomer feed rate into the polymerization chamber. Composites with thickness from 0.25 μm to 2 μm were obtained. The metal particles tend to grow with the (111) planes parallel to the substrate as can be found from the high intensity ratio between (111) and (200) reflections, also observed in similar synthesis.

[PLV-447] Synthesis of molybdenum oxide thin layer by laser ablation

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Molybdenum oxide (MoOx) is a transition metal-oxide (TMO) with a great technical interest due to its remarkable optical and electronic properties. MoOx has the potential to be used in a variety of applications in the field of crystalline silicon and perovskite solar cells, chemical catalysis applications and hydrogen separation. Besides TMO can be switch between two different optical states prompted by photochromic, thermochromic or electrochromic effect. Molybdenum oxide thin films have been prepared by different methods such as sol-gel technique, magnetron sputtering, pulsed laser deposition (PLD) and chemical vapor deposition (CVD). In this work we used the PLD technique to study the influence of the deposition pressure has on the parameters (mean kinetic energy and ion density) of the plasma generated by the laser ablation of Metallic molybdenum in an oxygen atmosphere, in order to optimize and control the synthesis of MoOx thin films. The results presented in this work are discussed as a function of the background pressure. For the ablation process, a Nd:YAG pulsed laser with a wavelength of 1064 nm was focused on the surface of Mo solid target for 20 minutes. The background gas was a mixture of 80% argon/ 20% oxygen. The pressure values were of 5 and 10 mTorr. Characterization of the thin films was carried out by Raman Spectroscopy, Scanning Electron Microscope (SEM), X-Ray Photoelectron Spectroscopy (XPS), X-Ray Diffraction (XRD) and Ultraviolet-Visible Spectroscopy (UV-Vis). According to XRD and Raman measurements, the crystalline structure depends on the pressure, besides XPS results show that the oxidation state in thin films is also influenced by the deposition pressure.

[PLV-545] Incorporation of potassium via hydrothermal in ZnO nanostructured thin films grown by PLD

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ZnO thin films were grown on glass substrates by laser ablation of a Zn metallic target in an O_2/Ar (20/80) atmosphere at room temperature. For the deposition process a Nd:YAG (532 nm) laser was used with 5 ns pulse duration and frequency of 10 Hz. The pressure in the chamber was kept constant at 2×10^{-2} Torr. Plasma parameters (mean kinetic energy and density of Zn ions) were calculated from "time of flight" curves obtained by Langmuir planar probe measurements. Zn ions density was kept constant while the mean kinetic energy was varied. Samples were hydrothermally treated (HT) using a KNO_3 solution in order to incorporate K into the ZnO thin films. Before HT, XRD patterns of the films reveal the presence of a strong peak corresponding to the (101) plane and a wide peak corresponding to the (002) plane, both of the Wurtzite phase of ZnO. After HT treatment, the (101) plane was no longer observed. XPS characterization shows the presence of K $2p_{3/2}$ in sample grown at mean kinetic energy 80 eV. Electrical and optical properties of the ZnO: K thin films were investigated.

[PLV-553] Optical study of the plasmas produced in a combined magnetron sputtering and pulsed laser deposition system during the growth of ZnO-Au films

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The deposition hybrid technique combining magnetron sputtering (MS) and pulsed laser deposition (PLD) has been used in recent years to prepare nanocomposite materials as thin films and to study their mechanical and tribological performances. Most of the reports have been focused on the films properties, and only a few of them report the study of the species into the plasmas produced during the deposition processes. In this work we evaluate the behavior of the species in the plasma by optical emission spectroscopy during the combination of the ZnO sputtering and gold laser ablation. The aim of this work was to study the effect of the background gas and MS plasma on the temporal evolution of the optical emission of the following species: neutral and ionic Au, neutral Ar and Zn atoms. Specifically, we recorded the temporal profiles of the emission lines corresponding to Au I (479.26 nm), Au II (405.28 nm), Ar I (763.51 nm) and Zn I (472.22 nm) at 5, 25, 35 and 45 mm from the Au PLD target surface. Also, the laser energy density was varied at 1.2, 3.6 and 5.4 J cm-2. The measurements were done under different conditions of the laser ablation of the gold target: a) under high-vacuum (4x10-4 Pa), b) under an argon atmosphere (0.67 Pa) and c) simultaneously with the ZnO sputtering process. Apparently, the argon is excited by the collisions with the Au ions, which is evident at short observation distances. Also, at the shortest distances to the Au target surface, we observed no changes in the temporal profiles, but at the largest distances the variations of the intensity and time positions of the profiles maxima were observed. In all environments, at 45 mm from the Au target surface (near the substrate surface), there was a notable increment of the intensity of Au I and Zn I emission, which suggested the rebound of neutral atoms of Au from the films surface exciting the neutral atoms of Zn in the highest density region of the MS plasma.

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PHOTOTHERMAL PHENOMENA (PTP)

Chairman: Mario Enrique Rodríguez García (CFATA-UNAM)

PHOTOTHERMAL PHENOMENA (PTP) ORAL SESSION

[PTP-524] Study of the Si/SixOy interphase stability by photocarrier radiometry spectroscopy

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Silicon oxide (SiO_x) is the most common passivation covering used in the manufacture of electronic devices based on silicon (Si) to prevent the diffusion of impurities into the bulk material and stabilize the interface. However, different types of defects dominate the electronic properties of the Si/SiO_2 interface, this fact converts the Si/SiO_2 interface in a not simple system due to the non-equilibrium distribution of the carriers charge across the of the Si/SiO_2 interface, that makes it sensitive to an optothermal phenomenon. In this work, it was investigated the thermoelectric stability of the Si/SiO_2 interface by photocarrier radiometry spectroscopy, in the linear regime of optical flow. It was found a diverse transitive phenomenon as a function of the lighting time. The results obtained can be used to understand the diffusion phenomena of impurities through the surface interface and bulk and the silicon oxide surface stability.

[PTP-528] Bragg Reflector fabrication monitoring by using in situ photoacoustic

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The Porous Silicon (PSi) is used to fabricate multilayer systems for photonic devices. One of the most common systems based is the distributed Bragg reflector (DBR). The quality and characteristics of the DBR of PS depend strongly on the fabrication process that it is usually by electrochemical etch in hydrofluoric media. This route could make the PS layers with no-controlled properties because it depends on of multiple parameters during the etching process such as current density, electrolyte composition, lighting conditions, temperature among other intrinsic and extrinsic parameters. The photoacoustic technique is useful for monitoring in situ the PS multilayer formation and measured in real time the properties of every single layer that are part of the DBR because the PA signal is directly related with the reflectance. In this work, it used a photoacoustic cell coupled to an electrochemical cell for monitoring in-situ de fabrication process of DRB based on PSi. It was used as an effective medium approximation (EMA) to calculate the refractive index of the layers, and it was simulated the optical response of the heterostructure. This procedure was made for design and characterize the DBR systems.

PHOTOTHERMAL PHENOMENA (PTP) POSTER SESSIONS

[PTP-16] Measurements of the thermal transport properties of heptane-isooctane mixtures

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Measurements of the thermal transport properties of heptane-isooctane mixtures in the liquid phase at room temperature and atmospheric pressure were performed. The thermal conductivity, k, was measured using the transient hot-wire (HW) method, and the thermal effusivity, e, was determined by the front photopyroelectric (FPPE) technique. Then, the thermal diffusivity, α, and the volume specific heat capacity (heat capacity per unit volume), C, were calculated using the well-known relationships $\alpha = (k/e)^2$ and $C = e^2/k$, respectively. We show that a correlation between these parameters and octane number exists, and that the obtained thermal parameters proved to be sensitive to detect molecular associations in binary hydrocarbon liquid mixtures. We also report about the thermal conductivity of mixtures of n-alkanes vapors and air showing that almost similar values are obtained for heptane and isooctane, so that octane number rating using the well-established binary mixtures of these substances becomes impossible with thermal properties measurements in the gas phase.

[PTP-56] Photoacoustic spectroscopy applied to the study of fisher rat blood with hepatic damage and the effect of spirulina treatment

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Photoacoustic spectroscopy (PAS) has been increasingly used for analysing biological samples, particularly optical absorption spectrum of blood has been associated with some diseases [1]. In the present study, the optical absorption spectra of Fisher rat blood, with liver cancer, are obtained by using photoacoustic technique, also the daily intake of Spirulina (*Arthrospira maxima*), as a protection liver damage, was evaluated. Through the amplitude of the characteristics peaks of blood α(585nm), β(550nm) and γ(420nm) it is possible to associate them with differences in concentrations of haemoglobin in the studied samples, by means of the peak ratios and [2], obtained from the optical absorption spectra of blood of each analysed group.

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[PTP-71] New hot wire prototype of small dimensions for thermal properties measurement of nanofluids

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Recently, the Transient Hot Wire Technique is a useful tool for thermal conductivity measurement. It has been implemented in several prototypes designed to test fluids quality, especially for nanofluids containing metallic and semiconductors nanoparticles.

To obtain measurement method, a new prototype of small dimensions that only needs 4 mL of a sample, was designed with the advantages that the test can be performed easily and quickly in a short period of time of only 5 minutes. The prototype is controlled by a LabView interface, which allows the user to control heating time and voltage used a wire, while the resistance and temperature graphs are displayed in a friendly GUI.

Thus, thermal conductivity, thermal diffusivity and temperature parameters can be accurately controlled on the device by the users and prototype performance is easy to manage in order to test nanofluids and fluids in general. Also, to ensure the tests reliability and precision, the prototype was calibrated by testing several well-known fluids, with already known thermal conductivities.

[PTP-77] Photoacoustic spectroscopy and its application in medicine

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The photoacoustic effect was discovered in 1880 by Graham Bell, but was only in 1976, the development of the first theoretical model to explain this phenomenon

In this effect, the gas is confined inside a chamber or cell with the sample inside this cell, it is illuminated with intensity modulated light. When the sample absorbs the light, raise its temperature in a modulated manner, causing a modified heat flow from the sample to the surroundings, towards the gas confined in the cell.

The energy supplied to the gas increases its temperature in a modulated way, causing pressure fluctuations in this gas, which can be detected by a microphone.

In this paper, the theory of the photoacoustic effect will be showed, as well as an application of photoacoustic spectroscopy in medicine, especially in the study of blood in diabetic rats. This technique is non-destructive, and it allows us to study biological materials "in vivo" and “in situ”.

[PTP-90] Characterization of thin samples with rare and frontal configuration using lock-in thermography.

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Infrared thermography is opening the way in the field of photothermal techniques due to its advantages over others, such as: non-contact with the material, it is not destructive, it manages to obtain a thermal map of the sample (which allows to characterize even anisotropic materials). In this work different materials are characterized by the lock-in thermography technique using an experimental system that allows the rear and front configuration without extracting the sample from the vacuum system. Some comparisons are made and the versatility of each one is checked. The thermal diffusivity of the samples is determined, analyzing some details that have been considered in previous studies for this experimental assembly, demonstrating that it is a fast and efficient experimental system for the thermal characterization of materials.

[PTP-99] PHASE RESOLVED METHOD APPLIED TO OPTICAL ABSORPTION SPECTRA OF RATS BLOOD WITH SEPTIC SHOCK

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Photoacoustic spectroscopy has become a very useful tool in the study of biological material since is not an invasive, non-destructive and suitable for these materials, due to its scattering of light that makes difficult to obtain its absorption spectrum by conventional spectroscopic techniques. The optical absorption spectra of the samples obtained by this technique evidence their own characteristics[1], in particular, when applied an analysis known as phase resolved method, in which is possible to observe optical absorption peaks of some components that constitute the sample. This method is based on the fact that there are different non-radiative des-excitation times corresponding to the components of the sample [2]. This method was applied in optical absorption spectra of blood samples from rats induced to septic shock, where absorption peak characteristics of blood components were found, such as the Soret band at 415nm and the cytochrome P450 at 450nm, the last component plays an important role in the evolution of septic shock and it is difficult to observe by conventional spectroscopic techniques, however, by applying this method it is possible to separate its optical absorption spectrum by making this component evident.

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[PTP-137] Photothermal techniques for thermal diffusivity and effusivity measurements of linear alcohols

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Thermal characterization of linear alcohols, from methanol to 1-decanol, was carried out by means of photothermal techniques; photopyroelectric technique, taking the sample´s thickness as variable, was used for thermal diffusivity measurements and photoacoustic technique, in the modulation frequency domain, was used for thermal effusivity measurements. Thermal effusivity values shown a decreasing behavior with the increase in size of the linear molecule, thermal diffusivity values, on the other hand, shown similar behavior but just up to 1-Pentanol from which these values start to increase. This peculiar behavior for thermal diffusivity was attached to the presence of the hydroxyl group and its relation with the molecule´s size.

[PTP-152] Self-normalized photoacoustic technique for thermal diffusivity measurements of materials consisting on thin layers

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A self-normalized photoacoustic (PA) technique for thermal diffusivity measurements of thin layered foils is presented. This methodology involves the analysis of the self-normalized PA signal as a function of the modulation frequency. This PA self-normalized signal consist in the ratio of signals in the transmission and front configurations. The thermal diffusivity for a steel foil, a silicon layer, different papers and a black paint on a glass substrate were measured for to illustrate on the applications of this methodology. Excellent agreement was obtained for thermal diffusivities reported in literature for similar materials.

[PTP-188] Spherification of silver nanoparticles in alginate: study optical and thermal properties

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Using the outer spherification method, composite microspheres of silver nanoparticles in an alginate matrix with different concentrations (0.010 - 0.030 mg / ml) were prepared. Metal nanoparticles were synthesized using the colloidal chemistry reduction method. Silver nitrate solution was reduced with sodium borohydride in the presence of sodium citrate as a stabilizing agent at room temperature. Spherical particles with average size in the nanometer scale (12 nm) were observed using transmission electron microscopy. Stabilized silver nanoparticles, immobilized and dispersed homogeneously in a microspherical matrix (21 x 103 μm) of alginate were obtained. The optical properties of the metal colloidal dispersion and the formation of the composite microspheres were evaluated using UV-Vis spectroscopy and optical microscopy. The properties of thermal diffusivity as function of the concentration of the silver nanoparticles were studied using thermal lens spectrometry. Higher values of thermal diffusivity of the microspheres were obtained with the increase in the concentration of metal nanoparticles. The behavior of the thermal diffusivity was corroborated using a theoretical model.

[PTP-219] Thermal diffusivity measurements by photoacoustic method of aluminum plates treated by plasma electrolytic oxidation

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Thermal diffusivity α, is a basic thermal quantity defined as the ratio of thermal conductivity to the product of specific heat c times the density ρ of the material. The measurement of this property is very important, as it can vary considerably with the particular composition and microstructure in a material during its production [1]. This thermal transport parameter determines the rate of heat diffusion in a material. The higher the thermal diffusivity is, the less time it takes for the heat to pass through the material [2], therefore its role is crucial in modern material design processes.

In this work, plasma electrolytic oxidation [3] has been applied to grow oxide layers on aluminum surfaces. The treatments have been performed applying 300 V pulses to samples immersed in electrolytic solutions of sodium disilicate and it has been investigated the influence of treatment on the thermal diffusivity of the samples. To obtain the sample thermal diffusivities, we used a photoacoustic method that considers the phase differences for heating occurring in the front and the rear face of the sample. The phase difference between the photoacoustic signals ($\Delta\varphi$) is given by the expression [1]:
$\tan(\Delta\varphi)=\tanh(l/\mu)\tan(l/\mu)$
where $\mu=\sqrt{(\alpha/\pi f)}$ is the sample thermal diffusion length, f is the light modulation frequency used to excite the sample, and l is the sample thickness. This method is useful to determine the thermal diffusivities of opaque thin samples of metal and semiconductors, being their temperature changes very small, an attribute particularly important in materials whose thermal properties varies significantly with temperature.

The results of the present study indicates that treated aluminum plate samples increase their thermal diffusivity when compared with the thermal diffusivity of pure aluminum.

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[PTP-301] Photoacoustic and modulated photoreflectance imaging of biased integrated circuits: voltage and temperature maps

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Photothermal reflectance microscopy has become a very well established technique for the characterization of thermal properties (thermal diffusivity, thermal conductivity, interfacial thermal resistance) of materials at the micrometer scale,[1,2] as well as for the investigation of the heat source distribution in optoelectronic and microelectronic devices in operation.[3,4]

In this work we propose an alternative technique that uses a combined thermoreflectance and thermoacoustic set-up for imaging biased microelectronic circuits, in particular, polycrystalline silicon resistive tracks grown on a monocrystalline Si substrate mounted on a test chip. Thermoreflectance images, obtained by scanning a probe laser beam on the sample surface, clearly show the regions periodically heated by Joule effect, which are associated to the electric current distribution in the circuit. On the other hand, the thermoacoustic signal, detected by a piezoelectric sensor located beneath the chip, also discloses the Joule contribution of the whole sample. However, additional information emerges when a non-modulated laser beam is focused on the sample surface in a raster scan mode allowing imaging of the sample.

The conventional experimental arrangement of the thermal reflectance microscopy is achieved by using an intensity modulated Ar^+ laser line as excitation, and a non-modulated He-Ne laser as probe, both superimposed and focused on the sample surface by an optical microscope (1.0 to 2.0 µm beam diameters). Typical Ar^+ beam power is 400 mW at the laser exit, resulting in a few mW to a few tens of mW at the sample surface, while the He-Ne laser power is 10 mW (less than 1.0mW on the sample). The reflected He-Ne beam is detected by a Si photodiode connected to a lock-in amplifier. The thermoacoustic signal is acquired by a pyroelectric/piezoelectric sensor. The distribution of this supplementary signal is related to the voltage distribution along the circuit, as shown by simulations performed using Advanced Design Software (ADS).

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[PTP-309] Photothermal images of corn grains through Photoacoustic and Photopiezoelectric Microscopies

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The use and implementation of photothermal (PT) techniques can provide information to characterize materials, their principal benefits are that they does not require a prior sample preparation and they are not destructive [1]. Among PT techniques, Photoacoustic Microscopy (PAM) and Photopiezoelectric Microscopy (PZEM) have been used to obtain images of homogeneous and inhomogeneous solids *e.g.* metals, semiconductors, and agricultural materials among others [2-6]. Therefore, in the present study thermal images of corn grains, with different characteristics (crystalline and floury), were obtained by using a portable PAM device and a PZEM system. The obtained images are shown in Figure 1, where it is possible to see three columns. The first column shows the sample optical images, the second and third columns show the PAM and PZTM images respectively. PAM and PZTM images have a color scale, which corresponds to differences in the PA and PZTM signals respectively, due to the different components in corn grain samples. The obtained images by PAM show a better image resolution in both grain varieties, when compared with PZTM images. In the case of PAM images it is possible to observe red zones within the grain contour because there is a greater signal amplitude.

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[PTP-391] Photoacoustic inverse problem for the reconstruction of images

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Se presentan los fundamentos físicos y planteamiento matemático del problema inverso fotoacústico seguido del uso de k-Wave, qué mediante el método de inversión temporal, reconstruye la presión inicial, que se generó por la absorción de un pulso electromagnético en una muestra (generalmente en el rango VIS-NIR). Esta presión se mide en diferentes posiciones alejadas del punto donde se originó por un tomógrafo fotoacústico automatizado hecho en casa y controlado por arduino a través de un teléfono celular. La señal inicial reconstruida se presentada mediante un presograma (imagen) en escala de grises con una resolución de un milímetro. Las muestras analizadas para hacer las pruebas de concepto de nuestro tomógrafo fotoacústico fueron huesos de rata Sprague-Dawley así como objetos metálicos y de acrílico. Durante las mediciones, las muestras fueron sumergidas en agua para lograr un acople de impedancias acústicas,. Para iluminar las muestras se utilizó un láser de Nd: YAG emitiendo a 532 nm y con una frecuencia de repetición de 6 Hz las señales acústicas fueron adquiridas con hidrófonos piezoeléctricos basados en PVDF.

This work presents the physical foundations and mathematical approach of the photoacoustic inverse problem and the use of k-Wave, that uses the time reversal method to reconstruct the initial pressure, generated by a source illuminated by pulsed electromagnetic radiation (generally in the VIS-NIR range). This pressure is measured in different positions away from the point where it was originated by a homemade automatized photoacoustic tomograph and controlled by arduino through a cell phone. The reconstructed initial pressure is presented in a gray-scale image and with a 1 millimeter resolution. The analyzed samples to make the photoacoustic tomograph proof of concept includes Sprague-Dawley rat bones, metallic and acrylic objects. During the measurement, the samples were submerged in water to achieve the acoustic impedance coupling. In our experiments, we used laser emitting at 532 nm with a 6 Hz repetition frequency and PVDF based hydrophone to acquire the acoustical signals.

[PTP-450] Photothermal characterization of mGO for laser asisted hyperthermia applications

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The hyperthermia is an alternative method in the treatment of the cancer, which consist in the heating of tissues by the use of hot water blankets, thermal chambers, catheters or blood perfusion depending on the localization of the tumor. The high temperature (42-45°C) can damage the cancerous cells while the health tissue experience no injury. Currently, this treatment is being approached in a different way in order to improve the localization of the thermal effect by injecting photosensitive nanoparticles in the tumor and then exposing the tissue to a NIR laser beam, enhancing the effects of hyperthermia. In this work, graphene oxide nanoparticles decorated with magnetite (mGO) in different proportions are being studied in order to be proposed as a nanomaterial alternative in laser assisted hyperthermia. The phase identification, microstructure, morphology and elemental composition were characterized by XRD, Raman spectroscopy, SEM and EDS respectively. Additionally, thermal properties were studied by the LFA method and photoacoustic spectroscopy. Finally, stable mGO suspensions were prepared in order to study the thermal behavior of the nanoparticles in the presence of a NIR laser at different power density.

[PTP-482] Finite sensor size effects in three-dimensional photothermal radiometry

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Photothermal radiometry has been widely to obtain lateral thermal diffusivity of solid materials. It is well known that the thermal field phase has a linear behavior when measured as a function of the distance to the excitation source, inside the excitation source, the phase is flat. In this paper we analyze the effect of the size of IR sensor on the measurement of the temperature field. Calculations developed show that the temperature field phase will remain flat when measured as a function of the distance to the excitation source, if the size of the sensor is larger than the radius of the excitation source. On the other hand, to observe the linear behavior, measurements beyond half the size of the sensor have to be performed, the slope is not affected. This demonstrates the symmetry property of the Green function, which states that the observation point can be exchanged with the source point and the result will be unchanged. Experimental results are performed using sensors of different sizes, particularly 50 μm X 50 μm, 1 mm X 1 mm and 4 mm X 4 mm.

[PTP-508] Study of Lager and Ale style commercial beers by photoacoustic spectroscopy

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The use of photothermal and photoacoustic techniques in theoretical and experimental aspects has boomed with the implementation of new technologies, with wide use in the investigation of various types of materials, whether solid, gases and liquids, the research developed demonstrates the possibility of use the technique of photoacoustic spectroscopy for the evaluation of beer types associated with the style that differentiates them, where from the study of the shape of the absorption spectra, these showed differences in a range of UV and Visible length showing values in The UVB band for the beers analyzed a similarity in the behavior of the amplitudes of the absorptions, and where respectively starting from the UVA band in the 325 approximately there were significant differences, these bands could be related to components such as proteins and flavonoids present; In addition, the study is complemented with UV-Vis spectroscopy and a comparison between the techniques used, where a distinction is found according to the tonality of the beer in both spectra.

[PTP-525] Determination of water permeability in starch films by photoacoustic technique

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The determination of the water permeability of starch films for different atmospheres is still an open problem that requires a detailed analysis. In this work a photoacoustic cell that allows the changes in the atmosphere conditions was developed to determine this parameter. Corn Starch-glycerol at 30, 40, and 50 ratios w/w where fabricated and studied by using photoacoustic. It was found a correlation of permeability coefficient, and glycerol contends. SEM images showed that the films are uniform and do not have a microporous formation. Mechanical properties showed that the films prepared with glycerol exhibit elastic and plastic regimens.

RENEWABLE ENERGY: MATERIALS AND DEVICES (RWE)

Chairmen: Issis Claudette Romero Ibarra (UPIITA-IPN)
Mario Fidel García Sánchez (UPIITA-IPN)

RENEWABLE ENERGY: MATERIALS AND DEVICES (RWE) ORAL SESSIONS

[RWE-111] "Heterogeneous direct transesterification, a novel method to obtain biodiesel"

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Nowadays, biodiesel production has emerged as one alternative fuel produced from vegetable oils and/or animal fats, is a sulfur-free, biodegradable, non-toxic and replaces the use of fossil fuels as a principal energy source and the air contamination main source. In this work the biodiesel was obtained by direct transesterification as new novel method in one pot (*in-situ*). The heterogeneous direct transesterification reaction is carried out with seeds as raw material, in the same reactor the oil was extracted and then it was transesterified. The biodiesel obtained is of high purity and the processes of purification, washing and neutralization are not necessary. No *n*-hexane is required for oil extraction. Thus, methanol as a reactant and as a solvent increased the greenness of the heterogeneous process, and the resulting biodiesel shows good purity and composition. In addition, no water is required to purify the biodiesel.

This process is a new novel method that facilitates the extraction and transesterification of the oil in one-pot obtaining 99.99% yields. Moreover, green metrics parameters of biodiesel showed that heterogeneous direct transesterification resulted in a seven times greener synthesis compared to conventional process. [1]

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[RWE-183] Development of polymeric materials based on polypropylene and magnesium micro-silicates for application in solar collector pipeline

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Energy saving and environmental care are of great importance in all countries. For this reason, the search for new sources of energy has been developed to replace those from fossil fuels. Among the renewable energies are: wind energy, geothermal, hydroelectric, tidal, biofuels and solar energy. In different regions, solar collectors made of polypropylene (PP) have a high durability, show good mechanical properties and are resistant to corrosion.On the other hand,micrometric talc can act as a thermal insulator, which in combination with other materials can retain heat at low temperatures. In this work, compounds of polyoropylene/microtalc (1.8 to 2 µm) were manufactured. by ultrasound-assisted extrusion 1.8 to 2 µ,. *The compounds were diluted to 5, 10 and 30% by weight. The obtained compounds were analyzed by X-ray diffraction, thermal analysis (DSC and TGA), heat capacity and scanning electron microscopy. X-ray results show the characteristic signals of PP and magnesium silicates in the corresponding raw materials. For the compounds, signals are shown at the 2θ angles of 12.45 °, 35.90 ° and 59.94 ° corresponding to the magnesium silicates. From the resulting thermal analyzes, for DSC the thermal transitions for all materials were recorded between 165.6 and 168.8 ° C. In the TGA analyzes, a weight loss of 99.7% was presented at 474 ° C for pure PP, and for the T-30 sample a loss of 83.4% was recorded at 489 ° C, showing that this and the different compounds they are thermally more stable than the PP. In the SEM images at the magnitudes of 2 000, 5 000 and 10 000X, can be seen that thanks to the ultrasonic assisted extrusion process there was a good dispersion of the particles in the polymer matrix. Regarding the modulated DSC analysis to calculate the Cp, and thus the thermal conductivity, an increase in temperature occurred when using 5% of talc, going from 0.14 (W / mK) to 0.34 (W /mK), improving the thermal conductivity of the compound.*

[RWE-197] Study of solar cells based on the Sb2(S1−xSex)3 absorber

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Semiconductor materials such as Sb_2S_3, Sb_2Se_3 and $Sb_2(S_{1-x}, Se_x)_3$ have recently attracted attention as solar cell absorber materials because of their p-type conductivity, high absorption coefficient and direct band-gap transitions. Band-gap values of 1.7 and 1.1 eV have been reported for Sb_2S_3 and Sb_2Se_3 compounds, respectively. Furthermore, since Sb_2S_3 and Sb_2Se_3 are isomorphous, the $Sb_2(S_{1-x}, Se_x)_3$ compound can be synthesized with intermediate properties between both compounds as function of the Se/(S+Se) compositional ratio. So far, low solar cell efficiencies of 5-7.5 % have been reported for solar cells using these absorber materials. In particular, these low efficiencies could be attributed to defects formation in $Sb_2(S_{1-x}, Se_x)_3$ bulk material and at the absorber/buffer interface. In this work, it is evaluated the impact of different Se/(S+Se) compositional ratios and absorber thicknesses on $Sb_2(S_{1-x}, Se_x)_3$ solar cell performance under radiative and non-radiative recombination mechanisms. Conditions for optimizating $Sb_2(S_{1-x}, Se_x)_3$ solar cell efficiency are presented and discussed.

[RWE-198] Growth of In2S3 thin films by hydrothermal method and their photocatalytic activity for hydrogen production

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Sulfide semiconductor photocatalysts have attracted much attention due to their excellent solar spectrum responses and high photocatalytic activities. Indium sulfide (In_2S_3) is an n-type chalcogenide semiconductor, which consists of elements with low toxicity, is one of most promising candidate material used for photo(electro)catalytic hydrogen production due to is favorable band gap (2.0 - 2.45 eV), which depends on the different kind of structures of the In_2S_3. In this work, we study the photocatalytic hydrogen production of In_2S_3 thin films grown by hydrothermal method. In_2S_3 were grown over TiO_2 substrates preciously deposited by DC magnetron sputtering. In_2S_3 were characterized by X-ray powder diffraction (XRD), UV-Vis spectroscopy, scanning electron microscopy (SEM) and their photocatalytic activity was evaluated using a chromatograph with a thermal conductivity detector (TCD) under UV light and simulated sunlight. Results will be discussed.

[RWE-199] Photocatalytic hydrogen production of Zn2SnO4 thin films deposited by DUPLEX SURFACE method

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Zn_2SnO_4 is a ternary oxide n-type semiconductor with a band gap of 3.6 eV, which has attracted considerable attention due to stable properties under extreme conditions, high electron mobility, and interesting optical properties, this makes suitable for gas sensors, solar cells, lithium-ion batteries and photocatalyst applications. Mostly, Zn_2SnO_4 has been obtained in powder form using different methods, but there are a few reports of Zn_2SnO_4 deposited in a thin film. In this work, we present the Zn_2SnO_4 thin films and their photocatalytic activity in hydrogen production. These films were deposit using Duplex surface method (SILAR + SPUTTERING) at low temperature. Sputtering is an exceptionally versatile technique suitable for combines with SILAR method and gets the deposition of high-quality, well-adhered films of a wide range with a cost-effective, sustainable way and reproducible method. Zn_2SnO_4 thin films were characterized by X-ray powder diffraction (XRD), UV-Vis spectroscopy, scanning electron microscopy (SEM) and their photocatalytic activity was evaluated using a chromatograph with a thermal conductivity detector (TCD). Results will be discussed.

[RWE-230] Influence of the substrate in the morphology and crystalline orientation of MoO2 flakes grown by chemically driven isothermal close space vapor transport

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Presently, molybdenum oxides are the subject of intense research efforts because of their interesting properties and promising applications in different areas. These cover catalysis, biomedical applications and, most interestingly,energy storage and harvesting.[1] For some of these applications, the crystal surface plays a decisive role, reason why the study of molybdenum oxide flakes has become a subject of interest. In a previous work, a new technique has been developed to prepare pure MoO_2 films in a chemically driven isothermal close space vapor transport configuration (CD-CSVT) using MoO_3 as the source.[2] In the present communication, the CD-CSVT growth of micrometer sized MoO_2 flakes is presented. It was observed that flakes orientation and growth strongly change when they are grown on different substrates. X-ray diffraction, high resolution scanning and transmission electron microscopy, including stereoscopic 3D images, transmission electron diffraction as well as optical microscopy, allowed to determine the crystalline direction and the orientation of the flakes facets deposited on sapphire c-cut, sapphire a-cut, Si (100) and Si (111) substrate. Triangular, standing rectangular, rhombic, “kite” shaped or not clearly faceted flakes including nano-belts and nanowires were obtained depending on the used substrate. As an application, after CD-CSVT growth, samples were in-situ tellurized and micrometric $MoTe_2$ (an important member of the transition metal dichalcogenides family) flakes were obtained.

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[RWE-271] Properties and oxidation of MoO2 films grown by chemically driven isothermal close space vapor transport

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Molybdenum forms different oxides with formula MoO_{3-x} and x ranging from 0 to 1. The more oxidized extreme (MoO_3) presents the orthorhombic structure, has n-type conductivity and a band gap of circa 3.0 eV.[1] On the other hand, the monoclinic structure is the more stable phase of the more reduced form (MoO_2). The electrical properties of MoO_2 are somewhat unclear since theoretical calculations predict a metallic behavior as a consequence of Fermi level crossing by Mo 4d bands[2] but an optical band gap has been found in absorption spectra. Both MoO_2 and MoO_3 present very interesting properties as catalysts while MoO_3 is being widely used as hole transport layer in either inorganic or organic solar cells. Usually, molybdenum oxide samples contain a mix of different phases, which makes difficult to associate a given measured property with a determined phase. We have developed a technique that allows to obtain pure MoO_2 by a chemically driven isothermal close space vapor transport technique (CD-ICSVT) using MoO_3 as the source.[3] We present an extensive characterization of the electrical and optical properties of these pure MoO_2 samples including measurement of resistivity as a function of temperature, ellipsometry, UV-VIS transmission and reflectance, surface photo-voltage spectroscopy, x-ray photoelectron spectroscopy and photoluminescence. The results were compared with those reported in the literature whenever this was possible. Moreover, samples were annealed in air to transform them onto MoO_3 films. Rutherford backscattering spectrometry and Raman spectroscopy allowed to confirm the presence of MoO_3 in the annealed samples. The properties of these samples were in turn studied and compared with the parental MoO_2 layers. Finally, different types of MoO_x based heterostructures involving Si substrates with different conductivities types were fabricated and the corresponding current-voltage characteristics are reported and analyzed.

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[RWE-276] Zinc oxide nanowires grown by Vapor-Liquid-Solid technique: Photocatalytic degradation of Ciprofloxacin antibiotic

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Nanomaterials have attracted interest due to performance in electronics, optics, photonics, and recently in photocatalytic degradation of organic pollutants. Unidimensional (1-D) materials, such as nanowires, offer a larger surface-to-volume ratio, and hence a higher photocatalytic activity through enhanced adsorption of target organic molecules onto the catalyst surface. Metal oxide semiconductors (MOS)-based nanowires are of interest due to the enhanced structural, electronic and optical they show in comparison with their bulk counterparts.

In this research project, ZnO NWs were grown using the vapor-liquid-solid technique. Aluminum-doped ZnO (AZO) and Au thin films were used as seed layer and catalyst, respectively. Samples were analyzed using X-ray diffraction (XRD), scanning and transmission electron microscopies, and photoluminescence spectroscopy (PL) for structural, morphological and optical properties. Additionally, photocatalysis tests were performed for the degradation of the Ciprofloxacin (CIP) antibiotic under UV-light. The photocatalytic efficiency of ZnO NW's is correlated with the aspect ratio of the samples.

[RWE-292] Inverse hydrogeochemical modelling and possible proposal for arsenic remediation in water for the Matehuala community in San Luis Potosí.

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The presence of arsenic in water is due to natural processes and some anthropogenic activities such as mining, where arsenic can be found in high concentrations. People exposed to arsenic can develop various diseases. In the community of Matehuala, in San Luis Potosí, arsenic concentrations have been reported up 150 mg/L. Therefore, there is a need to evaluate proposals tha help to reduce the concentration of the metalloid so that it can enter to the norm. The objectives of this study were: 1) to determine the mechanisms of arsenic mobility in water in Matehuala; 2) to stablish a proposal for remediation of arsenic in water. To achieve the objectives, an inverse hydrogeochemical model of arsenic in water was made. The use of electrodeionization techniques (EDI) is presented as a remediation proposal. For this, membranes and ion exchange resins were used. The EDI worked with synthetic arsenic solutions using a concentration of 15 ppm.

[RWE-350] Graphene oxide as catalyst in constructed wetland-fuel cells

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Power can be obtained from biochemical reactions at the electrode surface in a constructed wetland-fuel cell. Constructed wetlands are an efficient process for wastewater treatment; recently electrochemical cells have been implemented into lab scale constructed wetlands looking for an electrical current and to improve the treatment capacity of wetlands. The electrochemical current is the result of the bio-electrochemical reactions at electrodes; on one hand the organic matter oxidation at anode, on the other hand, the oxygen reduction reaction that takes place at the cathode. However, the latter reaction requires a catalyst to obtain a higher power from the wastewater treatment. In this work, the reduced graphene oxide (rGO) is studied as catalyst for the oxygen reduction reaction that takes place at cathode in a constructed wetland-fuel cell. Graphene oxide (GO) was synthesized under the improved Hummers method. GO is characterized by thermogravimetric analysis (TGA), X-ray photoelectron spectroscopy (XPS), by the measurement of its electrical conductivity, as well as, by energy-dispersive X-ray spectroscopy (EDS), by the specific surface area (BET) and by UV-vis. The reduction of GO is carried out using ascorbic acid as reductant. The same parameters of characterization are used to analyze the reduced GO. Finally, the rGO is used as catalyst at cathode of a lab scale constructed wetland-fuel cell in order to improve the performance of the bio-fuel cell, which is electrochemically characterized by means of linear and cyclic voltammetry, the measurement of anode, cathode potential as well as the cell voltage, power and current density. Cell voltage has achieved 615 mV and the power density 9.5 mW/m2 with no addition of rGO. The treatment performance will be evaluated before and after the addition of rGO.

[RWE-361] Nano-structured Diamonds films and Solar Concentrators for Solar Energy Conversion Applications

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The physics and applications of Nanocrystalline Diamond (NCD) films are been investigated due to their unique combination of properties such as high wear resistance, highest hardness relative to any other film, lowest friction coefficient compared with metal and ceramic coatings, chemical inertness, negative electron affinity, low work function, and the high electrical conductivity for boron doped and nitrogen grain boundary incorporated diamond films. The combination of these properties make doped diamond films suitable for many applications like electrodes for water purification, thermionic and field emission devices, and high power electronic devices. Boron doping of NCD films during growth has the drawback of Boron contamination of the chamber where the film is grown, which can only be used for the growth of B-doped diamond films. This presentation will focus on describing the results from research and development of a novel process for Boron doping large area NCD films by thermal diffusion after growth, thus eliminating the problem of Boron contamination of the diamond film growth chamber. An advance on characterizing other properties of NCD films is provided in this research for use in Photovoltaic Cells. These studies are focused on the optical properties of NCD films studying afterglow (AG), thermoluminescence (TL), optically stimulated luminescence (OSL) and relation with the PETE. This research is focused on understanding the chemical, structural and electrical properties of Nanocristalline diamonds films before and after doping with boron by thermal diffusion. The diamond films were grown by Microwave Plasma Chemical Vapor Deposition technique on Silicon (100) substrates. The boron doped diamond films were characterized by Raman, XRD, XPS, 4-point probe and C-V analysis. Moreover, progress in the Photo-Enhanced Thermionic Emission (PETE) from the Nanocristalline diamond films under solar concentration is provided in this research.

[RWE-372] Hybrid a-Si/polymer flat heterojunction for enhancement of current density in thin film solar cells

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An alternative to pure organic or pure inorganic solar cell are hybrid solar cells that combine organic and inorganic materials for exploit the advantages of both technologies, with the objective to obtain solar cells of low cost of fabrication and high performance. In this work, we present the results of investigation of thin film hybrid organic-inorganic photovoltaic structures based on flat heterojunction hydrogenated silicon (a-Si:H) and poly(3,4 ethylene dioxythiophene):poly(4-styrenesulfonate) (PEDOT:PSS) fabricated on polyethylene naphthalate (PEN). It has been demonstrated that the silicon/PEDOT:PSS interface is a good candidate for substitution of the fontal interface based on standard p-type a-SiC:B layers and structures based on this interfaces have shown promising results as a remarkable high short circuit current density as large as J_{SC}= 17.74 mA/cm^2, similar to those for pure inorganic amorphous silicon - based solar cell with complex pattering surfaces.

[RWE-411] KBiO3/g-C3N4 composites for hydrogen evolution

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One of the techniques that is used for H_2 production from water splitting is photocatalysis. Which consists in the activation of a semiconductor (photocatalyst) with light, leading to the generation of electron-hole pairs, which are responsible for the reactions. A promising photocatalyst for water splitting is g-C_3N_4. However, the g-C_3N_4 shows different photocatalytic activity by every batch obtained and as all photocatalyts, presents a charge recombination. Due to this, there has been efforts to modify the g-C_3N_4 using metals, sulfides and compositing with other semiconductors, in order to increment the photocatalytic activity of this material. In this work g-C_3N_4 and $KBiO_3$ were prepared for the formation of composites, in order to test their photocatalytic properties for hydrogen production.

g-C_3N_4 was obtained by polycondensation of melamine and $KBiO_3$ was synthesized by chemical substitution using $NaBiO_3$ and a 50% aqueous KOH. Composites of g-C_3N_4/$KBiO_3$ were prepared with different weight ratio of $KBiO_3$ (10, 20, 30, 40, 50, 60, 70 80, 90 %wt) assisted by microwave technique. The synthesized powders were characterized by X-ray Diffraction (XRD). The XRD analysis shows that $KBiO_3$ crystallizes in the cubic structure (PDF #00-047089). The product of polycondensation melamine the XRD pattern shows two main reflections at 2θ 13.1° and 27.4° indexed to (100) and (002) planes, respectively. The SEM images reveals that $KBiO_3$ sample exhibited a cube-like homogeneous morphology. On the other hand the sample of g-C_3N_4 presents an irregular porous structure. For the composites the presence of two both materials is observed in the micrographs. The photocatalytic test, resulted in an increase for hydrogen production with the composites rather than the materials separately. The higher production of hydrogen (820 μmol H_2 g^{-1}) was obtained with the ratio 40%$KBiO_3$/60%C_3N_4.

Key words: Photocatalysis, $KBiO_3$, g-C_3N_4, hydrogen evolution

[RWE-412] Effect of LiAlSiO4 on the photocatalytic hydrogen production of TiN-LiAlSiO4 films irradiated under simulated sunlight

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Nowadays, photocatalysis is one of the most promising alternatives to obtain clean energy using only sun light and semiconductor materials. Particularly, TiN is one of the diverse materials that has been attracted considerable attention in last decade due to its interesting physicochemical properties, chemical stability, and environmental friendly properties. Therefore, in the present work it was carry out the preparation by high energy mechanical milling of TiN-$LiAlSiO_4$ composites. Film preparation was carried out using a paste prepared with terpineol as organic binder an using different weight ratio of TiN:$LiAlSiO_4$ (90:10, 80:20, 70:30, 60:40, 50:50, 40:60, 30: 70, 20:80 and 10:90 wt.%), previously, the mixture was treated by mechanical milling at 200 rpm for 10 minutes. TiN-$LiAlSiO_4$ composites were characterized by several analytical techniques. XRD results did not showed any variation in the crystal structure of both semiconductor materials. All composites presented homogeneous distribution of the TiN and $LiAlSiO_4$ particles. On the other hand, the results of diffuse reflectance spectroscopy show that the Band gap values are in the interval 2.0 to 3.6 eV, which indicates that most composites could be activated under visible light. Additionally, the emission spectra of PL indicated that the samples with greater presence of TiN have a lower emission, which is related to a lower recombination of the pair hole-electron, which could be favorable for the photocatalytic H_2 production under simulated sunlight.

Keywords: *TiN, $LiAlSiO_4$, Photocatalysis; Hydrogen, Sunlight.*

[RWE-421] Enhanced conductivity of nitrogen-doped graphene for the application of the photocatalytic generation of hydrogen

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Increasing levels of greenhouse effect gases and its implications on the planet climate, compel scientific community to shift the focus on sustainable alternatives for energy production. Hydrogen is considered a promising alternative fuel for power generation and transportation that could be produced at affordable price. Artificial photosynthesis, which mimics the natural photosynthesis in terms of light harvesting, charge collection and carrier mobility, is gaining significant interest as cheap route for hydrogen generation. Nitrogen-doped graphene oxide has been pointed out as a material of choice for hydrogen photogeneration, because it's large surface area, continous light absoprtion from UV to NIR and high conductivity. From graphene oxide reduction for doping and conductivity improvement, contradictory reports suggested different reducing agents such as hydrazine and sodium borohydride. In the present work, chemically synthezised graphene oxide was doped with nitrogen using hydrazine and further reduced with sodium borohydride. XPS results confirms the presence of the nitrogen and boron in the samples and the bulk resistance decreased down to 30 ohm.cm when compared with GO and other samples which were reduced with either hydrazine or $NaBH_4$ alone. Samples were further characterized by BET, Raman, Infrared and UV-Vis spectroscopy. The results indicate that N_2H_2/$NaBH_4$ sequential reduction lead to nitrogen/boron co-doping and is a more suitable candidate for hydrogen photogeneration through artificial photosynthesis.

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Keywords: Artificial photosynthesis, hydrogen fuel, photocatalysis, graphene

[RWE-459] Electrical characterization of microbial fuel cells with graphene-based catalysts decorated with Fe and Ni magnetic oxides.

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The conversion of bio-electrochemical energy using microbial fuel cells (MFC) has become an emerging renewable technology, due to the use of electroactive bacteria present in organic matter that can be harnessed as a portable energy technology. However, the oxygen reduction reaction (ORR) is kinetically sluggish causing loss of potential in the performance of the fuel cell. Currently, transition metal oxides with the inverse spinel structure and carbon-based materials to promote electrical conductivity and catalysis of the ORR have been used. In the present work, GO was prepared by a modification of the Hummers method, followed by decoration with magnetite nanoparticles (Fe_3O_4) and mixed oxides (Fe/Ni) using the chemical co-precipitation technique. The graphene oxide with magnetite (GO-Fe_3O_4), was prepared with a precursor solution of Fe^{3+}/ Fe^{2+} with molar ratio 2:1; in addition, part of the sample was reduced with hydrazine at 80 ° C to observe the effect on the present crystalline phases. The graphene oxide with nickel ferrite (GO-$NiFe_2O_4$) was prepared with variations in the concentration of iron and nickel chlorides (2: 1, 18: 1 Fe^{3+}: Fe^{2+}/ Ni^{2+}). The materials were studied by X-ray diffraction, Raman spectroscopy, Fourier transform infrared spectroscopy and transmission electron microscopy to know the crystalline and molecular structure, as well as the microstructure. The crystallite size was found between 6-13 nm. The materials were characterized by cyclic voltammetry, showing catalytic activity for the ORR and their activity was also evaluated under an external magnetic field to compare the performance in the generation of electricity and an improvement in the current was observed after removing the magnetic field. The material was characterized by vibrating sample magnetometry showing the materials to be superparamagnetic. The MFC performance was evaluated in single chamber configuration where the best catalyst was Fe^{3+}: Fe^{2+}/ Ni^{2+} 2: 1, with a maximum potential of 397.7 mV and a current of -1.28E-4 A. The activity for the ORR depends on the crystalline phase and to the interactions between the M^{2+}: M^{3+} cations.

Acknowledgments: Financed with BEIFI-IPN, SIP project 20181187 and CONACYT 783100. The department CP2S- Équipe Matériaux Carbonés of the Faculté des Sciences et Technologies of the Institut Jean Lamour, CNRS-Université de Lorraine, France is acknowledged for structural and magnetic measurements.

[RWE-486] Influence of annealing temperature on Cu2SnS3 thin films grown by spray pyrolysis for photovoltaic applications

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Cu_2SnS_3 is a p-type semiconductor showing a direct band gap in the range of 0.85 - 1.6 eV, suitable for photovoltaic applications. Its constituent elements are nontoxic, earth abundant, and it exhibits different phases depending on the method of deposition and post-deposition annealing temperature. Cu_2SnS_3 thin films were grown by spray pyrolysis, using two different synthetic routes, the non-stoichiometric and stoichiometric. The study of the Cu_2SnS_3 phase transitions was carried out using different sulfurization temperatures (350, 400, 500, 560 and 600 ° C). The phase identification and the composition analysis was performed using X-ray Diffraction (XRD) and Energy dispersive x-ray spectroscopy (EDS). For the non-stoichiometric composition (Cu/Sn = 1.76) and a temperature annealing interval of 350-600 °C, the films were composed of a monoclinic Cu_2SnS_3 phase. On the other hand, for the stoichiometric composition (Cu/Sn = 2), the films were constituted of a tetragonal Cu_2SnS_3 phase as long as the temperature was in the range of 300 and 400 °C. When increasing the temperature up to 500 °C, the Cu content incremented and the orthorhombic Cu_3SnS_4 phase was formed. The Raman spectra showed the peaks at 292 cm^{-1} and 353 cm^{-1} for the monoclinic Cu_2SnS_3, 331 cm^{-1} for tetragonal Cu_2SnS_3 and 314 cm $^{-1}$ for orthorhombic Cu_3SnS_4. The optical band gap energy was 1.2 eV for monoclinic Cu_2SnS_3, 1.40 eV for tetragonal Cu_2SnS_3 and 1.60 eV for orthorhombic Cu_3SnS_4. X-ray photoelectron spectroscopy (XPS) was used to study the core levels of the constituent elements, surface contaminants, and ionization potential and valence band spectra. The conduction band was determined by inverse photoemission spectroscopy (IPES). The different films based on Cu, Sn and S are constituted by Sn^{4+} and Cu^{+} confirmed by the Auger parameter. The electronic band gaps obtained for the monoclinic, tetragonal and orthorhombic films were 1.23 eV, 1.33 eV and 1.54 eV, respectively, which agree with those obtained by UV-Vis spectroscopy. Also, the proximity of VBM to the Fermi level confirms the expected p-type nature of this compounds.

[RWE-500] CdTe mini-modules performance enhancement by subsequent annealing

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It is known that when CdS/CdTe solar cells are prepared they show important changes after heat treatment. In this work we study CdTe mini-modules of 5x5 cm^2 glass substrates with transparent conducting contact. The ZnO and CdS thin films were deposited by sputtering. The CdTe film was obtained by using CSS technique. The thin film structure was introduced to a vacuum chamber, and exposed to atmospheric gases, which contain chlorine to perform the activation process. The next step was the deposition of the Cu/Mo thin films as back contact. In order to finish mini-module, laser scribing and electric connection were done. Once the samples were ready, the annealing process was performed at T=300ºC during different times (20, 35, 50, 80 100 and 120 minutes).

In this work, we report how Isc, Voc, FF, and efficiency changed after each annealing process. The experimental data are discussed and an interpretation is exposed.

Keywords: CdTe/CdS mini-modules, heat treatment, photovoltaic parameters changes

Acknowledgment. This work has been suported by CONACYT- SENER under project LENERSE 254667

RENEWABLE ENERGY: MATERIALS AND DEVICES (RWE) POSTER SESSIONS

[RWE-9] Pt3Fe/C bimetallic alloy nanoparticles as electrocatalysts with improved activity for the oxygen reduction reaction

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The synthesis of octahedral and octopods nanocatalysts of Pt_3Fe for oxygen reduction reaction (ORR) in acid media is presented. Catalysts were prepared through chemical reduction with the correct amount of oleylamine, oleic acid, and precursor salts ($Pt(acac)_2$ and $Fe(acac)_3$). In one of the two syntheses, we use dibenzyl ether and tungsten hexacarbonyl ($W(CO)_6$) as the solvent and reducing agent respectively. Subsequent, both catalysts were dispersing in a carbon matrix (Vulcan Carbon) previously thermally treated. The presence of the alloy Pt_3Fe in the nanoparticles was proved by XRD. STEM micrographs showed the morphology of the nanoparticles with an average 7-9 nm for octahedral and 12-14 nm in size for octopods. The electrochemical performance of Pt_3Fe/C was evaluated by cyclic voltammetry, CO stripping and rotating disk electrode in $HClO_4$ as the electrolyte. Octopods of Pt_3Fe/C nanocatalyst showed the best catalytic activity regarding mass activity and specific activity than commercially available 20-wt% Pt /C-Etek® catalyst. Therefore, this finding suggests a methodology for producing a carbon supported octopods nanocatalyst, which could be used as a cathode electrode in a PEM fuel cell.

[RWE-10] Elaboration of bricks from reused Polyethylene Terephthalate (PET)

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Industrial processes are usually the major pollutants of the planet either due to the gases that are produced during the process or the waste they generate. One of the most polluting industries is the production of brick, which uses highly polluting fuels, which generate dioxins, massive volumes of particles, carbon monoxide, oxides of sulfur and nitrogen, among others, which pollute the atmosphere, bodies of water and soil.

Here, we report the elaboration of bricks based on cement and PET (polyethylene terephthalate); It is manufacture consists of crushing PET disposable bottles, recycled by environmental companies, which once reduced to a specific size, is mixed with cement and water in defined proportions and deposited in molds with specific measures in accordance with the Mexican Standard NMX-C-038-ONNCCE-2013 , after that they are dried in the open-air for 2 days and then a curing process is carried out for 7 days, which gives the brick characteristics of cohesion. After 7 days, the bricks are removed the water to store them in a cool place at room temperature for 28 days where they will obtain their characteristic properties. Finally, several cement and PET compositions were studied, different tests of compression resistance and water absorption were carried out. This type of mechanical tests were carried out according to the standard NMX-C-036-ONNCCE-2013, the results show that bricks with a composition of 50 percent cement-50 percent PET have a higher strength than conventional bricks commonly used in construction. In this work, we design and build a product that has excellent mechanical properties, easy to elaborate and can compete with the brick that is currently used in construction

[RWE-11] Tera Hertz emission simulation for food quality control application In-situ on solar dryer

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The solar drying method it's a way to preserve food in trend because is environmental friendly and low cost. However, the temperature of the process depends on weather conditions, Therefore the drying kinetics for different products like a fruits vegetables and meat is measured in laboratories but the method employed can't use in real conditions on solar dryers.

To determine the loss of water that exists in food inside a solar dryer is imperative because it allows conserve nutritional properties and increases storage time to generate food safety. Nowadays, to determine the weight loss of food in a solar dryer the chamber is opened and a sample of the loss of mass is taken with a scale, this has the effect of reducing efficiency of solar dryer and the rehydration of the food for the environmental nowadays determining the removal of moisture inside the drying chamber has been poorly studied.

Tera Hertz (THz) radiation is electromagnetic radiation whose frequency lies between the microwave and infrared regions of the spectrum this radiation is nonionic, non-invasive for organic materials. Based on optical properties at THz frequencies, condensed matter is largely grouped into three types: water, metal, and dielectric. Water, a strongly polar liquid, is highly absorptive in the THz region. So, this a promising radiation for quality control of solar dryers and in-situ monitoring food in dry process.

In this work we used the MEEP (MIT Electromagnetic Equation Propagation) which is an open-source implementation of the FDTD (finite difference time domain) method for numerically solving electromagnetic problems to study better theoretical THz we varied gap THz, properties dielectric samples of mango, stevia, grain coffee

The parameters obtained in this work are work thickness sample, absorption THz in simulate water atmosphere and THz gap for specific dielectrics and propose a sematic way for measure in solar dryers adapted without significative change. The graphs obtained by adjusted simulation model show the behavior of the drying curves for slice mango in different water content atmosphere respect to time and proposes standard control for monitoring lose moisture in solar dryer

Keywords: Environmental, Energy efficiency, Solar Devices, Tera Hertz, MEEP, Simulation.

[RWE-32] Micro and nanostructured hydrophobic materials based on polymer waste for oil spill remediation.

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The increasing number of oil spill accidents cause long-term ecological damages, particularly in aquatic environment. In recent years, interest in polymeric materials as methods of remediation of oil spills have increased due to their low cost, high stability and recyclability. Oil spill cleanup can be carried out by many methods and technics, being the sorbents the most attractive due to the possibility of collection and complete removal of the oil in situ from the water surface.

In this work, absorbent materials were prepared from polymer waste (recycled polyethylene terephthalate, PET, from bottles and recycled polyurethane, PU) using salt templates and hydrophobized using carbon nanotubes and silica nanoparticles. For the formation of the templates, sodium chloride was used, with three different grain sizes (table salt, ground table salt and sea salt). For the formation process, first enough water was added to the salt, this mixture was placed in molds and left to dry for 24 hours at room temperature, finally the templates were removed from the molds.

For the formation of the PET porous material, the salt templates were surrounded with PET and heated (250-260 °C), the polymer infiltrates the salt templates thanks to the capillary forces, once this process is completed, the salt templates was dissolved in water. For the formation of the PET-PU porous material, first it was necessary to prepare a suspension of PU in a solution of ethylene glycol and n-butanol, this suspension was mixed with PET, and the previous process was followed. SiO_2 nanoparticles were synthesized by sol-gel method (molar ratio $[H_2O]/[TEOS]=25.13$). Carbon nanotubes will be synthesized by spray pyrolysis method. The hydrophobization of the porous materials will be performed by the dip coating technique.

By means of infrared spectroscopy was possible to discard polymer degradation, due to the porous materials spectrums showed the same signals than raw materials (PET or PET-PU). It was possible to observe porous sizes thanks to SEM, for porous materials obtained from ground table salt template the porous sizes were between 50 nm-3 μm, from table salt template were between 1 μm-5 μm and from sea salt were between 2 μm-18 μm. The SiO_2 nanoparticles obtained had particles sizes less than 100 nm but they were in clusters (according to SEM data) and amorphous (according to XRD data).

[RWE-34] Comparative adsorption of asphaltenes onto metal oxides and mixed oxide.

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The hydrocarbons industry, specifically the oil industry, has a great impact on the economy and on the daily life of the human being, since the oil provides the great quantity of energy and materials used by us.[1,2] Actually, the availability of light oil fields[3] has decreased[4], so the heavy oil are the main alternative. However, this type of oil causes problems in equipment during the stages of extraction and refining of oil[5,6,4] due to high content of asphaltenes.

Different methods are being applied to counteract the adverse effects of asphaltenes[7], which can be classified as those that conserve asphaltenes in crude oil[8] and those removing asphaltenes from petroleum.[9,10] The removal of asphaltenes seems the most effective, since it does not require subsequent treatments and prevents re-precipitation of asphaltenes.[11] The selective asphaltene adsorption can lead to the best results, which could be implemented in refineries.[12,13]

In this work, we propose the synthesis of mixed oxide ($Ni_{(3/2)x}Fe_{2-x}O_4$) by means of the self-combustion technique. Its capacity to adsorb asphaltenes was evaluated and compared with nickel oxide and hematite, which were synthesized by controlled precipitation. The oxides were characterized by the techniques of X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR). Its morphological characterization was carried out by scanning electron microscopy (SEM). The asphaltene adsorption capacity was determined with the UV-Vis spectroscopy technique

The SEM micrographs revealed that hematite with a needle-like morphology which has 41 nm in width. Nickel oxide which has a spherical morphology and an approximate particle size of 112 nm and finally the mixed oxide having an irregular morphology with an average diameter of 128 nm.

Adsorption tests showed that mixed oxide ($Ni_{(3/2)x}Fe_{2-x}O_4$) is a good adsorbent compared to hematite and nickel oxide, both for asphaltenes with ether and amino functional groups, having an adsorption capacity of 961.95 and 547.05 mg/g respectively. In addition, the mixed oxide has a low affinity for oil which makes it selective to asphaltenes.

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[RWE-35] Nanocomposites adsorbents with magnetic properties for the separation of hydrocarbons from water.

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At the moment that there is an oil spill or that of some other hydrocarbon, the recovery of the spilled material is a priority, due to the economic losses, as well as the pollution caused in the place where it occurs [1-2]. As a response to a spill, different techniques and methods have been implemented, in addition to absorbent and adsorbent materials. Each of them has certain advantages and disadvantages in containment, remediation and cleaning. A recent proposal is the use of nanomaterials as adsorbent materials, which can be used in the adsorption of petroleum and other hydrocarbons [3], where the use of magnetic nanoparticles and carbonaceous nanomaterials is highlighted. Among the carbonaceous materials, carbon nanotubes present a great interest in the adsorption of petroleum due to its one-dimensional structure, large surface area and its oleophilic and hydrophobic nature. Within magnetic nanoparticles, maghemite is considered one of the most desirable materials for its stability to oxidation and its good magnetic properties [4]. So, in this project is proposed to obtain a composite based on these two materials, iron oxide / carbon nanotubes (gamma-Fe_2O_3/CNTs) as oil adsorbent material. First, maghemite nanoparticles were synthesized by chemical co-precipitation by oxidation of a magnetite solution [5]. Then, carbon nanotubes were synthesized by spray pyrolysis using a ferrocene / toluene solution at 800°C for 20 min [6]. Subsequently, the two materials were mixed by means of ultrasonic agitation to obtain the nanocomposite. Different tests were carried out to determine the adsorption capacity of the nanomaterials individually and of the composite; where contact adsorption, magnetic stirring and mechanical agitation are included. As preliminary results, an adsorption was obtained for the nanoparticles of 1.046 mg/g by contact and 54 mg/g by mechanical stirring. For the carbon nanotubes, an adsorption of 28.3 mg/g was obtained by magnetic stirring and 149 mg/g by mechanical stirring. Current pending work is being done on the different adsorption processes of the materials and the nanocomposite to determine their adsorption capacity on crude oil.

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[RWE-73] Improvement of optical and electrical properties of PCBM:P3HT absorber by mixing with CdS/TiO2 nanoparticles

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In this work, we proposed an strategy for the improvement of a light absorber based on a mixture of PCBM:P3HT semiconducting polymers. Improvement was achieved by blending CdS/TiO_2 nanoparticles (nps) with the PCBM:P3HT system. First stage consisted in developing a methodology for obtaining semiconducting CdS and TiO_2 nps; Chemical Bath Deposition (CBD) and co-precipitation techniques were employed, respectively. After obtaining CdS and TiO2 nps, second stage consisted in mixing these nps with the PCBM:P3HT system, and absorber films were prepared by the spin coating technique on glass substrates. Nanoparticles were characterized by XRD, XPS and SEM. Transmittance measurements of the absorber showed that light absorption is improved between 300 nm and 500 nm as the content of nanoparticles increased. In the case of electrical measurements, they showed that resistivity decreases as the content of the nanoparticles increased, reaching a value of $1x10^{-4}$, which is lower than the resistivity of the PCBM:P3HT polymer. Results demonstrated the potential of the proposed methodology for improving the optical and electrical properties of the PCBM:P3HT system for application in the fabrication of polymer-based photovoltaic solar cells.

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[RWE-107] Two chromogenic properties studies of Mo1-xTixO3-y thin films synthetized by sol-gel route.

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In this work, molybdenum trioxide (MoO_{3-y}) and titanium doped MoO_{3-y} ($Mo_{1-x}Ti_xO_{3-y}$) thin films were deposited on glass substrates by the sol-gel method (spin coating technique) with the aim to analyze the thermochromic response. Effects of the process parameters on the thermochromic properties of MoO_{3-y} and $Mo_{1-x}Ti_xO_{3-y}$ thin films were studied changing the annealing temperature (between 175 - 350 °C) and the annealing atmosphere (in air and argon). Another batch of samples were deposited in ITO (In_2O_3: Sn) with the objective to study the electrochromic properties. The changes in these properties were studied using cyclic voltammetry (CV) in a propylene carbonate (PC) solution containing 1 M lithium perchlorate ($LiClO_4$). The samples were characterized by means of different techniques as UV-Vis spectroscopy, X-ray diffraction (XRD), Raman spectroscopy, Transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) according to the characteristics of the film to be evaluated. The experimental results revealed that the MoO_3 and the $Mo_{1-x}Ti_xO_{3-y}$ thin films showed that the heat-treatment temperature, the annealing atmosphere, and titanium concentration will have strong influence on the thermochromic and in the electrochromic properties. The structural, optical and electrochemical characteristics were evaluated to been used as a smart window, temperature markers or as polarizers. On other hand, the objective of having widely characterized this oxide, will allow us to know all these properties and thus be able to apply MoO_3 in one of the layer that conform the solar cell panel.

[RWE-121] Effects of Mg concentration on the structural and optical properties of ZnO thin films

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In recent time it was demonstrated that Magnesium doped Zinc Oxide (ZnO:Mg) can be used as a window layer for thin film solar cells and it is now considered as the best candidate to substitute the typical Cadmium Sulfide (CdS). The main advantages of ZnO:Mg are the low light absorption and its non-toxic nature. In this work, we present the effects of Mg doping on the structural and optical properties of ZnO thin film deposited by reactive RF-Sputtering. The ZnO:Mg thin films were deposited on Corning glass substrates by using a Zn metallic target in Ar+O_2 gas atmosphere. The doping was performed in situ during the film deposition by placing sheets of metallic Mg on the Zn target. The amount of Mg was varied from 0 to 375 mg. The deposition was performed at 400°C with a working pressure of 20 mTorr and a RF-Sputtering power of 80 Watts.

The structural and optical properties of ZnO:Mg films were characterized using grazing incident X-ray diffraction (XRD) and optical absorption spectroscopy UV-vis, respectively.

XRD spectra show that ZnO:Mg thin films have a hexagonal ZnO structure (H-ZnO) according to JCPDF card number 361451, with preferential orientation along the (002) plane. When the Mg amount is increased, the crystallite size decreases from 27 to 17 nm (according to Scherrer equation); this can be reasonably attributed to the Mg incorporation in the ZnO film. The optical transmittance was measured in a range from 300 to 800 nm. The spectra present transmittance values between 80 and 90 %. The absorption edge shows a shift toward short wavelengths (less than 400nm) as the Mg amount raises, resulting in a bandgap increase from 3.2 to 3.7 eV.

Keywords: Mg doped ZnO, magnesium, RF-Sputtering

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[RWE-123] Study of the presence of a chemical complex in the electrodeposite of the cobaltphosphate complex as a water oxidation catalyst

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The in situ production of cobalt-phosphate complex (CoPi) demonstrates layers based on this catalyst have not reached its optimal thickness for water oxidation. It has already been studied that during the deposit procedure there is a limitation in solubility in the precursor solution, which at concentrations higher than 5 mM the presence of a precipitate is observed, wich it has a strong influence on the decrease of active cobalt species in solution that are needed to achieve the successful electrodeposition of the desired material and therefore its thickness growth is limited. So that, up to now, the thicker the CoPi layer the higher the catalytic activity for the range of explored thickness (1-4 µm).

In this work we study for the first time the use of a chemical complexing agent, at different concentrations, to improve the solubility of cobalt salts in the precursor solution and avoid the resulting precipitate at concentrations higher than 5 mM. It was observed that the presence of a chemical complexing agent not only overcome the problem of solubility limitation of cobalt salts, but makes possible an increase in the thickness of the deposited layers. The structural characterization of the films was carried out by X-ray diffraction (XRD) and Raman spectroscopy, as well as the morphology was obtained by Scanning Electron Microscopy (SEM). Our research is in progress to evaluate the water oxidation activity dependence on thickness of CoPi layers above 4 µm.

[RWE-129] Electrodes based on TiO2 nanostructures with Co3O4 Qds for photocatalytic oxidation of water

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The excessive use of fossil fuels as primary energy sources, as well as the environmental problems caused by their consumption, have generated in recent years the search for materials and devices that allow the use of alternative energy sources. Solar energy is very attractive and useful for the generation of fuels through water oxidation and CO_2 reduction reactions. Water oxidation reaction represents a major challenge since typical semiconductor materials used for this purpose that present high performance and efficiencies are commonly expensive, unstable or toxic, or if they are cheap and stable, their efficiency is regularly low or if, on the other hand, they are highly efficient and cheap then they are not photoactive and require external potentials, for this reason the search for economic, efficient and photoactive materials has increased.

This project shows the results of the methodology developed to obtain quantum dots (QDs) of spinel cobalt oxide (Co_3O_4) on nanostructured TiO_2 electrodes controlling the size of the quantum dot. The materials obtained were characterized structurally and optically and were also evaluated in the photocatalytic oxidation reaction of water in the visible and / or ultraviolet region of the solar spectrum.

[RWE-134] Obtention of heterojunction CdS/CdTe through chemical techniques for its application in photovoltaic devices

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Policrystalline photovoltaic devices based on the CdS/CdTe heterojunction are considered an excellent option due to their simplicity, low cost and their current efficiency of 21%. As a matter of fact, chemical techniques offer a lower cost process and a greater possibility of carrying out on a large scale. In this work CdS/CdTe heterojunction was performed through chemical bath deposition and electrochemical deposition over FTO glass substrates. CdS films were grown under different temperature conditions and thiourea concentrations. The obtained films exhibit good crystal quality, photoluminescence at room temperature and band gap of 2.31-2.55 eV. Films with the higher transmittance percent were obtained at 0.1 M and 70°C. CdTe layers were grown using a basic solution with EDTA as complexing agent, and -1.2 V was identified as the electrochemical potential for CdTe under the described conditions, exhibiting two vibrational modes, indicating a better crystal quality under this conditions. The obtained CdTe films present a band gap value between 1.33 eV and 1.40 eV, near to the expected value of 1.45 eV. Favorable conditions were found, resulting in a photovoltaic device with a 2% of efficiency that although it is a low value, shows the potential of the techniques to get a low cost solar cells.

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[RWE-200] Effect on the deposition parameters of cadmium telluride thin films by SILAR method as absorber material

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Cadmium telluride (CdTe) with a cubic structure has been considered as a chalcogenide p-type semiconductor material and an excellent candidate for photovoltaic energy applications at low cost due to a reduced and optimum band gap energy for solar energy conversion. Cadmium telluride thin films have been deposited on glass substrates by Successive Ionic Layer Adsorption and Reaction (SILAR), which is a simple and economical chemical method to enhance the use of precursors to get thin films over large areas. This SILAR method was performed by means of chemical precursors such as sodium tellurite as an anionic source and cadmium chloride as a cationic source along with two separated rinsing steps. The tellurite has been reduced to telluride by using rongalite as an environmentally friendly substitute to the hydrazine hydrate. Some conditions were achieved to find the optimum parameters for the thin film formation such as the number of cycles, the temperature of the deposition, the temperature and time of the thermal treatment, the pH of the precursor solutions and the subsequent cleaning in the as-deposited thin films. The thin films were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), ultraviolet-visible spectroscopy (UV-vis) and X-ray photoelectron spectroscopy (XPS). The XRD spectra of thin films confirm a CdTe polycrystalline material with cubic structure and the grain sizes were in a range from 15 to 35 nm. The optical transmittance and the bandgap energy values were attained from the UV-vis analysis, it demonstrated a reduced transmittance typical for an absorber material and the bandgap energies ranged from 1.1 to 1.5 eV. SEM micrographs demonstrated uniform and distributed grains agglomerating all the surface on the glass substrate without pinholes or cracks in the thin films. Further XPS analysis helped to confirm the CdTe chemical composition in the thin films according to the effect of pH in the anionic precursor solution. Current-voltage measurements have been required to get electrical characteristics of thin films and their potential application as an absorptive capacity for solar cell technology.

Keywords: Chalcogenides, cadmium telluride, semiconductor material, successive ionic layer adsorption and reaction (SILAR) method.

[RWE-207] Effects of agitation time of complexing agent, time and deposition temperature in structural, morphological and optical properties of the SnS thin films by chemical bath deposition method (CBD).

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In the present work we have investigated the effect of agitation of the complexing agent in the deposit of thin films of SnS by chemical bath. For the chemical bath tin chloride dehydrate ($SnCl_2 \bullet 2H_2O$) and sodium thiosulfate pentahydrate ($Na_2S_2O_3 \bullet 5H_2O$) were used as precursors of Sn and S respectively and as a complexing agent triethanolamine (TEA), the deposit was carried out at a temperature of 35 °C, a time of 5 hrs and an agitation of TEA from 1 to 20 minutes.

The structural, compositional, optical and morphological studies were carried out by techniques such as X-ray diffraction, X ray fluorescence (XRF), UV-Vis spectrometry and scanning electron microscopy (SEM). The best results were shown at an agitation time of 16 minutes. The X-rays showed good crystallinity with cubic structure, lattice parameters of *a*: 5.82 Å, a crystal size of 8.26 nm, while the composition of the SnS film by XRF was rich in Sn. The energy gap was calculated with a value of 1.65 eV close to that reported.

Studies were also carried out on the effect of temperature of 25 to 50 °C and the time of deposit from 1 to 8 hrs. on the thin film with better agitation time. The best results were found at 35 and 40 °C, and in 3, 5, 6 and 7 hours of deposit.

For the study of the effect of temperature, the X-rays revealed polycrystalline films with cubic structure, lattice parameters from 5.82 to 5.79 Å and energy gap in a range of 1.62 to 1.66 eV in the best films. However, when raising the temperature to 40 °C the films increased their crystal size to 25 nm, decreasing at 45 and 50 °C up to ~5.3 nm. While the atomic composition was better at a temperature of 35 °C with 73% Sn and 27% S.

The X-rays of the different deposition times showed polycrystalline films with cubic structure and an increasing crystal size with respect to the time ranging from 8 nm to 36 nm. The lattice parameters of these films were similar. It was observed that in 3 hrs the best composition was found with 65% Sn and 35% S, while from 5 to 7 hrs the composition remains at 73% Sn and 27% S, despite this, from 5 to 7 hrs the films show a higher crystallinity according to X-rays. The energy gap varied between 1.6 to 1.7 eV, which is within what is reported for SnS with cubic structure.

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[RWE-221] n-type polymorphous silicon thin films for applications in HJT solar cells

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Polymorphous silicon (pm-Si:H) materials have considerable advantages in absorption, photoconductivity and photostability with respect to conventional amorphous silicon (a-Si) due to nanometer sized crystalline Si inclusions embedded in an amorphous silicon matrix. These properties are very useful for the implementation of present material in photovoltaic industry. As well the structure of pm-Si:H improves the transport conduction properties with respect to amorphous silicon, even after being in a prolonged exposure to solar radiation. In this work, pm-Si:H thin films were obtained at a lower temperature of 350 °C using dichlorosilane as a precursor in plasma enhanced chemical vapor deposition (PECVD) and were doped with phosphine (PH_3). Deposition pressure was varied from 1 to 2 Torr and the RF power of the source was varied from 100 to 150 W. Ultra-thin films deposited on p-type silicon and glasses were characterized by different techniques such as FTIR, AFM and optoelectronic properties. Based on the results presented in this work, the best open circuit voltages (Voc) of the films were obtained for the samples deposited at chamber pressure of 2 Torr. The AFM results showed that the average surface roughness decreased as in effect to the increase in chamber pressure. n-type thin films were obtained and an increase in photoconductivity of the thin films under solar illumination was obtained. At the same time the samples also shown good chemical stability. The possible application of these materials could be applied to the new generation of HJT silicon solar cell structures.

[RWE-222] Synthesis and characterization of different silicon nanowires compounds for use in 3th generation of solar cells

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The nanowires are structures that have the great advantage of allowing particles like electrons, holes or photons propagate freely along the dimension unconfined, which has caused a deep interest for application in solar cells which could serve as channels unidirectional conduction through the device. The most methods for synthesis of nanowires involve the use a metal catalyst such as "guide" unidirectional growth. Gold has been widely used in this regard but the atoms can incorporated into silicon induce deep level electrical defects. However, had investigated other materials that can function as catalyst to carry out the growth of nanowires as tin, aluminum, gallium, indium an others. Tin has a low eutectic point (232 °C), does not have deep impurity level in the band gap of Si and is removed easily after the synthesis through the reaction Sn + H2 -> SnHx. In this work, tin films were deposited varying the thickness of Sn on p-type silicon (100) and SiO2 substrates by thermal evaporation. Subsequently, they were attacked with a hydrogen plasma to reduce the tin oxide and to form Sn droplets. After the hydrogen plasma treatment, the nanowires were fabricated by PECVD system. To study the differences in the morphology of the nanowires depending on the thickness we used scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

[RWE-234] Black silicon solar cells with different surface passivation states

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It is well known that, in crystalline silicon solar cells, the surface treatments are very important and have great relevance in the final efficiency of the devices. Black silicon solar cells are the terminology used for naming the crystalline silicon solar cells with different grades of surfaces texture, plasma annealing and combinations of different thin films as antireflection and passivation coatings. In this work we prepared silicon solar cells with diverse grade of chemical surface treatment and different hydrogen plasma annealing. On the other hand, various combinations of thin films passivation coating were deposited by plasma enhance chemical vapor deposition as SiO_2/SiN_x, pm-Si/SiN_x, SiN_x.Spectral response, surface reflectance, I-V curves in dark and under illumination were measured. The results are discussed as a function of different passivation states.

[RWE-242] Synthesis and Characterization of ZnO nanowires by VLS deposited on ZnO:Al-TCOs for their application as photoelectrode in a DSSC

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In modern materials science, ZnO is a semiconductor material with suitable physical, electrical and optical properties for different applications such as gas sensor, optoelectronic, photocatalysis and photovoltaic devices. Traditionally, mesoporous TiO2 is used for photoanode electrode in DSSC, however, ZnO is a potential alternative to TiO2 due to its wide direct band gap (Eg) energy of 3.37 eV, as well as very high electron mobility and high electron diffusion coefficient. In addition, ZnO can be obtained with a wide range of shapes and morphologies by various techniques. In particular, VLS (vapor-liquid-solid) is an attractive technique because it offers excellent control over size, shape, location and high crystalline quality of nanostructures obtained. This work presents the synthesis and characterization of ZnO nanowires (ZnO nws) obtained by VLS method. The ZnO nws were grown on transparent conductive oxide (TCO) substrates composed by Al doped ZnO (AZO) which was deposited by magnetron sputtering to room temperature. Of the results obtained by X-ray diffraction, (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM), UV-vis spectroscopy and four points probes, the AZO films presented a roughness surface, a low electric resistivity (~10-4 Ω cm) and a high optical transmittance (~80%), these values are suitable for application as TCOs. On another hand, the ZnO nanowires showed a highly c-axis preferred orientation (0002) which is perpendicular to the substrate. The diameter size was 70 nm approximately and lengths as long as 6 μm were obtained, the aspect ratio was higher than 70. These results are suitable for the sensitized process and their application as photoelectrode in a DSSC.

[RWE-251] Cu2ZnSnS4 thin films obtained from a single stage SILAR process

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The quaternary sulfide Cu_2ZnSnS_4 (CZTS) has been studied as absorber layer in thin film solar cells, due to its band gap energy, as well as large absorption coefficient, which are ideal for highly efficient solar energy conversion devices. Successive Ionic Layer Adsorption and Reaction (SILAR) is a wet chemistry technique with a lot of potential for multi-element compounds, since the reactions can be controlled in a way similar to Atomic Layer Deposition (ALD) technique. One of the major issues regarding the thin film deposition of CZTS by the SILAR technique is the direct achievement of the quaternary, without post-deposition treatments. All the literature available in this subject, reports the deposition of precursor films, which need thermal sulfurization treatments. In this work, several conditions of the deposition process were explored, including pH control, reactive concentration and immersion time. Samples were characterized by X ray diffraction, scanning electron microscopy, Raman spectroscopy and X-ray photoelectron spectroscopy. The results showed that control of pH is relevant to the incorporation of the elements, as well as the relations of solutions concentration and differenced immersion time play an important role on the direct deposition of CZTS.

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[RWE-254] Design of three biopolymer electrolytes using an ionic liquid

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Currently there is growing interest in the production and use of new materials from renewable sources. Natural polymers have excellent features environmental, such as biocompatibility, biodegradability and non-toxic. In recent years, research on chitosan , which is a linear poly(aminesaccharide) obtained from the deacetylation of chitin, considered as the second most abundant natural polymer and the main component of the exoskeleton of crustaceans and insects For some applications, such as electrolyte polymers, glass transition (Tg) of chitosan temperature is in the range of its thermal decomposition, so the determination of this temperature is difficult by conventional techniques . To modify these properties it has resorted to the functionalization of chitosan using the amine from its structure. Thus it has quaternized with various alkylating agents to generate a cationic polymer . It was sulfonated with 1,3-propanesultone to generate a polymer anionic and introduce an ampholytic group to increase the dissociation of the lithium salt .Three different biopolymer electrolytes were obtained formulated with lithium salts and organic solvents. 96% degree of deacetylated chitosan (DAC), sulfonated chitosan (QS, 96% functionalized), and sulfobetaine chitosan (SBC, 46 % functionalized) was mixed with an ionic liquid (IL) and glycerol. The latter acts mainly as a plasticizer and the ionic liquid not only behaves as a plasticizer but also contribute to increase the conductivity of the biopolymer. It was considered all the chitosan derivatives as a support of the electrolyte and the functionalization could have mainly helped to dissociate the lithium salt. Ionic conductivity increased dramatically when the ionic liquid Is added achieving values on the order of 10^{-4} S/cm. The ability of IL to dissolve the lithium salt is demonstrated. In all cases the chitosan derivatives have a role as a support of the electrolytes. Sulfonated chitosan (QS) are soluble in water and organic solvents. Both of the functionalized chitosan, sulfonated and sulfobetaine (SBC), are amorphous polymers, and SBC shows to have the ability to dissolve the lithium salt. The highest conductivity was depicted of 1.4 x 10^{-4} for SBC/$LiPF_6$/ system with the molar ratio of 1.00 /0.15/2.00, respectively.

[RWE-278] Optical and structural characterization of spray pyrolyzed SnS thin films synthesized by different sulfur precursors

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SnS thin films were deposited on soda-lime glass substrates by spray pyrolysis technique at 200, 250, 300, and 330 °C substrate temperatures. Three different precursors were used as sulfur sources: thiourea ($CS(NH_2)_2$, 0.17M), sodium thiosulfate ($Na_2S_2O_3$, 0.27M), and sodium sulfide (Na_2S, 0.17M), while $SnCl_2$ (0.08M) and NaOH (4M) were used as tin precursor and buffering agent respectively. The thin films were characterized by optical transmittance, X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), and Energy Dispersive Spectroscopy (EDS). Band gap values ranging from 1.59 to 1.88 eV were obtained. The XRD analysis showed orthorhombic SnS phase with preferential orientation on the (111) direction. The FE-SEM micrographs showed not well defined grains and agglomerated material. SnS thin films synthesized with $Na_2S_2O_3$ and Na_2S showed cracks along the deposited surface. Furthermore, the Sn_2S_3 secondary phase was detected in these samples. Thin films deposited with thiourea showed better results than those deposited with the other sulfur sources.

Keywords: Tin sulfide, spray pyrolysis, thiourea

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[RWE-279] The effect of tin impurities on CdS/CdTe thin films solar cell

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The doping of CdTe has been investigated with different materials such as Sb, As, Mg, Se, Bi. Sn-doped CdTe is a promising intermediate band photovoltaic material, therefore the optoelectronic and structural properties have been investigated in this work. Tin was co-sublimated with CdTe films by close-spaced sublimation (CSS) process in Ar environment to avoid Sn oxidation. CdTe:Sn was deposited on a superstrate structure, glass/ITO/ZnO/CdS, and Cu/Mo bi-layer was used as back contact. The amount of tin doping was kept constant. Well shaped and uniform grains were found by Field Emission Scanning Electron Microscopy (FE-SEM) analysis (about ~ 3 μm). Also it was observed a morphological changes between as-deposited CdTe and Sn-doping CdTe. Energy Dispersive X-ray Spectroscopy (EDS) and X-ray Photoelectron Spectroscopy (XPS) showed presence of tin in the CdTe films. X-rays Diffraction (XRD) revealed peaks corresponding to the SnTe compound, as well as CdTe peaks strongly orientated along the (220) and (311) directions. The CdTe:Sn and as-deposited films showed a band gap of 1.49 eV. The measured efficiency of CdTe:Sn solar cell was 5.4%.

Key words: CdS/CdTe, solar cell, doping, tin.

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[RWE-293] microwave-assisted hydrothermal synthesis of BiFeO3 powders for potential application in photocatalysis

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Among of the oxide metals, the bismuth ferrite ($BiFeO_3$ or BFO) has received great interest in photocatalysis. In this work we present the influence of the microwave assisted-hydrothermal synthesis method in the microstructural characteristics of the BFO that promote its potential application in heterogeneous photocatalysis. Samples were structural and microstructural characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), elemental mapping (EDS), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS) and reflectance techniques. The rhodamine-B degradation reaction under visible radiation conditions was monitoring with UV-Vis spectrometry.

[RWE-331] The effect of humidity content in the air atmosphere applied during the activation process of the solar cells

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An important step prior the back-contact deposition is the activation process which is considered to be necessary to obtain high photovoltaic conversion efficiency. The activation process consists in the chlorine incorporation into the CdTe absorber layer. Such incorporation is usually obtained exposing the CdTe surface to chlorine compounds at high temperature (between 380 and 420 °C). Among others, one of the possible compounds for this purpose is difluorochloromethane ($CHClF_2$), which is a stable, non-toxic gas, under normal condition. These characteristics make the $CHClF_2$ suitable for industrial production.

Therefore, in this work, we address the effect of humidity when air is mixed to the $CHClF_2$ during the activation process. Several solar cells were fabricated by the same process with the structure of ITO/ZnO/CdS/CdTe. The solar cells were then activated at 400°C ranging the relative humidity level from 0% (dry air) to 40%. After the activation process the morphological changes on the surface of the CdTe were analyzed by Field Emission Scanning Electron Microscopy (FE-SEM) and X Ray Diffraction (XRD). The solar cells were finished depositing a Cu/Mo back contact and the current-voltage (J-V) characteristics was measure. The FE-SEM characterization show enhanced grains coalescence as the air relative humidity increases. Furthermore, the XRD show more randomized crystal orientation as relative humidity increases. Finally, the J-V characterization clearly indicates that solar cells performance decreases as air relative humidity increase. The best solar cells performance was registered for the dry air activation treatment exceeding an efficiency of 10%.

Keywords: CdTe, activation process, solar cell.

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[RWE-336] MgCl2 and TeCl4 as alternative thermal treatments of CdTe thin films to be applied on solar cells

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The CdTe morphological surface is characterized by grains with twins, in this way the activation of CdTe thin films is an essential process using a chlorine compound. $CdCl_2$ thermal process is the most used element in CdTe technology. As was mentioned recrystallization of this material is an important step in photovoltaic devices process for this purpose a $MgCl_2$, and $TeCl_4$ thermal treatment are investigated as activation processes of CdTe thin films. The morphological, structural, and electrical properties of the CdTe thin films recrystallized are reported. Scanning Electron Microscope (SEM) measurements reveal some morphological improvements, as CdTe grains increase from 2.5 µm to 5 µm. Also, a noticeable defects (twins) decrease on the grain surface. X-Ray Diffraction (XRD) study confirms the improvement of the structural composition of the CdTe grains in the (111) orientation, compared with the as-grown CdTe thin film and some devices with these thermal treatments were developed.

Keywords.

CdTe, Thermal treatments, CdTe recrystallization

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[RWE-339] Obtaining of CdS/CdSe bilayers thin films by CBD on flexible PET substrates

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The multilayer structure CdS/CdSe has attracted the attention in recent years to the great potential it presents as a window layer in solar cells based of CdTe. There are many techniques that can be used for the synthesis of semiconductor materials, being the CBD (Chemical Bath Deposition) one of those that offers great simplicity in its operation parameters, as well as low production cost and the possibility of carrying out on a large scale. In the present work CdS:Mn films were obtained, CdSe and the multilayer CdS:Mn/CdSe on substrates of PET/In_2O_3:Sn by CBD. The HRTEM images shows that the CdS:Mn films obtained by chemical bath are of polycrystalline nature, present the hexagonal phase of the CdS. The Raman spectra indicate that the CdSe films on PET/In_2O_3:Sn and CdS:Mn present a hexagonal phase. In addition, the HRTEM results indicate the presence of nanoparticles for both the CdS and CdSe films. Photoluminescence spectra indicate that the band gap value for CdS films is 2.22-2.29 eV and for those of CdSe it is 1.7 eV. Favorable conditions were found, showing the potential of the CBD for obtaining multilayer films at low cost.

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[RWE-340] Cu(Al1-XGaX)Se2 thin films by electrodeposition for photovoltaic applications

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Wide-bandgap quaternary semiconductor chalcopyrites can be of interest for photovoltaic application. In order to avoid the use of expensive In and to explore new tunable wide-band gap chalcopyrite semiconductors, $Cu(Al_{1-X}Ga_X)Se_2$ (CAGS) thin films have been studied. The electrodeposition technique is suitable for the manufacture of thin films due to its characteristics of cost-effectiveness, time-saving, and displaying high-quality in fabrication with appropriate parameters. In the present work novel $Cu(Al_{1-X}Ga_X)Se_2$ ($0 \leq x \leq 1$) thin films have been achieved by electrodeposition on FTO glass substrates and FTO with CdS. There films were grown using an acid solution with triethanolamine (TEA) as complexing agent, and - 0.65 V was identified as a reduction potential for obtaining the CAGS films. The x-rays diffraction analysis shows that polycrystalline CAGS thin films with chalcopyrite structure have been obtained and Raman spectroscopy indicates the presence of two vibrational modes characteristic of the CAGS, the first band presents a shift towards green, this indicates a partial substitution of atoms of Ga by Al. Spectroscopy UV-VIS indicates that the optical transmission decreases and the band gap energy shifts toward smaller values as the Ga content increases. Photoluminescence spectra indicate that the band gap value for CAGS films is 1.8-2.5 eV.

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[RWE-344] The effects of RF-Sputtering power and temperature on the optical, electrical and morphological properties of ITO thin films.

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The ITO is used as contact in thin film solar cells; however, high temperatures are used during its deposit to obtain a material with good characteristics, therefore, when deposited on materials sensitive to temperature such as kesterite or CIGS, it generates modifications in their structures or chemical composition. For this reason, the effect of the Sputtering power, temperature and the post thermal treatment on the physical properties (morphological, electrical and optical) of ITO thin film was investigated. The ITO films were deposited on Corning glass substrates by RF-Sputtering technique from ITO target with 4N purity in Ar atmosphere. Deposition was performed at a working pressure of 20 mTorr, sputtering power of 80 Watts with set temperature at 200°C, and 90 Watts with two different temperatures, 200 and 300°C. After deposition the films were annealed at 200°C in two different atmospheres (air and nitrogen) with time 35 minutes. The morphological, electrical, and optical properties of the ITO thin films were characterized by Atomic Force Microscopy (AFM), Hall Effect and UV-vis spectroscopy, respectively. The spectra present transmittance value over 90% and band gap values between of 3.21 to 3.60 eV. On the other hand, when the power and temperature increase, the electrical resistivity decreases from 16.9 $\times10^{-4}$ Ωcm to 11.0$\times10^{-4}$ Ωcm. The morphological characterization showed a change in the geometry of the grains on the surface of the material. After of thermal treatment, it was observed a shift in the transmittance spectrum towards longer wavelengths and an increase in its band gap value, from 3.21 to 3.5 eV. The resistivity increased in the thin film treated in air; while, the resistivity of the samples treated in nitrogen decreased.

Keywords: ITO, Sputtering power, Thermal treatment

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[RWE-390] Effect of type of substrate on the physical properties of CZTS thin films deposited by spray pyrolysis with a perfume atomizer

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Nowadays thin film photovoltaic technologies comprising $CuInS_2$ (CIS), $CuInGaSe_2$ (CIGS) and CdTe rely on elements that are rare in the earth (e.g. In, Ga, Te), toxic (e.g. Cd), and expensive. Cu_2ZnSnS_4; commonly abbreviated as CZTS is a promising material for low-cost thin film solar cells, due to its suitable bandgap energy of around 1.5 eV and large absorption coefficient of over 10^4 cm^{-1} [1,2].

Successful deposition of CZTS thin films from non-toxic precursor solution by mean of an automatized spray pyrolysis system with a perfume atomizer is demonstrated. The effects of two different substrates, on the surface morphology, band gap energy and crystalline structure of thin films deposited were studied. Glass (Corning) and polyimide (DuPont™ Kapton® HN 500) were used as substrates for deposit of the CZTS thin films. The thin films were characterized by means of XRD, SEM, AFM, and spectroscopy of UV-Vis. All films were deposited at 350 °C due to that the substrates of Kapton support a maximum temperature of 400 °C. The results obtained of CZTS/Kapton thin films could have potential applications in flexible solar cells.

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[RWE-395] Comparison between CdS nanowires obtained using gold or bismuth nanoparticles as catalytic materials

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One-dimensional nanostructures of semiconductor materials are being the subject of intense research due to their excellent electrical and optical properties that allow their applications in different optoelectronic devices as LEDs and solar cells [1]. In particular, CdS nanowires have been obtained using Au and Bi nanoparticles in very thin layers of these metals in order to catalyze the nanowire growth [2]. Gold is probably the most used catalyst but other metals are being successfully used. In this work, the preparation of CdS nanowires using gold or Bi nanoparticles as catalysts is reported. A comparison is made between the optical and morphological properties of the obtained nanowires with the these metals. CdS nanowires present the hexagonal phase and a vapor-liquid-solid technique was found to be the responsible mechanism for the nanowires growth. Different morphologies were obtained in dependence of the growth parameters and the type of catalyst. The nanowires are strongly luminescent with both, near band gap and defect induced emissions which were studied in a wide range of temperatures. Transmission and scanning electron microscopy were used to study the morphology and stoichiometry of the different nanostructures.

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[RWE-429] Development of carbon materials for potential supercapacitors application

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In matters of energy storage, the supercapacitors are the most promising devices to reach high energy and power density in comparation with REDOX batteries, the way to obtain materials for this application with a controlled porous structure are chemical activation of carbon. A chemical activation of waste coffee grounds was done with conventional microwave using FeCl3 as chemical agent at different power steps (120, 180, 240, 300, 360 W) at 8 min and constant mass concentration of 1:1.5 g. FT-IR shows the effects on the surface chemistry indicating that the power to reach carbonization effect is 300 W at 8 min, SEM micrography shows that after this point a visible mesoporous structure with pores between 10-30 nm can be formed. This work has been partially supported by project SIP-IPN 20180219.

[RWE-449] Influence of pH value on growth of SnS thin films deposited on flexible plastic substrates by CBD for solar cells applications

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Tin sulfide (SnS) thin films were deposited on two types of plastic and flexible substrates such as acetate and PET. SnS is a semiconductor material very attractive for solar cells applications due to its abundance, no toxicity and inexpensive while PET and acetate are inexpensive and easy to obtain. Chemical bath deposition was the used technique to obtain thin films of SnS at various pH values from 8.5 to 11 on PET and acetate substrates. Tin chloride and thioacetamide were used as precursors of SnS compound in aqueous solution. Ammonia concentration was varied in the chemical bath to adjust the pH and improve the films adherence. Deposition temperature and ammonia concentration are parameters that promotes optical, structural and electrical changes on SnS films and determines its deposition time. X-ray diffraction measurements were done to observe the crystalline structure, preferred orientation plane and to calculate the crystal size of SnS films. Specular transmittance and reflectance measurements were done to evaluate the absorption coefficient and band gap. The SnS films could be deposited on large-area foils (up to 100 cm^2) and cut into any size and shape easily, without any degradation or detachment.

[RWE-456] Influence of flow rate and thermal annealing in nanostructured ceria thin films obtained by spray pyrolysis.

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In this work, nanostructured ceria thin films have been prepared in glass and silicon substrates by ultrasonic spray pyrolysis using cerium acetylacetonate as metallo-organic precursor dissolved in anhydrous methanol. The influence of flow rate in the structural, optical and electrical properties of films was analysed. The morphology, structure, optical and electrical properties were studied using scanning electron microscopy, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), photoluminescence (PL) and impedance spectroscopy (IS). The influence of thermal annealing at 900 ºC on the structural properties of films was evaluated. The substrate temperature were optimized for obtaining uniform and homogeneous nanocrystalline films with grains sizes smaller than 20 nm. The flow rate modified the morphology and the grain size of prepared films. By XPS were demonstrated the presence of Ce^{3+}, even in treated films. The Ce^{3+} concentration do not depend on the grown temperature. The different signals observed in PL after the thermal annealing are associated to the presence of defects induced by levels in the band gap created by the Ce^{3+} atoms. The low values of total conductivity and activation energy measured by IS are related to the nanometric grain size.

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[RWE-465] Study of photoluminescence in off stoichiometric SiOx films deposited by sputtering on silicon solar cells to increase the conversión efficiency by spectral shift effect

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Nowadays, photovoltaics energy (PV) is one of the most attractive options for generating electricity using clean and renewable energy. However, PV is not yet economical compared to energy obtained through conventional sources. Therefore, it is essential to reduce manufacturing costs of solar cells and photovoltaic modules. The fundamental spectral losses in a single-junction solar cell made of semiconductor material such as silicon can be large. This is a result of the mismatch between the incident solar spectrum and the spectral absorption properties of the material. Several routes have been proposed to overcome this intrinsic property of semiconductor solar cells and thereby increasing the power output of solar cells. All these methods or concepts concentrate on a much better use of the solar spectrum. Applications of low dimensional structures such as the use of Si nanocrystals to the photovoltaic have been proposed as a very promising way to increase the efficiency of the solar cells. One of the possible implementations of low dimensional structures to solar cells is to assure down conversion of high energy photons, which are otherwise thermalized and wasted for conventional solar cells. We have shown that the use of siilcon rich oxide films (SRO) with high photoluminescence deposited by LPCVD on the solar cell surface can increase the energy conversión efficiency. These films have the optical property of absoption below 300 nm radiation (UV), so that the absorbed energy by the SRO film is then reemitted as red light (photoluminescence); but silicon solar cells have a greater response in the spectral range from 500 to 1000 nm, so that the redshift of the short wavelengths offers an increase in the energy conversión efficiency of the silicon SC. On the basis of the previous knowledge, that silicon solar cells covered with off-stoichiometric SiOx films showing high photoluminescence offer a higher energy conversión efficiency, in this work we present a study of the photoluminescence properties of SiOx films deposited by RF sputtering and their posible application to silicon solar cells. The main goal of this work was to get the experimental conditions in temperature, power and presure in order to obtain a good photoluminescence in the deposited films, and then using them as the cover of previously fabricated pn junction silicon solar cells. A comparison of the electrical and optical characteristics of silicon SC with a layer of conventional SiO_2 and silicon SC covered with a SiOx obtained by sputtering is presented. Results on measurement of the open circuit voltaje and short circuit current under UV light illumination is also presented. The results demonstrate that the red luminescence of the SiOx films produces large enhancement of current and voltage, with improved performance in the UV range.

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[RWE-472] Thermoelectric properties study of zinc oxide doped with aluminum (Zn1-xAlxO)

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ZnO is an n-type semiconductor with a wide band gap (3.3 eV), wurtzite crystal structure, high electron mobility and thermal conductivity, is cheap and non-toxic. Due to its characteristics, ZnO has important technological applications such as sensor, photocatalyst, varistors, UV protection and thermoelectric devices. However, in order to improve the thermoelectric performance of ZnO is necessary increase the electrical conductivity but at the same time introducing dispersion centers through doped to decrease the thermal conductivity. In this way, zinc oxide doped with aluminium ($Zn_{1-x}Al_xO$) was synthesized by Pechini method using $ZnCl_2$ and $AlCl_3$ as precursors, citric acid and ethylene glycol; then was calcined at 500 °C. Several experiments were carried out with different weight percent of aluminium (0.1, 0.3, 0.5, 1.0 and 2.0 wt. %) to evaluate the composition effect on the structural, optical and thermoelectric properties. X-ray diffraction patterns show the wurtzite type structure of ZnO and its vibrational modes are observed in Raman spectra. Elemental composition was evaluated by X-ray Photoelectron Spectroscopy. Energy band gap of each sample was calculated from Diffuse Reflectance spectra by Kubelka-Munk and Tauc methods. The thermoelectric properties such as electrical conductivity, Seebeck coefficient and thermal conductivity were evaluated and used to calculate the figure of merit ZT which reached a maximum of 0.5.

[RWE-502] Synthesis and characterization of laminar oxides as cathodic materials for lithium batteries

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Efficient energy production, storage, and distribution are major global challenges. Li-ion batteries with their wide range of applications are a promising solution. However, the ability of Li-ion batteries to successfully address the growing energy storage demands relies on the development of new and efficient electrode materials. A common problem in lithium ion batteries is a loss of the specific capacity when a passivation layer forms on the negative electrode and a fraction of lithium, extracted from the positive electrode, is bound irreversibly on the negative electrode in the initial charge of the cell. Lithium laminar oxides as bismutates and cuprates show a high theoretical specific capacity between 274-530 mAh/g depends on the phase. The oxides were prepared via ceramic synthesis method. In this work, we synthetized lithium bismuth and cuprate oxides (Li_xBiO_y and Li_2CuO_2) as cathode materials. Materials were characterized using X-ray diffraction, scanning electron microscopy, nitrogen adsorption-desorption (BET model) and X-ray photoelectron spectroscopy. Cathodes were assembled as combi cells and electrochemically evaluated.

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[RWE-503] Development ultra-thin solar cells of CdS/CdTe by the magneto-planar-sputtering (MPS) technique.

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The impact of transparent and conductive materials, as well as thin film-semiconductor materials in daily life has increased in the last years, due to their applications on thin film transistors, transparent electronics, touch and flat panel displays, and specially solar cells. For this last application they consist, as a primary film, on a wide band gap degenerately doped metal oxides, and thus, they are known as transparent conductive oxides (TCO). Fluorine-doped SnO_2:F (FTO) is the most commonly TCO used in commercial CdTe-solar cells, as it is deposited during glass manufacturing and it is in general inert to subsequent processing. Usually, a double layer structure is used, which consist on a highly-doped primary layer and a nominally-un-doped secondary layer. It has been shown that the secondary layer increases efficiency and/or reproducibility of the solar cells, and prevents diffusion of atoms from the underlying highly-doped substrate. By the MPS technique it is possible to grow p-type CdTe as an ideal absorber material for high efficiency low-cost thin-film polycrystalline solar cells. Moreover the n-type CdS semiconductor continues being the best matching partner for these ultra-thin film solar cells. These three materials, SnO_2, CdS and CdTe, can be sequentially deposited by the sputtering technique, to get a uniform deposition and scalability of thin films in the order of 35 nm, 50 nm and 600 nm, respectively. The main objective of this work is to develop ultra-thin solar cells of CdS/CdTe with a buffer layer of SnO_2 by the MPS technique. Our processed hetero-structures were characterized by XRD, UV-Vis and electrical measurements. We present the materials characterization results as well as PV-performance of our solar cells. The authors gratefully acknowledge the project SIP-20180374 and CONACyT-Sener to the project P25 and P37.

[RWE-532] Nanoscopic characterization of the silicon pv solar cells

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Solar power as Renewable could grow and becoming economically feasible source of energy. The cost effective, including installation, maintenance, integrated design, and manufacturing photovoltaic solar cells, starts to attract more industry attention. The impact of the science especially physics are most obvious field to play mayor part in solar cells research and development. However, to reach the efficiency improvement require material free from defects in manufacturing at nanoscale. In turn understanding these elements is built on background quantum information of small structure arrangement. The high quality resolution probe of the material could reveal this correlation between the local electrical properties due to surface defect, carrier density, grain size, grain boundary, structure, compositions, impurities and the performance of the device.

The development of the electronic microscopy using induced current (EBIC) is one of the powerful technique which offer surprising results showing the local properties of the sample with small resolution during cell operation. The results of this technique is the outstanding contribution of this research showing the the influence of surface passivation and metal impurities, nano defect in materials, could affect drastically, electric activities such the minority carrier diffusion length. The test samples used are modules of PV technologies. Commercial mono-crystalline and poly-crystalline PV installed, to measure the electron beam induced current and local imaging area of solar cell.

Keywords: PV solar cells, EBIC, renewable energy

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[RWE-541] Planar Perovskite solar cells with new conjugated polymers as hole transporting layer.

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Recent studies have reported perovskite-based solar cells with promising photovoltaic efficiencies; the simplest device configuration employs a crystalline and well-oriented thin film of organo-lead perovskite that acts both as light absorber and carrier conductor, sandwiched between two electrodes. Nevertheless, it is well known that in order to efficiently collect the charges generated after photon absorption an electron transporting layer (ETL) and hole transporting layer (HTL) are prerequisite. Along the literature the most accepted configuration employs a mesoporous TiO_2 nanoparticles layer as ETL, and a Spiro- OMeTAD doped with lithium salts layer as HTL with FTO and Gold as electrodes. Most recently, the feasibility of using PEDOT:PSS as a HTL and fullerenes as ETL in planar inverted devices with Aluminum electrode is been proved, but despite of the competitive power conversion efficiencies of the devices issues as limited photocurrent due to not perfect level alignment as well as the low charge mobility of the organic materials can arise yet. In the present work preliminary performance results of perovskite based inverted solar cells with a carbazole derivate polymer as hole transporting layer and $PC_{61}BM$ as electron transporting layer are shown as an alternative to based water PEDOT:PSS.

[RWE-548] Postsynthesis Modification of Hexacyanocobaltates(III) Open Metal Sites for Hydrogen Storage

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Transition metal hexacyanocobaltates are porous materials with open metal sites and a wide variety of pores. In this work, manganese(II) and cobalt(II) hexacyanocobaltates(III) have been selected to explore the interactions between the open metal sites located in their pores and the guest molecules: hydrogen, carbon dioxide and several solvents. An experimental setup was designed and implemented to conduct post-synthesis modification of the solids with ozone. Samples were dehydrated, ozonized and saturated with solvents in situ. Ozone molecules acted on the open metal sites changing their oxidation state, causing a contraction of the unit cell and inducing a stronger interaction of the molecules of water and methanol with the lattice. This strengthening prevented the lattice from being evacuated without compromising its framework stability. The decomposition temperature decreased in all ozonized samples as a consequence of the elongation and weakening of the cobalt-carbon bond. Active infrared and Raman bands were used to monitor the interaction between the open metal sites at the framework surface and the guest molecules. The cell contraction and the presence of residual solvent molecules in the porosity reduced the hydrogen and carbon dioxide retention capacity of the samples.

[RWE-556] Semitransparent thin films of SrCuSeF with potential application in photovoltaics devices

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Semitransparent solar cells have been developed in recent years and have the advantage that can be used by replacing the coatings for the several PV-device ultra-thin-films used in the windows to decrease the light transmission. These solar cells would be used to absorb the radiation and convert it into electrical energy usable; in addition the PV-device can produce a thermally more comfortable environment. For the construction of these cells one of the indispensable requirements is that each one of the layers of materials, that compose it, is sufficiently thin and possesses a good efficiency. Recently, transparent conductive oxides, such as: SrCuSeF and BaCuSeF, have been studied because they are widely promising in this field and they have a wide band gap and have a high p-type conductivity. In this work we study SrCuSeF, p-type semiconductor material, for its potential application as semitransparent back contacts of optoelectronic devices, such as the specific case of solar cells and radiation detectors. The characteristics and physical properties of our first thin layers of SrCuSeF obtained by the pulsed laser deposition (PLD) technique are presented. The layers were characterized by the structural, morphological and electrical measurements.

Keywords: back contacts, semitransparent solar cells, p-type semiconductor material

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SCIENCIE DIVULGATION (SCD)

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[SCD-393] Nanociencia en el cascarón de huevo: Lo que no sabías

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Resumen

¿Sabías que el cascarón de huevo se encuentra conformado por infinidad de cristales romboédricos formados por carbonato de calcio?

¡Así es! El cascarón de huevo se compone por aproximadamente un 95% de carbonato de calcio ($CaCO_3$) el cual es uno de los materiales cerámicos más abundantes producido por los organismos vivos y que debido al perfecto control de factores de temperatura, presión y presencia de moléculas orgánicas en dichos organismos, se une a más moléculas formando romboedros superpuestos que dan lugar a la formación del cascarón de huevo.

Es este acomodo característico el que permite utilizar al cascarón de huevo para producir partículas de metales, polímeros u otros cerámicos a escalas nanométricas quienes; posteriormente se utilizan para eliminar contaminantes como: metales pesados (cadmio, plomo, arsénico, níquel, cobre, cromo, etc.) colorantes, fármacos o derivados del petróleo del agua y suelo.

Por otro lado, también es posible tener partículas nanométricas del cascarón de huevo y la inherente presencia de proteínas tales como colágeno promueve que puedan ser aplicadas en el área médica como transportador de fármacos, para regenerar células o para sustituir las prótesis metálicas.

En el presente trabajo se muestra una pequeña descripción morfológica obtenida en un microscopio electrónico de barrido y algunos resultados sobresalientes en materia ambiental, médica e industrial. Con esta información podrás conocer que hay detrás de los ricos huevos que disfrutas por las mañanas.

[SCD-394] ¿Para qué sirve la ciencia de materiales en México?

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El desarrollo de la humanidad hizo necesario que el conocimiento se sistematizara para resolver los problemas asociados con la evolución. Es posible identificar la historia de la humanidad a través de eras asociadas con los materiales. Los términos edad de piedra, edad de bronce, edad de hierro son términos familiares. Una de las explicaciones del atraso de los pueblos subdesarrollados en las diversas regiones del mundo es que no transitaron por las eras asociadas con la evolución en el conocimiento de los materiales. En México es claro que fuimos conquistados por una sociedad con un conocimiento superior en el manejo de los materiales.

La transmisión del conocimiento se ha acelerado en esta época y en México podemos encontrar sistemas para la producción de materiales con aplicaciones tecnológicas de punta. Sin embargo, en contraste con las sociedades desarrolladas, es difícil encontrar aplicaciones de dispositivos para resolver los problemas que enfrentamos en nuestra vida cotidiana.

En esta platica describiremos rápidamente la evolución de la ciencia de materiales a nivel mundial. El conocimiento necesario para trabajar en esta área y el desarrollo de un prototipo de sensor de luz ultravioleta desarrollado en los laboratorios del Departamento de Física del Cinvestav-IPN en colaboración con el Instituto de Ingeniería y Tecnología de la Universidad Autónoma de Ciudad Juárez

[SCD-402] Desarrollo de Nanosatélites en Universidades Mexicanas

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Actualmente las Universidades Mexicanas desarrollan un gran número de proyectos satelitales con fines de investigación dentro de sus aulas, proyectos que en el pasado era casi imposible desarrollar en cualquier Universidad que no contara con los recursos financieros suficientes.

Con el desarrollo de nuevos estándares de construcción satelital, como la norma CubeSat, ha sido posible que casi cualquier Universidad pueda desarrollar sus propios satélites, pues se ha reducido en gran medida el costo de fabricación y el tiempo de construcción.

En este proyecto se presenta una descripción de la estructura general de un satélite así como del estándar CubeSat para construcción de satélites que ha sido muy usada en los últimos años en proyectos satelitales dentro de las Universidades.

También se describe el proyecto AztechaSAT-1 basado en la plataforma CubeSat. El proyecto se denomina AzTechSat-1, en alusión a nuestra cultura Azteca (Az) y también constituye un reto Tecnológico (Tech, por sus siglas en inglés) del primero de varios proyectos Satelitales (Sat-1), auspiciado por la Administración Nacional de la Aeronáutica y del Espacio (NASA, por sus siglas en inglés) y la Agencia Espacial Mexicana (AEM). El AzTechSat-1 es un nanosatélite de clase CubeSat de 1U (un cubo de 10cm) administrado, diseñado y construido por un equipo interdisciplinario de estudiantes de ingeniería y otras áreas de la Universidad Popular Autónoma del Estado de Puebla (UPAEP). La AEM tiene dentro de sus funciones ser enlace con otras agencias extranjeras, y para este proyecto en particular con la NASA, realizará todas las gestiones correspondientes para el buen desarrollo y éxito del proyecto, además de que también hará las gestiones con otras instancias del gobierno federal mexicano, para el buen desarrollo y operación del nanosatélite AzTechSat-1. El AzTechSat-1 tiene como misión principal enviar datos a la constelación de GlobalStar y esta a su vez bajará los datos colocándolos en la nube para su recuperación más ágil. Esta es una nueva tecnología que será probada en 2019, el compromiso de NASA es llevar el satélite a la Estación Espacial Internacional y de ahí liberarlo en su órbita correspondiente.

[SCD-442] Biodiesel: Una alternativa de biocombustible en México.

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El tema de los biocombustibles se ha ido retomando en últimos años, esto debido a que son una alternativa para sustituir a los combustibles fósiles que están escaseando y además generan altos niveles de contaminación ambiental [1]. En al año 2010, la Secretaría de Energía comenzó a evaluar la posibilidad de desarrollar un programa de fomento al uso de biocombustibles como fuente de energía renovable. Actualmente en el país se está incursionando en la producción de bioenergéticos desde la obtención de la materia prima hasta el procesamiento y obtención de los biocombustibles [2]. Uno de los bioenergéticos que se está produciendo en México es el biodiesel, el cual se obtiene a partir de aceites vegetales y/o grasas animales mediante la reacción de transesterificación. En esta reacción una molécula de aceite reacciona en presencia con un alcohol de cadena corta en presencia de un catalizador.

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[SCD-458] El hidrógeno y la energía del futuro

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El hidrógeno aparece en la actualidad como una de las fuentes de energía renovables, aunque en México casi no se menciona. El hidrógeno va a tener un papel importante en el futuro cercano, sobre todo en el almacenamiento de la energía eléctrica. Entre sus principales ventajas con respecto a otras energías renovables está su posibilidad de generar energía de forma continua con una eficiencia superior al 50 %. Pero para su implementación a gran escala aún existen varios aspectos que deben ser mejorados. En esta plática se expondrán de forma general las distintas etapas y problemáticas que tiene la transición a una “economía del hidrógeno”; desde la obtención del hidrógeno y su almacenamiento, hasta el diseño de celdas de combustible para su transformación en energía eléctrica. Se comentarán los distintos tipos de celdas de combustible, haciendo énfasis en las llamadas de celdas de estado sólido, y los aspectos científicos (materiales y tecnologías) en los que se está investigando en cada caso. Recientemente ha crecido el interés en utilizar materiales nanoestructurados, debido a los cambios en las propiedades físico-químicas que producen las restricciones en su tamaño. En esta presentación se exponen además algunos resultados obtenidos en el crecimiento de algunos materiales nanoestructurados en películas delgadas para electrolitos y su posible aplicación en celdas de combustible de temperatura intermedia (~ 600 °C). Los materiales fueron obtenidos por la técnica de rocío pirolítico en su variante ultrasónica y se observó que la disminución del tamaño de grano permite reducir la energía de activación del material y aumenta la conductividad, que es uno de los objetivos fundamentales de las investigaciones en el campo de las celdas de combustible.

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[SCD-469] Recubrimientos Autolimpiables: Ciencia, Tecnología e Impacto en la Sociedad

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La historia nos marca la importancia de la ciencia en el crecimiento de un país, aunada a las tecnologías que surgen de la misma. Partir de una idea acompañada de un fundamento científico, su evolución para generar conocimiento y dar lugar a desarrollos tecnológicos, permite crear oportunidades para la generación de riqueza a partir de la investigación y el desarrollo académico. La comercialización de tecnología es la culminación de un amplio espectro de actividades multidisciplinarias, desde las investigaciones a escala de laboratorio hasta la producción, tomando en cuenta las cuestiones no tecnológicas relacionadas con la comercialización. A manera de ejemplo, se presentan las experiencias en el paso a través del desarrollo tecnológico de un proyecto enfocado a recubrimientos funcionales, los cuales tienen importancia debido a sus múltiples aplicaciones en el sector de energía, construcción, automotriz, entre otros. Su impacto no se limita al área científica y tecnológica, converge en el ámbito económico, ambiental y social.

[SCD-471] Experiencia Universitaria en el Desarrollo y Lanzamientos de Sondas de Exploración Volcánica

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El desarrollo de sistemas de monitoreo y exploración en volcanes activos por medio de lanzamiento de sondas es un esfuerzo en conjunto con diferentes áreas de estudio. La universidad UPAEP, a través de la oferta educativa en licenciaturas y posgrado pone en marcha proyectos en los cuales profesores y alumnos trabajan en conjunto para obtener mejores resultados de los problemas que afectan la salud y seguridad de la población de zonas volcánicas del territorio mexicano y su medio ambiente. Aunado a lo anterior la UPAEP lleva a cabo convenios con otras Instituciones nacionales e internaciones a fin de fortalecer la transferencia de conocimiento docente-estudiantes. Entre las áreas que destacan son la ingeniería mecatrónica, electrónica, biónica, medicina y administración. El involucramiento de diversas áreas de estudio facilita el análisis profundo de los riesgos y amenazas que prevalecen en las zonas volcánicas de nuestro país.

La UPAEP ha estado diseñando un sistema de monitoreo para observación de volcanes desde el 2014, específicamente para la región de Puebla y la zona volcánica circundante, y se ha probado parte del desarrollo tanto la parte electrónica, estructura y software en ocho lanzamientos con Sondas de Exploración Espaciales que alcanzaron hasta una altitud de 40 km. A partir de la implementación y uso de diferentes fuentes tecnológicas es posible obtener información suficiente para medir y comparar los datos arrojados por los sensores bioquímicos y visuales instalados en las sondas. La información obtenida destaca el incremento o decremento de las partículas suspendidas en el aire; el monitoreo visual de las modificaciones geográficas de la superficie terrestre y crecimiento de la mancha urbana alrededor de los volcanes. Además se utiliza la modelación cartográfica utilizando la realidad virtual, para recrear diferentes escenarios de riesgo humano y ambiental.

Los proyectos de investigación extracurricular impulsados por la UPAEP a través de los docentes investigadores, hacen posible que los estudiantes se desarrollen en ambientes profesionalizantes, con mayor seriedad y carácter hacia la investigación de los problemas que aquejan la salud y desarrollo social acompañada de una actitud más humana, consciente de las necesidades y desafíos que nos rodean.

La comunidad de estudiantes y profesores de la Universidad UPAEP, reconoce que la amenaza volcánica es un problema con carácter multidisciplinario que posibilita el conocimiento interdisciplinario para la capacitación, evaluación y retroalimentación científica; que puede difundirse en espacios de interés público a fin de facilitar la prevención de eventualidades entre los habitantes de las zonas vulnerables y también el enriquecimiento del conocimiento empírico que impera entre los habitantes, es decir el conocimiento de los volcanes que se ha transmitido por generaciones en los pueblos aledaños a las faldas volcánicas, sus creencias, costumbres y tradiciones. Dado que para conocer el fenómeno geofísico y llevar a cabo planes de prevención exitosos es importante que también se respeten las creencias de sus habitantes, pues nos permite conocer el misticismo que circula alrededor de los volcanes.

[SCD-507] Materiales multifuncionales con aplicaciones en medioambiente y energía

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Una de las grandes problemáticas que enfrentamos en la actualidad es el aumento de las emisiones de gases de efecto invernadero (GEI) en la atmósfera, lo cual afecta el medio ambiente y la salud humana. En materia de energía y cambio climático México propone en el Plan Verde "*reducir las emisiones de gases de efecto invernadero, impulsar y fortalecer el mercado de las energías renovables y realizar acciones de adaptación al cambio climático para la población*". Para lograr este objetivo es necesario el desarrollo y uso de nuevos materiales aplicables a tecnologías enfocadas en energías renovables y ambientales.

En esta plática se presentan estrategias para la síntesis y evaluación de materiales que por medio de un proceso de quimisorción puedan capturar CO_2 (un gas de efecto invernadero), que funcionen como catalizadores heterogéneos en la generación de energéticos limpios (biodiesel y gas de síntesis, $CO + H_2$), tratamiento de agua y que puedan ser usados como cátodos en dispositivos de almacenamiento de energía como baterías de ion litio. Los materiales se caracterizaron estructural y microestructuralmente por medio de diversas técnicas espectroscópicas. Además, se presentan resultados de la evaluación de cada uno de estos materiales en diversas aplicaciones ambientales y energéticas.

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[SCD-519] Conceptos de Manufactura aditiva aplicados a la industria aeronáutica

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La manufactura aditiva (MA) o impresión en 3D es un método fabricación donde las piezas se construyen a partir de la adición de material, capa por capa basado en un modelo computacional (CAD). Este concepto de fabricación es contrario a los procesos tradicionales como torneado, frezado o maquinados de cualquier tipo, donde se remueve material de la pieza hasta darle la forma y dimensiones deseadas. La MA permite fabricar piezas de gran complejidad y de diferentes tipos de materiales como metales, polímeros, cerámicos o materiales compuestos. En la industria aeronáutica la MA ha permitido la integración de elementos reduciendo el número de piezas que se utilizan en una turbina y con ello se reduce el peso y los gastos de combustible. A pesar del potencial que tiene esta tecnología, la MA aun tiene grandes retos que resolver desde el punto de vista científico. En esta platica se muestran algunos conceptos básicos de la MA y su estado actual en el mundo y en México. Además, se presentan resultados parciales de investigaciones que se están desarrollando en este tema.

[SCD-522] Bioelectrónica, BioMEMS y BioChips: Posibilidades de Desarrollo para México

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Actualmente el término "Internet de las cosas" (Internet of Things) representa un concepto bastante amplio en las telecomunicaciones, que también se utiliza para describir el protocolo de intercomunicación y control de un arreglo de sensores posicionados en una persona, para el seguimiento continuo de los signos vitales. Estas nuevas aplicaciones son el producto de una fase más de desarrollo dentro de la tecnología de los circuitos electrónicos (chips). Actualmente la Electrónica moderna se desarrolla en base a la tecnología de los chips, la ingeniería de software y la ciencia de materiales, principalmente.

Los Sistemas MicroElectroMecánicos (MEMS, MicroSistemas) surgen como una nueva tecnología interdisciplinaria, a partir de la ya consolidada industria de los circuitos integrados (CI´s, chips) o Microelectrónica. Esta nueva tecnología ha dado cauce al desarrollo de sensores y actuadores que se fabrican en combinación con bloques de CI´s para el procesamiento de sus señales eléctricas (Sensores inteligentes). En sus inicios, los MEMS presentaron aplicaciones restringidas hacia áreas de electromecánica: pero posteriormente, con el desarrollo de nuevos materiales compatibles con los chips, los Microsistemas se han diversificado hacia áreas tales como biología, óptica, fluídica, medicina, comunicaciones, e Internet de las cosas, entre otras. Hasta la fecha, los prototipos MEMS totalmente integrados con amplio uso industrial son enfocados hacia aplicaciones específicas, algunos ejemplos clásicos son los acelerómetros que detonan las bolsas de aire cuando ocurre una colisión vehicular, los cartuchos para inyección de tinta en las impresoras y recientemente los dispositivos microfuídicos para el análisis portátil de los signos vitales.

En un contexto general de investigación y desarrollo, los MEMS representan un amplio campo de estudio. En otro contexto de interés público, los dispositivos (Microcomponentes) MEMS para aplicaciones médicas (BioMEMS) representan un campo de desarrollo estratégico porque se proyecta como un mercado con potencial muy alto. La tecnología de BioMEMS permite el desarrollo de Microcomponentes con posibilidades de interacción con el cuerpo humano, utilizando materiales inertes o de alta pureza química por los requisitos de biocompatibilidad. Los primeros dispositivos BioMEMS fueron fabricados en 1970 consistiendo de sensores de presión arterial micromaquinados en silicio. En la actualidad, los trabajos de investigación en BioMEMS han derivado en una gran variedad de procedimientos en síntesis de materiales y métodos de fabricación, que utilizando técnicas de miniaturización de fluidos han conducido al desarrollo de la tecnología denominada “Lab on a chip”. Este tipo de tecnología incrementa la precisión en el análisis bioquímico, posibilitando nuevas capacidades de análisis clínico de tipo ambulatorio. En esta conferencia se abordan proyectos de desarrollo de tecnología de Microelectrónica y sus aplicaciones en Microsistemas y BioMEMS, utilizando la Tecnología nacional PolyMEMS INAOE®, los cuales por sus características de innovación y bajo costo resultan de muy alto interés para nuestro país.

[SCD-537] Óxidos de Cobre y Zinc para fabricación de dispositivos electrónicos

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El uso de semiconductores para la fabricación de dispositivos electrónicos ha favorecido parte del desarrollo tecnológico actual. Si bien el silicio se ha consolidado como material base en la microelectrónica y los dispositivos electrónicos, es cierto que continuamente se buscan alternativas que puedan contribuir al desarrollo tecnológico, mejorando las prestaciones con las que se cuenta actualmente. En esta plática se comentará acerca de dos óxidos semiconductores que por sus propiedades han llamado la atención de diferentes grupos de investigación. Entre las posibles aplicaciones se encuentra que los semiconductores óxido de cobre y óxido de zinc, por su alta sensibilidad superficial, han sido propuestos para la detección de gases que son tóxicos o explosivos. Por otra parte, cuando tecnológicamente el óxido de cobre se une con el óxido de zinc, se forma un dispositivo que comúnmente se conoce como diodo. Este dispositivo electrónico es fundamental en diversas aplicaciones, entre las que se encuentra la conversión de corriente alterna a corriente directa, así como también en celdas solares.

SEMICONDUCTORS (SEM)

Chairmen: Máximo López (CINVESTAV-DF)
Salvador Gallardo (CINVESTAV-DF)

SEMICONDUCTORS
(SEM)
ORAL SESSION

[SEM-23] MBE-grown InAs/GaAs and InGaAs/GaAs heterostructures for THz sources development

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The development of new mechanisms that allow the generation of Terahertz radiation (THz), represents a new area of work and research of great interest due to the great impact that is expected in the coming years in various scientific areas. One of them is the communications area where new higher capacity data transfer technologies are currently being developed, for example, mobile networks and THz Wireless communication [1].

To satisfy the increasing demands of coherent THz sources, several mechanisms of THz radiation such as solid-state oscillators, quantum cascade lasers, optically pumped solid state devices and novel free electron devices, have been proposed. On the other hand, the devices based on semiconductor InAs/GaAs and InGaAs/GaAs structures has the potential to generate THz emitters due to the small effective mass of InAs carriers that might be cheaper, powerful and more stable, as compared with the nowadays technologies. [2] In this work, we study the molecular beam epitaxial growth of InAs and InGaAs on semi-insulating GaAs substrates to promote a high electron mobility. For InAs/GaAs structures, 1-μm-thick InAs layer was deposited with a growth rate of 0.86 μm/h. At the early stages of the InAs growth, the surface showed a streaky (2x4) reconstruction, which evolves to a (4x1) RHEED surface reconstruction once surpassing the InAs/GaAs critical thickness. This surface suggest that the growth proceeded under In-rich conditions either because the substrate temperature was high or the As-beam equivalent pressure was low. According to the (-10) and (01) diffraction spots the InAs lattice relaxation started at 0.37 nm and concluded at 1.85 nm. As reported previously, [3] most of the misfit dislocations caused by lattice mismatch disappear in the first 0.2 μm of InAs growth and hereafter the smooth surface is recovered as can be proved by the RHEED technique. Atomic force microscopy images of the samples confirmed that in spite of the built-in strain, the InAs surface heterostructures are smother than those of the GaAs homostructures. Finally, prelaminar characterization of the THz radiation emission of the heterostructures after excitation by ultrashort pulses is presented.

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[SEM-217] Lifetime determination of CdTe optical phonons by resonant raman spectroscopy

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We present a Resonant Raman Spectroscopy (RRS) study of LO and 2LO optical phonons in zincblende CdTe substrates with surface roughness of 279 and 430 nm. For the experimental data, the observed intensities dependence of the 2LO optical phonon frequencies and linewidths for each one surface roughness is analyzed by fitting the RRS line shape with a lineal superposition of Lorentzians functions, an excellent agreement between experimental data and model is reached. The lifetimes of both the LO and 2LO phonons are measured from the line width [full width at half maximum (FWHM)] values obtained through a Lorentzian fit of the RRS profiles. The 2LO mode relaxation lifetime is found to occur via electron-phonon decay, with an appreciable dependence of surface roughness. The LO phonon lifetime is does not depend on roughness. The results obtained are a tool that contributes to the understanding of the line shape of the Raman spectrum and its use for surface analysis to investigate optical phonon lifetimes in semiconductors.

[SEM-326] First Principles Study of Electronic and Optical Properties of Semiconductor Quantum Dots of Indium Phosphide

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The physical and chemical properties of semiconductor nanoparticles have opened a great number of applications such as biological markers, LEDs, transistors, solar cells, etc. Among the II-V and III-V semiconductors, indium phosphide (InP) is, probably, the only material that offers a broad range of emissions similar to those of CdSe but without their intrinsic toxicity. Nevertheless, its quantum behavior has not been yet completely understood. Using the software suite ABINIT with the Density Functional Theory (DFT) framework, we have studied the relationship of the electronic structure and optical properties with the size of InP quantum dots (QDs). As a first step, we have calculated the InP bulk properties (structural parameters, electronic structure and phonons relation dispersion) to demonstrate the accuracy of our model with the Augmented Plane Wave (APW) method. Then, we have modeled stoichiometric InP QDs with diameter sizes in the range between 1.50-3.0 nm. Next, the computational results were used to examine and deduce the electronic properties, density of state (DOS) and localized molecular orbitals HOMO and LUMO. With this, it was demonstrated the quantum confinement and its improvement with the passivation effect on the quantum dots. We suggest a reliable analytical equation to describe the change of energy band gap as a function of size to valid our experimental results. Also, we have calculated the phonons dispersion, refractive index and dielectric constant, and their dependence with the size of each modeled QD. Finally, we present a comparison of our theoretical calculations with the UV-Vis and Raman spectra of colloidal InP QDs that were synthesized.

[SEM-374] ON THE POSIBILITY OF PROBING THE TEMPERATURE OF A TWO DIMENSIONAL ELECRON GAS

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The hetero-structure AlGaN/GaN contains a two dimensional electron gas (TEG) that spontaneously forms at its interface but completely contained in the GaN side. This electron gas displays an electron concentration and mobility around 10^{13} e-cm^{-2} and 1000 cm^2/V-s, respectively. The quasi-triangular potential well that contains it is about 10 nm wide. The HEMT produced with it is able to handle a power density of a Mega-Watt/cm^2, with a lineal current density of 1 A/mm of gate width. At such current density the electron gas temperature in the TEG, should be quite different from the lattice temperature eve if this is carefully kept at room temperature. To now it has not been reported a method to determine the two dimensional electron gas while conducting such high current densities. Here we propose an experimental way to explore and probe its temperature in an extremely simple procedure. Just taking advantage of the High Electron Mobility Transistor (HEMT). We have found the TEG temperature increases in a way proportional to the square of the current being handled and that for a current density of 10^6 A-cm^{-2}, the TEG temperature is around 500 K. Full details of the procedure to extract the TEG temperature will be given and discussed in this presentation.

[SEM-408] Study of the Band-to-Band, and Interband transitions of GaNAs/GaAs MBE grown heterostructures

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In recent years, great efforts have been made to improve the efficiency of photovoltaic devices, which has led to extensive theoretical and experimental studies of novel materials and new designs of solar cells. To date, the highest power conversion efficiencies have been achieved with multi-junction solar cells, called tandem cells. This technology comprises the absorption of photons of various energies allowing to capture a larger region of the solar spectrum. An alternative to achieve this same objective is the use of highly mismatched alloys (HMA) where the decoupling in electronegativity and size of the atomic radios, generates a splitting of the host material conduction band. The lower energy band is called the intermediate band (IB). Thus, the splitting allows the absorption of photons of three different: VB-IB, IB-CB and VB-CB. An important advantage compared to tandem solar cells is that the multiple absorptions of photons is achieved in a single p-n junction.

In this work, the MBE growth of GaNAs and the optical quality inferred from the VB-IB, IB-CB and VB-CB transitions are reported. The Nitrogen concentration N% in the allows was chosen close to 2%, since around this value the IB energy is suitable for photovoltaics applications. The lattice disorder measured by Raman spectroscopy was related to the incorporation of nitrogen in the GaAs matrix. The strain induced disorder leads on considerable discrepancies for determining %N by High-resolution x-ray diffraction (HRXRD), photorreflectance (PR) and spectroscopic ellipsometry (SE) spectroscopies. PR and SE of the samples revealed the transitions VB→IB and VB→CB, besides of spin-orbit $E_0+\Delta_0$. Temperature dependence PR measurements were performed in order to evaluate the activation energy of the fundamental transitions and to differentiate from extended to localized states. Low frequency Raman shifts of the resonance LO and TO modes suggested that the films are under tensile strain, which explains the low wavelength shifts of the optical transitions.

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[SEM-533] A Hybrid Structure for X-Ray Detection

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Recently, it has been a great increase in the use of radiation detectors for various applications, such as in medical imaging and charge particle detectors. Furthermore, most of the developed detectors are expensive, which limit its use. However, cost-efficient material, which can be deposited over flexible substrates, as well as in large area, have been attracted special interest, especially hybrid structures which are capable to enhance the behaviour of organic materials at a very low cost.

In this work, we present a hybrid-organic/inorganic structure for detection of X-Ray composed by lead sulphide (PbS) nanocrystals acting as the X-ray converter and Poly[2,5-bis(3-tetradecylthiophen-2yl) thieno[3,2-b]thiopheno] (PBTTT-C14) used to transport the generated carriers to the contacts. The advantage of using this material is the ability to be deposited at relatively low temperatures on flexible substrates, compared with vacuum or high temperatures methods.

Optical and electrical characterization will be showed, such as XRD, profilometry, ellipsometry, photoresponse measurement and conductivity. Also, in order to demonstrate its behaviour as detector, this structure was exposed to X-rays with energy of 34.5 keV for 2 seconds, showing a good response.

Keywords: X-ray detector, Hybrid Organic/Inorganic Structure, PBTTT:PCBM:PbS

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[SEM-550] MBE growth of GaAs thin-film detectors for ionising radiation

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Detectors for ionising particles have versatile applications, e.g. in particle physics experiments[1] and medicine[2]. Since the electron mobility in crystalline GaAs is almost 6 times higher than that in crystalline Si, single crystal GaAs based detectors have the prospect for providing high speed detection compared to conventional Si detectors. In addition, the larger bandgap, high density and large atomic number Z of GaAs allows the realisation of detectors with a better absorption efficiency and radiation hardness[3]. Nevertheless, the quality and the impurity level of the crystal is critical for achieving a good detection performance[4].

We have grown high quality and low dopant concentration single crystalline p-i-n GaAs ionising particle detectors by Molecular Beam Epitaxy (MBE). The highly sensitive CV measurement method was used to characterise the doping levels and detect the full depletion voltage. By introducing compensating dopants, a minimal impurity level of 1×10^{13} cm^{-3} was achieved, which results in low full depletion voltage and low leakage current levels. Supercontinuum laser Transient Current Technique (TCT) measurements suggest a charge collection time of less than 2 ns in GaAs. This is much shorter than that for Si which is typically 20 ns before irradiation[5].

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SEMICONDUCTORS
(SEM)
POSTER SESSION

[SEM-65] Oxygenated Amorphous Cadmium Sulfide Thin Films Grown By R.F. Sputtering

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Oxygenated amorphous cadmium sulfide (CdS:O) thin films were grown by radio frequency sputtering on corning glass substrates using the rf sputtering technique in a controlled plasma of N_2. Films were characterized by X-ray diffraction (XRD), photoluminescence (PL) and optical absorption (OA). The spectra of PL and OA show that the band gap E_g of the films depend on the oxygen concentration. E_g can be changed in a controlled way in the range from 2.4 to 2.7 eV. The film composition was measured by energy dispersion spectroscopy (EDS) using a Perkin-Elmer (JSM-6300) system.

[SEM-110] Physical properties of sputtered indium-doped ZnO films deposited on flexible transparent substrates

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Indium-doped zinc oxide (IZO) polycrystalline thin films were grown on polyethylene terephthalate (PET), polyethylene naphthalate (PEN), and as reference on 7059 Corning glass substrates at room temperature by radio frequency magnetron sputtering from a target prepared with a mixture of ZnO and In_2O_3 powders. The structural, optical, and electrical properties of the films were analyzed and compared. The IZO polycrystalline films showed n-type conductivity. The electrical resistivity drops significantly, and the carrier concentration increases as a consequence of In incorporation within the ZnO crystalline lattice. In both cases the changes are of several orders of magnitude. The resistivity obtained was $3.1 \pm 0.5 \times 10^{-3}$ Ohm-cm for an IZO sample grown on PET with a carrier concentration of $3.1 \pm 0.7 \times 10^{20}$ cm^{-3}, the best mobility obtained was 27.7 ± 0.8 $cm^2V^{-1}s^{-1}$ for an IZO sample grown on PEN. From the results, we conclude that n-type IZO polycrystalline films with high transmittance, high mobility and low resistivity were obtained on flexible transparent substrates

[SEM-126] Synthesis and characterization of materials based on the Cu-CdO-V2O5 ternary, in the high Cu content regime

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From the ternary system Cu-CdO- V_2O_5, different proportions in weight (*wt*) of these reactants were chosen to fabricate, six samples in the high copper content region. These were labeled according to the *wt* of the compounds used in the order Cu, CdO and V_2O_5 as follows: M1:40-50-10; M2:50-40-10; M3:60-30-10; M4:70-20-10; M5:80-10-10; M6:85-05-10.

The X-ray diffraction spectra showed the polycrystalline structure of the materials produced, the compound Cu_2O was present in all the samples, and the compounds $CuCdO(VO_4)$, CuO and Cu_3VO_4 for the samples M3-M6, were identified. Using Raman spectroscopy, the existence of VO_4 units and the Cu_2O was confirmed. On the other hand, the emission spectra showed luminescent bands related to charge transfers from the oxygen *2p* orbitals to vanadium *3d* orbitals, within the same VO_4 units. In addition, emissions due to charge transfer between *s* and *d* orbitals from Cu^+ ions were identified. The presence of these Cu^+ ions on the surface of the synthesized materials was corroborated by X-ray photoelectron spectroscopy. On the other hand, the electrical conductivity as a function of the temperature, was studied. Through the analysis of these plots, was found that this kind of materials, especially the samples M5 and M6 that have a higher copper content, are in the typical values range for semiconductor materials, which present conductivities in order of 10^{-8}-10^{2} $(\Omega{\cdot}cm)^{-1}$.

[SEM-150] Synthesis and characterization of SnS thin films by SILAR method as absorber material for photovoltaic applications

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Tin sulfide (SnS) is considered a chalcogenide p-type semiconductor material with orthorhombic crystal structure, it can be used in the fabrications of photovoltaic devices such as solar cells, due to its microstructural, optical and electrical properties. In addition, both Sn and S are abundant in nature and non-toxic. Tin sulfide thin films have been fabricated by Successive Ionic Layer Adsorption and Reaction (SILAR) method using chemical precursors as SnSO4 as cationic source and Na2S as the anionic source. Various conditions were experienced to find the optimum conditions for the deposition of the thin film, as were the number of cycles and temperature of the deposition, temperature and time of thermal treatment, pH of the precursor solutions and post cleaning on the formed thin film. For CdS/SnS heterojunction CdS has been acted as n-type material as window layer, and SnS as p-type material as the absorber layer. The deposited thin films were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), ultraviolet-visible spectroscopy (UV-vis), and x-ray photoelectron spectroscopy (XPS). The XRD studies confirmed the presence of orthorhombic SnS, as well as allowed to calculate the grain size in the thin films deposited, it is in a range from 15 to 25 nm. The order of the optical transmittance and the bandgap energy values were calculated from the UV-vis analysis, the bandgap energies were in the order 1.1-1.3 eV. SEM studies reveal that the SnS films exhibited uniformly distributed grains over the entire surface of the glass substrate for more time on the thermal treatment. Additional XPS studies helped to confirm the SnS chemical composition according to the effect of the thermal treatment

Keywords: tin sulfide, chalcogenide, thin films, successive ionic layer adsorption and reaction, SILAR, semiconductor, solar cell

[SEM-220] Study of morphological, optical and structural behavior of ZnO thin films deposited by spray pyrolysis at different temperatures of substrate

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Semiconducting metal oxide materials have showed interesting and novel properties. These properties have helped the researchers to improve their potential in devices as thin film transistor, spintronics, solar cells, gas sensors etc. [1-2].

Successful deposition of ZnO thin films from non-toxic precursor solution by mean of a spray pyrolysis system with an automatized perfume atomizer is demonstrated. The effects of three different temperatures of substrate, ranged of 300 to 400 °C, on the surface morphology, optical transmittance, band gap energy and crystalline structure of thin films deposited were studied. Irregular grains with cracks and voids can be observed by mean of images of SEM to 300°C. When the temperature change to 350°C hexagonal grains o crystallites appears on the surface of the films and a combination of hexagonal and round grains can be observed to 400°C. On the other hand, the band gap energy values obtained were 3.11, 3.18 and 2.91 eV to 300, 350 and 400 °C respectively. These values were slightly minor than the value reported of 3.22 eV. The optical transmittance showed low values between 30 to 50 % in the range of 300 to 700 nm of wavelength. However, the ZnO thin films deposited to 350 °C, could have potential applications as gas sensor according to results obtained.

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[SEM-262] Enhancement of the photoluminescence of InP quantum dots passivated with mercapto-based acids (MSA and MPA) for biological markers

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The study of the optical and structural properties of indium phosphide (InP) quantum dots (QD's) are of great scientific interest due to their unique physical and chemical properties. One of their main characteristics is the photoluminescence (PL) blue shift due to quantum confinement effects as the QD size decreases as compared to the Bohr exciton radius. Through a passivation process it is possible to improve PL efficiency and ensures an increased shelf-life of the InP QD`s, because it provides a physical barrier between the optically active core and the surrounding medium, thus generating QD's that are less sensitive to environmental changes, surface chemistry, and photo-oxidation. Consequently, this type of materials are good candidates to use as non-conventional biological markers in which the color will depend on the QD size. In this work, we have studied the effects of passivation with mercaptosuccinic (MSA) and mercaptopropionic (MPA) acids in InP semiconductor quantum dots through the use of optical and structural characterization techniques. From the PL spectra, we were able to observe an increase in the emission intensity before and after the passivation process. Also, a blue shift of the absorption spectrum according to the QD size was observed. The direct band gap energy of the samples was calculated according to Tauc's model, obtaining values in the range between 2.1-2.4 eV. Finally, using high-resolution transmission electron microscopy (HRTEM) we were also able to estimate the size and shape of InP quantum dots.

[SEM-281] Phosphorous and boron activation in polymorphous silicon thin films obtained by PECVD starting dichlorosilane as a gas source

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In this work, the incorporation of dopants into amorphous silicon (a-Si) used dichlorosilane as precursor in PECVD system has been shown. Intrinsic polymorphous silicon has been deposited, as reference for optical, electrical and morphological properties, using the same precursor as silicon source. After the characterizations, the polymorphous silicon thin films were doped with phosphine to get "n" type thin films. On the other hand, samples were deposited again and were doped with diborane, to form "p" type thin films. All of the samples were deposited at a pressure value of around 6 E-6 torr. We found the incorporation of phosphine in the silicon matrix at a RF power of 100-130 Watts and high pressures values (till 2 Torr). On the other hand, in case of diborane, the boron incorporation was possible using the RF power from 50 W to 130 W. To know the approximate concentration of boron and phosphorous, we measure the open circuit voltage (Voc). However, in case of thin films doped with boron it is more complex to create electrical active sites inside the matrix and in that case, it is necessary to find suitable conditions (for example annealing of the samples) to improve the junction created to enhance the Voc voltage.

[SEM-302] Growth of cadmium telluride films on flexible molybdenum substrate by close space vapor transport technique

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Films of polycrystalline CdTe were grown on 100 μm thick molybdenum flexible substrates by close space vapor transport technique. The deposition conditions were source temperature of 600°C, substrate temperature of 480°C, under an atmosphere of 100 mTorr and 80 mTorr of O_2/Ar 50%/50% gas mixture, 15 minutes time deposition. Prior the CdTe deposition, the molybdenum substrates were subjected to a chemical treatment with HCl solution or with $NH_4OH:H_2O$, or thermal treatment at 700°C during 15 minutes under air atmosphere, or a simple conventional cleaning with solvents (acetone, isopropyl alcohol and deionized water, 5 minutes each in ultrasonic bath). The thickness of the CdTe films varied in the range of 1 μm to 3 μm with grain sizes in the order of microns. The obtained films were characterized by X-ray diffraction, scanning electron microscopy and atomic force microscopy. The results of the structural properties and morphology of the CdTe lead us to the best substrate conditions to grow CdTe film suitable for applications in flexible solar cells.

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September 24th-28th , Playa del Carmen, Quintana Roo, México

[SEM-342] Synthesis and characterization of Cadmium Telluride thin films by SILAR method for solar cells applications

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One of the most important chalcogenides p-type semiconductor materials is the Cadmium Telluride (CdTe) which possess a reduced bandgap energy and a high optical absorption coefficient for solar cells applications. CdTe thin films have been deposited on glass substrates by Successive Ionic Layer Adsorption and Reaction (SILAR) method using chemical precursor solutions such as sodium tellurite with sodium hydroxymethylsulfinate (rongalite), which is an excellent environmental friendly substitute to traditional hydrazine hydrate (as reducing agent), as anionic source, and cadmium chloride as cationic source. In this work, we study the effect of several conditions such as the bath deposition temperature, immersion times in precursors and rinsing, pH of the precursor solutions by using hydroxides, as well as post-annealing, on the structural, morphological, optical, chemical and electrical properties of CdTe to achieve a high quality thin film as absorber layer for solar cells applications. The XRD spectra revealed that the samples show CdTe cubic zinc blende structure and a strong preferentially (111) orientation, as well as the grain size of the films deposited, were in the range from 10 to 30 nm. The optical properties of all the samples assessed by UV-vis analysis helped to determine the optical transmittance under 10% and energy bandgap values from 1.1 to 1.5 eV. The surface morphology of CdTe thin films was investigated by scanning electron microscope (SEM) and it reveals that the films exhibited more grains well distributed over the entire surface on the substrate for higher hydroxide molar concentration. Also, a higher post-annealing can improve and adjust the CdTe thin film properties.

Keywords: Successive Ionic Layer Adsorption and Reaction Method (SILAR), Cadmium Telluride (CdTe), Semiconductor Material, Thin Films.

[SEM-364] Hybrid organic solar cells of the type OTC/TiO2/PTB7:PC71BM/MoOx/Ag

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The present work contributes to the knowledge and to the technological implementation of the organic and hybrid solar cells belonging to the third generation of solar cells that, within the use of solar energy by means of the photovoltaic effect are being widely studied in the present century, due to its enormous potential to cover the present and future needs of clean electric energy at a reasonable price. For the development of the project were not found, within the studies reviewed, identical solar cells in terms of materials and process to those obtained here, so the initial deposit conditions for each of the films that make up the cell, were obtained of an extensive literature review on studies with the PTB7 polymer and the like. After the development of the cells, we worked on improving them, taking as a base the study with the best operating parameters; this improvement being the result of experimentation on: the active layer in aspects of importance as thickness and thermal treatment, the hole transport layer (in this project MoO3 was used) in thickness, the electron transport layer (in this project TiO2 was used) in thickness and finally the finished cell in thermal treatment. Specifically, an organic solar cell with an inverted structure was developed and improved using PTB7 polymer, and as an acceptor, a fullerene derivative, PC70BM, obtaining a maximum efficiency of 2.88%; CdS and FeS2 nanoparticles were also synthesized to be used in the development and improvement of hybrid solar cells, obtaining maximum efficiencies of 0.0036% and 0.0115% respectively; and finally, inverted structure organic solar cells with active layer PTB7:PC70BM:NP were developed and improved using the synthesized nanoparticles of CdS and FeS2 and obtaining efficiencies of 2.25% and 1.2% respectively.

[SEM-369] Development of a composite material based on TiO2 for the detection of glucose

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The present work a composite material based on TiO2 was developed to obtain a non-enzymatic biosensor for the detection of glucose, it was manufactured with TiO2 nanotubes (NTs-TiO2), which were synthesized by the chemical anodizing technique and sensitized with silver oxide nanoparticles (Ag2O3), by means of the reactive RF-Sputtering technique. The morphology of the electrode, was examined by scanning electron microscopy (SEM), the diameter of the NTs-TiO2-Ag2O3, was 98.07nm. The electrocatalytic properties of the electrode prepared to oxidize glucose were investigated by cyclic voltammetry (CVs) and chronoamperometry. By the technique of cyclic voltammetry (CVs) the voltage of -0.71V was obtained and with chronoamperometry the sensitivity of the composite material based on TiO2 was calculated, which was of 3.885 μA * cm-2 * mM-1, with a range linear from 20-250 mg / dL and a detection limit of 1.1 mM. In addition, the non-enzymatic type glucose sensor shows good stability and repeatability.

Key words: Biosensor, Titanium dioxide, Non-enzymatic, RF-Sputtering, anodized.

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[SEM-381] Energy non-equilibrium, recombination, quasi-neutrality, and transport phenomena in bipolar semiconductor

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A detailed analysis of nonequilibrium energy influence on transport in semiconductors was carried out. Special attention was paid to the effect of this nonequilibrium on recombination and the quasineutrality condition. In particular the recombination has the same form for band-to-band and Shockley-Read-Hall transitions; the only difference between these expressions is the different lifetime. For both type of recombinations, the homogeneous in space energy nonequilibrium and the space charge does not affect the transport of charges, changing, of course, the nonequilibrium concentrations of electrons and holes. The lifetime can be introduced only for the band-to-band recombination at the quasineutrality condition.

[SEM-440] Photocatalytic degradation of methyl orange over SnO2-graphene nanocomposites prepared by hydrothermal method

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Water pollution is caused mainly by the discharge of wastewater that contain synthetic dyes, a growing threat to our environment and public health [1]. In recent years, photocatalysis method has been developed as an alternative for dyes degradation owing to its simplicity, low toxicity and high efficiency. The SnO_2, is a well-known n-type semiconductor with a wide band gap of 3.6 eV. The SnO_2 nanoparticles exhibits unique optical and electrical properties due to its high surface to volume ratio. The high band gap energy and high stability of SnO_2 nanoparticles make it a unique photocatalyst. However, photocatalytic activity of the SnO_2 could be enhanced principally increasing the dyes absorption and the separation of the charge photoinduced. Recently to obtain better photocatalyst has been combined the semiconductor with graphene to enhance the photocatalytic activity, due to high conductivity and large area effective [2]. Various approaches have been developed to synthesis of SnO_2 nanoparticles, but, the hydrothermal method is a simple and inexpensive technique for large scale production. In this work, we report the synthesis in situ of SnO_2-graphene by hydrothermal method. The samples are prepared using tin chloride as SnO_2 source, deionized water as solvent and acetic acid as catalyzer with 1:30:4 molar ratio, respectively. The solution was mixed with different content of GO (2.5, 5, and 10 mg). The samples were processed at 200º C during 6 h using a steel autoclave covered by Teflon. The photocatalytic degradation studies in methyl orange (MO) are done using a UV light lamp (10 W). To know the structure and morphology the nanoparticles were characterized by X-Ray Diffraction, Transmission Electron Microscopy and Fourier-Transform Infrared Spectroscopy. The photocatalytic studies show that the increase amounts of GO on the nanoparticles of SnO_2 leads to an increase in photocatalytic activity of the synthesized nanocomposites. Also, the sample with best results corresponding to SnO_2 with 10 mg of GO with the 100% degradation of MO in 60 min. The results obtained show the high potential to be applied in organic pollutants degradations in water source.

Keywords: tin dioxide, photocatalysis, graphene oxide, methyl orange.

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[SEM-451] Synthesis and characterization of Mn doped ZnO nanowires

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Currently ZnO-based materials have been receiving considerable attention due to their potential applications in spintronics, light-emitting diodes, UV detectors, cosmetics and biomaterials. Doping has been a widely method to improve the electrical, optical and magnetic properties of semiconductors. For spintronic applications, the design of a transparent piezoelectric dilute magnetic semiconductor (DMS) has been pursued through a small amount doping of a transition metal (TM) ions in ZnO. Thus, ZnO nanostructures doped with manganese (Mn), ZnO:Mn having variable doping concentration by different molar ratio Zn:Mn have been synthesized by termal evaporation and condensation technique using zinc powder and manganese oxide at 750 ^{0}C for 60 minutes and nitrogen gas as carrier at atmospheric pressure. The as-synthesized Mn doped ZnO nanowires have been characterized by X-ray diffraction (XRD), energy dispersive x-ray (EDS), scanning electron microscopy (SEM) and electron spin resonance (ESR). XRD revealed that the sample posses hexagonal wurzite estructure. From the Rietveld refined XRD spectra, the lattice parameters average crystallite size was obtained. In this range of doping concentrations all samples show an expansión of the lattice parameters relative to the bulk samples. Optical absorption studies showed an increment in the band gap with increasing Mn content, and olso give evidence for the presence of Mn^{2+} ions in tetrahedral sites. All $Zn_{1-x}Mn_xO$ ($0.01 \leq x \leq 0.25$) samples were paramagnetic at room temperature. No peak corresponding to other impurities or catalytic particles was detected according to those obtained by EDS measurements. The last fact leads us to assumme that the vapor-solid (VS) mechanism is the route for growth and formation of those zinc structures.

[SEM-468] p-type transistors fabricated using transparent oxide thin films and processes of photolithography

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p-type SnO was used as active layer to fabricate thin film transistors (TFTs) through photolithography processes. The deposition conditions to obtain p-type SnO thin films (~25 nm) by DC reactive sputtering were a relative partial pressure between 7% and 21% (N_2 and/or O_2), a total working pressure of 1.8 mTorr and a plasma power of 30 W. The deposited thin films were oxidized after annealing at 250°C for 30 minutes. The dielectric gate was Al_2O_3 (~15 nm), deposited by atomic layer deposition. Drain and source electrodes of the TFT were ITO (140 nm)/Ti (10 nm) thin films deposited by sputtering. The TFTs were characterized using a Keithley 4200-SCS analyzer and a Cascade Microtech Summit probe station at room temperature. Hall measurements showed p-type carrier concentration (Nh) of around 1×10^{18} cm^{-3} when the O_2 was used as the reactive gas, but if the reactive gas was N_2 the Nh was around $1x10^{19}$ cm^{-3}. The Hall mobilities was between 0.35 and 2.64 cm^2 $V^{-1}s^{-1}$, depending on the N_2 and/or O_2 flow rate during deposition. A change in the Hall mobilities was associated with the preferred crystalline orientation in the SnO films from (101) to (110). The SnO-based TFTs showed p-type behavior with low threshold voltages in the range from 1.76 to 3.50 V. The TFTs mobilities in the saturation regime were in the range of 0.12 and 1.32 cm^2 V^{-1} s^{-1}. The current on/off ratio (I_{ON}/I_{OFF}) was in the order of 10^2, approximately. The large values of the interface trap density contributed to the high I_{OFF} and the low I_{ON}/I_{OFF} of the TFTs.

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[SEM-475] Glucose biosensor manufactured with titanium oxynitride by the reactive rf-sputtering technique

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TiO2 is a semiconductor focused on the industry as a pigment for paints, cosmetics, pharmaceuticals, paper, food products; In the area of thin films it has a wide range of applications. On the other hand, thin TiN films exhibit a combination of high hardness, chemical and metallurgical stability, excellent wear resistance, and a vast range of optical and electronic properties. Thin films of TiOxNy have recently attracted attention, having optical and electronic properties that can be modulated depending on the ratio Nitrogen to Oxygen (N2 / O2). TiOxNy coatings with high Nitrogen content have been used in many applications, such as antireflective coatings and biomaterials.

In this work thin films of TiOxNy were deposited on glass and titanium substrates using the reactive RF-Sputtering technique. The electrochemical biosensors shown high sensitivity, fast response times, and stability for the determination of glucose concentrations. The main goal is to evaluate the use of TiNxOy thin films obtained by the RF-Sputtering process for the construction of enzimatic and nonenzimatic biosensors.The results includes the optical and electrochemical characterization of the samples.

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[SEM-511] Influence of the growth temperature on the properties of AlGaAs deposited by R.F Magnetron Sputtering

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The effect of the substrate temperature, from 250°C to 550°C, on the optical and structural properties of AlGaAs thin films deposited on glass and Si substrates by R.F magnetron Co-Sputtering of GaAs and Al targets was studied. The characterization of the films was carried out via XRD, Raman spectroscopy and optical absorption in the UV-Visible range. The influence of the temperature on the crystallite sizes and micro-stress was evaluated by XRD. The X-ray diffraction spectra show that the films are polycrystalline with preferential orientation (111). The Raman spectra show a behavior of two modes, corresponding to vibrational modes TO and LO of GaAs and AlAs, respectively. The modes TO-AlAs and LO-AlAs, are originated on the ternary alloy. The UV-Vis optical measurements showed the presence of AlGaAs layer with a typical band gap around 1,45 eV.

[SEM-538] Study of thermal oxidation of copper sheets

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Copper oxide is a semiconductor with several applications such as gas sensing, photocatalysis, capacitors, and heterojunctions. There are two major structures of copper oxide, which are cuprous oxide (Cu_2O) and cupric oxide (CuO). We have performed thermal oxidation of copper sheets in the range of 200-1000 °C. Copper oxide was characterized by X-ray diffraction, Raman scattering, Scanning Electron Microscope, Energy Dispersive Spectroscopy, and Hall measurements. Structural analyses show that independently of the growth conditions, copper oxide samples show a mix of Cu_2O and CuO. Morphological measurements show a compact surface without formation of nanostructures or nanoparticles. Hall measurements showed that te copper oxide exhibits a p-type conductivity.

SURFACES AND INTERFACES (SIF)

Chairmen: Leonardo Morales de la Garza (CNyN-UNAM)
Mario Farás Sánchez (CNYN-UNAM)

SURFACES AND INTERFACES (SIF) ORAL SESSIONS

[SIF-108] Fabrication and characterization of non-enzymatic glucose sensor based on ZnO thin films deposited by sputtering

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In the present work, we developed a non-enzymatic glucose biosensor using zinc oxide (ZnO) thin films deposited on titanium substrates by the sputtering technique. Films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), cyclic voltammetry (CV), and chronoamperometry. The films were deposited on titanium substrates with grow times of 10, 15, 20, and 60 min at room temperature. Structural properties demonstrated that the deposition time influences the crystallographic planes, thin films with times of 10, 15, and 20 min have preferential orientation on (002), while for the 60 min sample the preferential orientation change to (100). SEM images show uniform morphology for all samples. The grow time affects the thickness, results in an increase in the sensitivity of the non-enzymatic glucose biosensor based on ZnO/Ti. The electrochemical device showed a sensitivity of 9.38 $\mu A\ cm^{-2}\ mM^{-1}$ with a linear response range of 2.20 mM to 12.10 mM.

[SIF-117] Chemical characterization of biofunctionalized platform of a-SiC:H for biosensing application

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The development of highly sensitive and cost-effective miniaturized sensors requires advanced technology with knowledge in chemistry, biology and materials sciences. The biofunctionalization of silicon materials and derivatives allows a good biocompatibility for the biomolecules immobilization; therefore these materials could be used for biological recognition, selective and reproducible biosensing systems, such as inmunosensores. Thin films, such as hydrogenated amorphous silicon carbide (a-SiC:H) has unique physicochemical properties and could be use in the creation of new recognition and transduction processes for chemical and biological sensors. The a-SiC:H was used as slid support, it was functionalized by Self- Assembly Monolayers (SAMs) method for chemically modifying surface with amino and aldehyde groups to immobilize antibodies. This functional platform show chemical and topography differences in each step in the process, which could impact the detection of specific targets in the surface. Morphological analysis and chemical mapping were studied by Atomic Force Microscopy (AFM) and Scanning Electron Microscopy with Energy Dispersive Spectroscopy (SEM-EDS). In this context a comparative chemical analysis , could provide a quality information about the fuctionalized platforms to assembly biomolecules for biosensors.

[SIF-209] Resistance to corrosion and wear of coatings 140MXC-530AS and 140MXC-560AS produced with the technique of electric wire arc spraying

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In this research, the corrosion and wear resistance of two dissimilar coating mixtures (140MXC-530AS and 140MXC-560AS) produced with the with the technique of electric wire arc spraying was evaluated by means of salt chamber tests according to ASTM B-117, potentiodynamic polarization (TAFEL), electrochemical impedance spectroscopy (EIS) and abrasive and adhesive wear under ASTM G-65 and ASTM C-633 standards respectively. The mechanical behavior of the deposits was also determined by the microhardness tests established by the ASTM E-23 standard and pin on disk.

As results it was established that the 140MXC-560AS mixture had an above-530AS 140MXC mixture 66% in corrosion tests behavior; while in the test adhesive wear the best performance as presented 140MXC-530AS mixture with 24% compared to 140MXC-560AS mixture because the specific surface roughness in these coatings. As for the mechanical behavior of deposits increased 21% in microhardness and 94% reduction in the coefficient of friction (COF) in 140MXC-560AS mixture compared against 140MXC-530AS mixture was observed.

[SIF-370] Laser-induced periodic surface structures formation: numerical investigation of the temperature dynamics in metals and dielectrics and subsequent stress build-up estimations

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To get insight into laser-induced periodic surface structures (LIPSS) formation, the relaxation of a periodic modulation in the temperature profile is investigated numerically on surfaces of two different kinds of materials (metals and dielectrics) upon irradiation by an ultrashort laser pulse. The periodic temperature modulation is assumed to originate from the interference between the incoming laser pulse and the surface-scattered electromagnetic wave, considered as the main mechanism of LIPSS formation [1]. Modulation of energy deposition can yield periodicities in stress distribution, melting, and ablation before the final heat dissipation [2,3] and thus influence the surface relief formation.

Dissipation dynamics of absorbed energy deposited on the surfaces of fused silica and gold, as typical examples, and the corresponding stress build-up is studied using a simplified two dimensional approach [2]. It is based on the two-temperature model (TTM) and considers the mechanisms of laser light absorption and relaxation specific to each material. The TTM is coupled with the Drude model for the evolution of optical properties of the irradiated materials. The stress build-up is estimated from the local temperature evolution.

The development and decay of the lattice temperature modulation, which can govern the LIPSS formation, is followed during electron-lattice thermalization time and beyond. It is shown that strong temperature gradients can form along the surfaces of materials under study within the fluence range of LIPSS formation in experiments. The analysis of stress resulting from the temperature modulation distribution reveals considerable difference of stress amplitude and modulation for the two materials. Implications of modulated stress build-up are discussed. Considerable changes in optical properties as a function of time are also found for gold which amplifies the modulation of energy coupling along the irradiated surface.

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[3] I. Gnilitskyi et al. Appl. Phys. Lett. 109, 143101 (2016).

[SIF-377] Correlated Measurement using AFM techniques inside a SEM by Quantum Design

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AFSEM™ is an atomic force microscope (AFM), designed for integration in a SEM or Dualbeam (SEM/FIB) microscope. Its open access design allows for simultaneously operation of SEM and AFM measurements inside the SEM vacuum chamber; this complimentary corelative measurement capability allows for unique characterization possibilities of any sample.

AFSEM enables the combination of these two most powerful analysis techniques to greatly extend correlative microscopy and analysis possibilities. It allows simultaneously imaging of samples with high resolution, create true 3D-topography representations, and accurately measure heights, distances and even material properties, all while maintaining the large SEM field of view to position. The optimized AFSEM workflow (with practically no reduction of the SEM uptime) ensures highest possible effectiveness, while the powerful control software allows for optimized and intuitive measuring, system handling, and data analysis.

This tool is of great interest to study subtractive tomography and could be used with Dual beam systems.

SURFACES AND INTERFACES (SIF) POSTER SESSIONS

[SIF-28] Adsorption of dyes on two metal oxides: WO3 and TiO2

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There are different techniques for treatment water contaminated with organic dyes. One of them is to remove the dye by the adsorption process. Adsorbent materials such as activated carbon, zeolites, clays and chitosan have been used in recent years. However, the use of metal oxides as adsorbent materials has been little explored since their use has been focused on heterogeneous photocatalysis. There is evidence that metal oxides are highly adsorbent but it is still necessary to carry out more detailed studies of the adsorption process on these materials. In this work, the adsorption of two dyes, methylene blue and acid orange 7, on the surface of nanoparticles of tungsten oxide (WO3) and titanium oxide (TiO2) is studied . Through an experimental statistical design, the effect of four factors on the adsorption capacity of WO_3 and TiO_2 is investigated. The factors are pH, the initial concentration of dye, C_0, the amount of adsorbent, x, and time, t. With the results of the experiment we propose a regression model for the adsorption depending on the factors involved, Ads = Ads (pH, C0 x, t). In addition, a response surface methodology is used to find the points that lead to maximum adsorption, that is, the optimal adsorption conditions. Finally, a comparative study of the adsorption capacity of both oxides is made.

[SIF-85] Surface morphological study of TiO2-Fe2O3 thin films obtained by Sputtering

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Using a magnetically assisted Torus cannon of 50.8 mm in diameter, a titanium target high purity was placed, obtaining in this way an exposed surface of 2,026.8 mm^2 on which small pellets of 13.5 mm^{2}of surface were incorporated with approximately 1 mm thickness, until reaching a surface of 1,916.4 mm^2 of Titanium and 110.4 mm^2 of iron, that is: 94.55 and 5.45 % of exposed area respectively for each of the elements. All this configuration within a Sputtering system with the purpose of generating thin films of $Ti_{1-x}Fe_x$, on ceramic substrates 250x750 mm (corning glasses) in non-reactive atmosphere of Argon.

In this way, it was possible to obtain nine samples in the form of thin films, with thicknesses of approximately 230 nm, of metallic gray color characteristic of Titanium, with very little apparent difference between each of them at first glance, subsequently, each sample was divided into pieces of 10x10 mm for subsequent studies and thermal treatments, which consisted in submitting each fraction of the different samples to temperatures of 550°C in an uncontrolled atmosphere (oxidant) for a period of six hours, obtaining new samples totally different in physical aspect, ranging from transparent corresponding to a phase of TiO_2, to brown shades due to the presence of different iron oxides contained in thin films synthesized. Studies made in each of the samples by EDS reported the presence of oxygen with a small variation, while a clear decrease of Titanium against a gradual increase of Iron in the different samples synthesized.

Studies carried out on all samples using physical, microstructural and morphological characterization techniques, show the presence of phases of the different compounds present, in the form of oxides or as alloys between them, and the most important of this work, the superficial morphological change due to the gradual presence of iron, which promotes the agglomeration and crystallization of each sample to a greater or lesser degree depending on the content of this element in the different samples.

[SIF-127] Evaluation of properties in steel with hard coating under hydrogen

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In this study, on ASTM A36 steel surface whit hardened, at 950 °C for 5h and 7h; through dehydrated paste-pack boriding process. Then, They were investigated, the behavior of the specimen hardened superficially in the microstructure, the hardness, the present XRD phases and characteristics by three point bending. Simultaneously, was investigated the hydrogen permeation effect on the coating formed in the surface of the material and the mechanical characteristics were evaluated by three point bending and hardness. Obtained a layer sawn with the time and temperatures study; likewise the growth of FeB/Fe2B layers. There is a hardness change of the boron coating subjected to hydrogen permeation and without hydrogen permeation for each time and temperature. The three-point test showed changes in properties with the coating formed on the surface of the study material subjected to hydrogen permeation and without hydrogen permeation. Showing that the coating boron an efficient alternative to lessen the effect by hydrogen permeation.

[SIF-176] Surface texturization of SS316 L by Ion implantation

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Utilizing the Pelletron accelerator at IFUNAM, 1 MeV Au ions were implanted into 316L stainless steel, used for medical applications. With an ion beam current of 200 nA, at room temperature, a fluence of 1.17×10^{17} cm^{-2} was reached. Three different angles of incidence, 32°, 45°, and 62° were chosen, and the surface texture was observed by SEM and AFM. The observations suggest mass flow at the surface. Additionally, in regions corresponding to different incidence angles, distinctive patterns are produced, in accordance with observations made in experiments with other materials and ions at lower energies. The support of DGAPA-UNAM project IN111717 and K. López, F. Jaimes and J.G. Morales is acknowledged.

[SIF-177] Indication of mass flow in the bombardment of metals

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When the surface of a solid is bombarded with energetic ions, it undergoes a series of modifications determined by the experimental parameters. Patterns such as ripples, grids and pits appear, clearly visible by conventional techniques such as SEM and AFM. There is a wide variety of experimental parameters, both for the impinging ions (type of ion, energy, fluence, arrival direction) and the solid surface (chemical composition, density, crystal orientation, curvature) that affect the formation of patterns. Heavy ions from a medium energy (MeV) accelerator typically have energies in the interval of 5 to 300 keV/amu, which places them between two extremes. For lower energies, up to ~ 1 keV/amu, where nuclear stopping prevails, continuum theories have provided explanations of many observed patterns, based mainly on the presence of sputtering and surface diffusion. At the other extreme, for energies ≥ 1 MeV/amu, electronic stopping dominates, producing deformation and mass flow, which lead to pattern formation on the surface. In the intermediate range there is a competition between nuclear and electronic stopping. Evidence of the existence of mass flow in several experiments at intermediate energies is presented, suggesting the prevalence of electronic stopping. SRIM calculations of stopping powers support these observations. The effect is observed in the bombardment of Ti, the alloy Ti-6Al-4V, stainless steel and amorphous SiO_2. The support of DGAPA-UNAM project IN111717 and M. Galindo, K. López, F. Jaimes, M. Escobar and J.G. Morales is acknowledged.

[SIF-235] Study on the effect of ball burnishing on roughness, surface hardness and corrosion resistance of ASTM F75 alloy

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The ball burnishing is a process in which the surface of a material is compressed causing plastic deformation, and therefore changing the mechanical and chemical surficial properties. The ASTM F75 alloy is widely used in the health field as surgical implant, where it is exposed to physiological fluids which are corrosive media. Therefore, improving the corrosion resistance is desirable in order to extend its lifetime. In this work, we propose the ball burnishing as a mechanical treatment to improve mechanical properties (roughness and surface hardness) and corrosion resistance. The influence of the two most important parameters of the ball burnishing was studied, i.e. force and number of tool passes. Tests were conducted in one of the faces of cylindrical ASTM F75 alloy samples (ø 25.4 mm x L 12 mm). The ball burnishing process was carried out in a conventional lathe, and samples were faced with tungsten carbide inserts before the surficial treatment. Roughness measurements were carried out in a Mitutoyo SJ-310 equipment, showing a decrease up to 86 % in samples with the highest number of tool passes. Surface hardness, measured in a microhardness tester HV-1000 of Sinowon, evidenced an improve up to 69% for those samples that were burnished with the greater force. Finally, corrosion tests in a VersaSTAT3 equipment demonstrated that the corrosion current ($icorr$) decreased up to 84% in burnished samples with respect to control samples. The analysis of these mechanical and chemical properties shows that the ball burnishing as a suitable process to improve the performance of the ASTM F75 alloy for implant applications, even more, it is an economic and ecological process.

Keywords: ASTM F75, Ball burnishing, Roughness, Surface hardness, Corrosion resistance.

[SIF-311] Characterization of opaque samples by reflection imaging complementary to optical and electronic microscopy

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The reflection image of a flat and polished surface was obtained using a conventional optical microscope, with the sample illuminated from above by a light source. The analysis of the optical image shows morphologic features, similar to the image obtained with scanning electron microscopy. In this work we observe the image of light reflected by a piece of wood. Since the sample is an opaque material, the light is absorbed completely when exceeding the penetration distance. The diffuse reflectance of back-scattered light contains information of the shape, topography and color of the surface. Even though the reflection imaging is not better than the optical transmission microscopy or the scanning electron microscopy, it has complementary information useful for the characterization of materials. We obtained a colored topographic image of live opaque samples up to 40X amplification.

[SIF-359] Synthesis of silver nanoparticles using PVP and chitosan using the polyol method

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Many routes water basis synthesis towards the shape-controlled of silver nanoparticles and microstructures have been used to form nanometers to micrometers shapes. At this work, were changing parameters conditions during the synthesis by the polyol method, the experimental parameters were changed: precursor stirring time, molar ratio (Ag, PVP and chitosan molar concentration), injection rate of PVP solution using ethylene glycol as the solvent or chitosan solution (using water and acetic acid as solvent), reaction time, reaction temperature and molecular weight of PVP.

The metallic nanoparticles (NPs) and larger nanostructures (NSs) have many useful properties. Especially silver, for the anti-bacterial action. Here, we report the shapes and sizes of the structures obtained by Scanning Electron Microscopy micrographs. Furthermore, the chemical species are reported by X-ray Photoelectron Spectroscopy data and the spectra obtained shows the metallic and ionic concentration of different samples. Some orientation shapes seem to grow with dimensional forms as a result of the temperature. Spheres, wires and ramifications are presented.

[SIF-432] CeO2-TiO2-Graphene oxide composites for supercapacitor applications

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Electrochemical double-layer supercapacitor (EDLSC) devices store charge by adsorption of electrolyte ions onto the surface of electrode materials. The absence of difussion-controlled redox reactions in these devices allows to fast response to changes in potential and leads to high power. EDLSCs have been used for applications which require rapid power delivery and recharge. Graphene has unique 2D structure and exotic intrinsic properties such as excellent electrical conductivity and large surface area. Superior chemical stability and broad electrochemical window make graphene-based composites attractive electrode materials for supercapacitors. In the present contribution, a novel electrode material, CeO_2 –TiO_2-graphene oxide composite was synthesized by the hydrothermal method at 120ºC. Structural and morphological studies were made using X-ray diffraction, Raman spectroscopy and scanning electron microscope. Cyclic voltammetry, charge-discharge profile and cycle life stability were studied by using electrochemical work station. The composite material exhibited electric double layer capacitance (EDLC) behavior with specific capacitance around 160 Fg-1 in 1 M KOH aqueous electrolyte. High rate capability, good cycle stability up to 2000 cycles and reversibility had been observed.

Acknowledgements. Financial support from SIP-IPN 20181187 project is granted. SEM/EDS and XRD were performed at CUV-BUAP and Raman at CIDS-BUAP.

Keywords: Supercapacitors, EDLC and graphene oxide based composite

[SIF-484] Peculiarity of TOF–SIMS analysis of biological cells and tissues

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Intensive investigations of different biological objects have been performed in last decade in the entire world by using the Time-of-Flight Secondary Ion Mass-Spectrometry (TOF-SIMS) method. Ion beam sputtering of an analyzed surface with monitoring of secondary ions lets it possible to get a true 3-dimentinal distribution of any elements of the Periodic Table with a high lateral and in-depth resolutions, and with a record sensitivity. This became possible due to a new generation of Time-of-Flight SIMS instruments, equipped with a pulsing Liquid Metal Ion Gun (LMIG) with heavy metal ions like bismuth and gold. The lateral resolution up to 80 nm is achievable with such ion sources; the heavy ions irradiation results a quit high secondary ion emission from organic materials. All this is necessary for effective elemental analysis of cells, tissues and microorganisms. But, a wide application of the SIMS method in biology and medicine is limited still by absence of an effective sample preparation technique. There is a high vacuum inside any SIMS instrument; this no suggests measurements of any liquids and “entire” bio-samples. Therefor different dehydration techniques are applied for sample preparation. Cryo-sectioning of frozen-dried samples is another alternative. Still there is no a common protocol of the bio-sample preparation and different laboratories demonstrate different techniques.

In this report we demonstrate experimental results of elemental analysis obtained by the SIMS method for different cells. The cells culture (3T3-F44A2 line) were dehydrated and fixed on crystal silicon substrates by using Glutaraldehyde (2% in PBS) and Paraformaldehyde (3.5% in PBS). After fixation, the samples were washed by using different methods and dried in a nitrogen atmosphere. TOF-SIMS analysis of lateral distribution of selected elements in cells was performed by a TOF-SIMS-V instrument from Ion-TOF Co. A pulsed finely focused bismuth ion beam with energy of 30keV and beam diameter of around 200 nm was used. First, the analyzing area was selected by using a secondary electron image obtained for a 500x500 mm scan. Then, secondary positive ions emitted from 100x100 mm areas were monitored to analyze the metallic elements distribution in cells, and negative secondary ions - to analyze halogens and non-metals distributions. Considerable difference between two fixation agents used was found. Obtained results let us conclude applicability of the sample preparation technique used in this study for future studies.

[SIF-512] Surface treatment of magnesium pieces through the “Sand-blast” technique

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The automotive industry in recent years has taken great interest in lightweight materials with the purpose of reducing weight, fuel consumption and the increase in the efficiency of automobiles. In this way, Magnesium has been studied for its implementation, because it possesses attractive properties, such as low density, high strength-weight ratio and excellent castability, however, the main drawbacks for its application are its low surficial hardness and the very low corrosion resistance . In this work, we report the implementation of the "sand-blast" technique for surface treatment of magnesium pieces to improve surficial hardness and to modify the corrosion resistance. The sand-blast surface treatment technique was applied on 1” x 1” polished magnesium sheets. The surface hardness, measured in a micro-hardness tester HV-1000 from Sinowon, showed an improve up to 44% .Corrosion experiments were carried out using a saline solution according to ASTM D1141-98 as a corrosive medium, and Tafel curves were obtained using a potentiostat in a configuration of three electrodes, showing a significant change in the Mg samples as function of the experimental parameters of the “sand-blast" technique.

Key words. Magnesium, corrosion, Sandblast, surface treatment.

[SIF-526] Application of the plasma electrolytic oxidation technique for surficial modification of Mg pieces.

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Mg has been widely studied to develop biodegradable implants, however, its main disadvantage is the rapid degradation in physiological fluids due to corrosion, therefore, in this work we report the development of the plasma electrolytic oxidation (PEO) setup and its application for preparation of TiO_2 coatings on Mg substrates with the aim of improving its corrosion resistance. For deposition of TiO_2 coatings, a conductive solution was prepared by dessolving 1-2 gr of NaOH in 1 L of deionized water, after that, 5 gr of titanium dioxide were dispersed in 1 L of deionized water, finally, both solutions were mixed. The PEO process was conducted in Mg pieces (99.8% purity) with 1 cm^2 in size. For voltage reference a platinum electrode was set at 0.5 cm from the Mg pieces. The platinum electrode was grounded and positive voltages were applied to the Mg pieces. The PEO process was applied for 15 min with a current of 50-75 mA/cm^2. After that, the Mg pieces were subjected to electrochemical corrosion tests in order to determine the effectiveness of the PEO process. Micrographs showed the surface modification after the PEO process, this modification depending on the experimental conditions. Tafel studies showed a decrease on the corrosion current in PEO processed pieces in comparison to control samples. Results demonstrated that developed PEO setup is effective for improving resistance corrosion of Mg, with the possibility for covering non-flat pieces, which is the main drawback of other deposition techniques.

Key words. Mg,TiO_2, PEO, corrosion.

[SIF-549] Bi2Te3 topological insulator: high vacuum vs atmospheric pressure

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Recently, a new state of matter has caught the attention of the scientific community: the topological insulator. With little more than a decade that the first material of this class was experimentally obtained, there are still many expectations about it. The surface states of these materials confer them unique exotic properties which makes them promising candidates for the future development of spintronics and quantum computing, among other potential applications.

Bismuth telluride (Bi_2Te_3) is one of the best known and studied topological insulator. It is a narrow gap semiconductor that has been widely studied for its thermoelectric properties. Among the different techniques used to obtain this material, molecular beam epitaxy stands out because allows a very precise control of growth parameters with low density of defects. However, it is a sophisticated and expensive system.

In this work, Bi_2Te_3 grown by physical vapor transport from its elementary sources, Bi and Te, is proposed as an alternative technique, under either high vacuum (HV) or atmospheric pressure (AP). The layers were characterized by different techniques to evaluate its structural properties. As a result, it is concluded that, as a consequence of the different transport regime, films grown at atmospheric pressure presented better crystal orientation.

[SIF-552] Towards an ISO standard in cluster ion depth profiling of organic materials using secondary ion mass spectroscopy (SIMS)

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In many technological and biological samples it is necessary to understand the distribution of organic chemical species as a function of depth and to combine this with laterally resolved surface chemistry to provide three dimensional representations. A method to do this is secondary ion mass spectrometry. Argon cluster ion beams can provide sputter depth profiles through organic material without causing significant damage. In order to reconstruct a depth profile or three dimensional image it is important to establish the depth scale in the depth profiling experiment. For this purpose, the sputtering volume yield is required.

The sputtering volume yield defines the ratio between the areic dose of primary ions and the sputtered depth. The depth scale can then be determined from the primary ion current, the sputtered area and the sputtering time. It also depends on sample temperature, the material being sputtered, the cluster source identity, kinetic energy and angle of incidence

This poster describes a draft International Standard that will specify a method by which the argon cluster sputtering yield volume of a specific organic material shall be measured and reported. The method requires one or more test samples of the specified material as a thin, uniform film of known thickness on a flat substrate which has a different chemical composition to the specified material. The International Standard will be applicable to test samples in which the specified material layer has homogeneous composition in depth and using instruments in which the sputtering ion beam irradiates the sample using a raster to ensure a constant ion dose over the analysis area. The international standard is being developed by ISO TC201 (surface chemical analysis) /SC6 (SIMS) and is expected to be published by March 2019.

THEORY AND SIMULATION OF MATERIALS (TSM)

ChairmEn: Raul Esquivel (IF-UAM)
María Teresa Romero de la Cruz (FCFM-UAdeC)
Ariadna Sanchez (UAEH)

THEORY AND SIMULATION OF MATERIALS (TSM)
ORAL SESSIONS

[TSM-57] Structural, electronic, and magnetic properties of the CrN (001) surface: First-principles studies

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Spin-polarized, first-principles total energy calculations have been performed to investigate the structural, electronic and magnetic properties of the chromium nitride (001) surface. Different approximations were used to treat the non-classical exchange correlation energy: LDA, GGA, LDA+U ($3\text{ eV} \leq U \leq 5\text{ eV}$) and GGA+U ($1\text{ eV} \leq U \leq 4\text{ eV}$). It was found that LDA+U with U= 4 eV describes correctly the structural, electronic and magnetic properties of bulk CrN. The CrN (001) surface has been investigated, employing the surface formation energy (SFE) formalism. For the surface in the cubic phase, three different structures were found to be stable: an ideally terminated surface, one with no nitrogen atoms in the second layer, and one with half of the nitrogen atoms missing in the second layer. In the case of the orthorhombic surface, only the ideal surface is stable in all the range of the chemical potential. Density of States (DOS) calculations show a metallic behavior for all the stable surface structures, with the main contribution around the Fermi level coming from Cr-d orbitals. The effect of nitrogen vacancies is clearly observed with an increase in the metallic behavior in the structures having less nitrogen atoms.

[TSM-92] Theoretical study of hydrogen adsorption on graphyne doped with N and transition metal atoms: the quest for novel singles atom catalysts

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In this theoretical work, we present the results from Density Functional Theory (DFT) calculations on novel system formed by graphyne-γ (GY-γ) with defects and doped with N and transition metal atoms (M). Systems with vacancy defects present a widening on the band gap. We found that the properties of the GYM family may be tuned, from a semiconducting to a metallic character. This may be due to the presence of N atoms in acetylenic linkages. The adsorption of metallic atoms in the GY-substrates is very favorable for the Pt atom. The system with vacancy defects presents high values in the adsorption energy (-6.84 eV) of the Pt atom. All the M@GY-complexes shown to generate thermodynamically stable system with different electronic properties, which can be further confirmed by *ab initio* Molecular Dynamics simulations. The catalytic character of the series of Pt@GY-complexes under study was tested by assessing the capability to absorb the H_2 molecule on the M@GY-complexes (single atom catalysts). It was discovered that the Pt@GYN-β complex represent the model that was able to absorb the H_2 molecule (-0.80 eV) onto the surface, due to the modified electronic structure after the N and Pt-doping. The minimum energy path (MEP) was also studied, in order to find the energy barriers in the dissociation of H_2O molecule. Such M@GY complexes represent potential candidates to be implemented as catalysis in devices such as fuel cell materials. All calculations were made using the Quantum-Espresso 6.1 computer code.

Keywords: Density Functional Theory, Fuel Cells, Energy storage.

[TSM-120] NO2 and SO2 adsorption on Cu/ZnO(0001): DFT study

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Due to the importance in reducing environmental pollution, especially NO_2 and SO_2, we have studied the adsorption of these contaminants for their elimination in the atmosphere. We perform ab initio calculations of NO_2 and SO_2 adsorption on copper deposited on zinc oxide (0001) surface. The calculations were carried out by means of computational modeling using the Quantum ESPRESSO package that works within the framework of the Density Functional Theory (DFT). Ultrasoft pseudopotentials were used to model the electron-ion interaction. The exchange-correlation functional was treated by the generalized gradient approximation (GGA) with the parametrization of Perdew-Burke-Ernzerhof (PBE). We used an optimum value of K points of [551] and 50 Ry cutoff energy. Several sites were tested for the molecules adsorption. The electronic properties of the most stables configurations were calculated. The adsorption energies values show that chemisorption take place for both molecules.

Key words: Cu, DFT, NO_2, SO_2, ZnO.

[TSM-138] Effect of Bismuth in the interaction of water with SrTiO3(001)-2x2 surface, a DFT study

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Density functional theory (DFT) calculations were performed to investigate the effect of Bismuth (Bi) in the interaction of water molecules with $SrTiO_3$(001). We are interested in the interaction that take place on this material surface because, after adding Bi this material presents photocatalytic activity. We have proposed the study of $SrTiO_3$(001) surface, using a supercell with slab geometry. Other surfaces and adatoms remain as further work. We considered a surface periodicity of 2x2. A H_2O molecule per surface, per supercell is used, conserving the inversion symmetry. Then one Bismuth atom per surface was added without and with water molecules. The calculations were carried out using the PWscf code of the Quantum ESPRESSO Package. Adsorption energies for different configuration were calculated. Electronic properties were studied by calculating the density of states (DOS), projected density of states (PDOS), band structure, Löwdin charges and charge density maps. Results show different types of interactions between the molecule and the selected surface sites: chemisorption or physisorption.

[TSM-147] X-FEM numerical modeling of the c-Al0.66Ti0.33N-M2 system under normal mechanical contact.

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The interfacial fracture toughness and tribological behavior of TiAlN/Interface/M2 system was analyzed by instrumented nanoindentation, finite element method (FEM) and Extended Finite Element (XFEM). The numerical model is constituted by hard coating/interface/substrate and a Berkovich indenter. Substrate assumed is M2 tool steel and the interface was modeled using the cohesive zone model. The hardness and elastic modulus were measured for each system using instrumented nanoindentation and scratch test methods. Additionally, the interfacial fracture toughness was calculated using the two characterization techniques mentioned above.A fractographic analysis on the scratched and nanoindented specimens was made to validate the failure mechanisms observed numerically by scanning probe microscopy and scanning electron microscopy.

Keywords: Cohesive zones, Nanoindentation, XFEM, Interfacial fracture.

[TSM-462] Structural, electronic, and vibrational properties chiral nanotubes upon adsorption of chiral amino acids

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Chirality is one of the most interesting properties present in every physical or chemical system. A lot of work has been done to determine the chirality and analyze the properties of chiral objects, such as atomic clusters [1], organic molecules, and most recently carbon nanotubes, both theoretically and experimentally. The optical properties of Single-Walled carbon nanotubes have already been studied [2], thus enabling the study of chirality in those structures. In this work we study the enantioespecific adsorption of chiral amino acids on Single-Walled carbon nanotubes, taking advantage of previous chirality studies already conducted on metal nanoclusters and Single-Walled carbon nanotubes, and presenting their structural, electronic, and vibrational properties.

[1]. Jesús Pelayo, Robert L. Whetten, and Ignacio L. Garzón. “Geometric Quantification of Chirality in Ligand-Protected Metal Clusters”, J. Phys Chem. C, 2015, 119 (51), pp 28666-28678.

[2]. Ariadna Sánchez y Cecilia Noguez. “Understanding Optical Activity in Single-Walled Carbon Nanotubes from First-Principles Studies”, J. Phys. Chem. C, 2010, 114, pp 9640-9644.

THEORY AND SIMULATION OF MATERIALS (TSM) POSTER SESSIONS

[TSM-38] The bond force constants of carbon nanomaterials calculated by density functional theory

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After the discovery of C_{60}, the energetic stability of smaller fullerenes with outstanding physical properties have been proved. Among them, C_{60} and C_{20} are known to have the most regular cage geometry; their mechanical properties can have dependence with the dimension and geometry. The bond force constant of fullerenes and graphene are computed using density functional theory (DFT) with the generalized gradient approximation proposed by Perdew, Burke and Ernzerhof for the exchange-correlation potential. Here a self-consistent total energy method was implemented in the SIESTA code. DFT predicts dependence between bond force constants and structural conditions, indicating that the bond force constant can increase if the bond lengths and geometry change inside of carbon nanostructure. The bond force constant computed here can serve as an input to molecular mechanics or finite element codes of larger carbon molecules.

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[TSM-124] Initial stages of the aluminum nitride nanostructure formation on the GaN (111) surface

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Aluminum nanostructure formation on the gallium nitride (GaN (111)-(2x2)) surface has been investigated by first principles total energy calculations. Studies have been performed within the periodic density functional theory as implemented in PWscf code of the quantum espresso package. The electron-ion interactions have been modeled according to the pseudopotential approach and exchange-correlation energies are treated within the generalized gradient approximation according to Perdew-Burke-Erzenholf parameterization. The aluminum (Al) coverage varies from ¼ to 1 monolayer (ML). The Al adsorption on the surface takes place at high symmetry sites with T4 being the most stable geometry. The Al incorporation into the GaN atomic structures occurs by displacing the first layer Ga atoms, with Ga becoming the new adatom to be adsorbed on the surface at high symmetry sites having the T4-2 as the most favorable structure. Surface formation energies (SFE) are calculated, which indicate that the AlN bilayer formation on top of the surface is the most favorable structure. Moreover the Al chain on the Ga terminated surface may be formed with SFE energy value similar to that of the Al layer under a Ga layer. To explore electronic properties the density of states and projected density of states are calculated of the most favorable structures. At the Fermi level the density of states displays no energy gap indicating that surfaces are metallic.

[TSM-186] First principle calculations of structural and electronic properties of ZnO nanotubes

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One dimensional (1D) nanomaterials including nanotubes (NTs), nanowires, and nanorods have been attracting interest due to their electronic and mechanical properties that give them great potential for nanotechnology applications. Specially the structure-properties dependence related to chirality in these nanostructures is very important. Structural and electronic properties of zigzag and armchair single walled ZnO NTs have been studied by first-principles calculations. This study was performed using density functional theory (DFT) as implemented in the PWscf code of the Quantum ESPRESSO Package. The formation energies values suggest an increase in ZnO NTs stability with the increase of diameter. The structural results show a contraction in the relaxed nanotubes. As part of the electronic properties study DOS, PDOS and band structure were calculated. ZnO NTs PDOS show that most of the electronic states in the valence band are mainly composed of O-2p orbitals and in the conduction band are mainly composed of Zn-4s orbitals.

[TSM-187] DFT study of the CO2, NO2 and SO2 molecules on ZnO monolayer

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Two dimensional (2D) nanomaterials have unique physical and chemical properties. These properties give them great potential in catalytic, electronic, optoelectronic, high performance electrodes, nanocomposites, and sensors. 2D materials provide a large specific surface area for the adsorption of molecules, making them efficient in sensing applications and catalyst. Increasing the number of gas molecules adsorbed on the nanostructure leads to a strong improvement of the sensitivity, catalytic properties and pollutant remotion through adsorption. Zinc oxide (ZnO) is a semiconductor material with a wide bandgap of 3.37 eV. ZnO also has high sensitivity, chemical stability, and low cost. In this work we focus in the study of the adsorption of the molecules CO_2, NO_2 and SO_2 on ZnO(0001) 2D nanostructure, in order to find its possible potential as pollutant gases remotion. The calculations were performed in the density functional theory (DFT) framework as implemented in the PWscf code of the Quantum ESPRESSO Package. Adsorption energies, DOS, PDOS, band structures and charge density maps for CO_2, NO_2 and SO_2 molecules on different ZnO sites were calculated.

[TSM-249] Hydrogen chemisorption and repulsion energies on MgxZn1-x alloy (0.9 ≤ x ≤ 1.0) as a function of temperature (T= 0, 200, 400, 600, 700 K)

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In this work, the magnesium-zinc alloy was studied, when temperature is increased from 0 to 700 K, obtaining its chemisorption and repulsion energies for concentrations of magnesium x = 0.90, 0.92, ..., 1.0, applying Density Functional Theory (DFT). The procedure consisted in building a bulk crystal structure which is cleaved in the direction of the plane (110). Further, a supercell was built, to interact hydrogen molecules on his surface. Result of enthalpies are used to obtain the chemisorption and repulsion of hydrogen molecule on the surface of the metallic alloy as a function of Magnesium (Zinc) composition and for temperatures from 0 to 700 K. We used CASTEP and DMol3 modules, of the molecular simulation program Materials Studio 6.0 in our calculations.

[TSM-260] Unidirectional anomalous transmission of light beams through a photonic structure with anti-symmetric density of states

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In this paper the numerical simulation of a two-dimensional photonic crystal constituted by an array of GaAs bars immersed in air, describing a structure with square periodicity and asymmetries in the direction of the predetermined propagation occurs. This structure has an unidirectional anomalous transmission of incident electromagnetic waves in the plane of propagation, whose frequency falls within the limits of the border between the Visible-Near Infrared (Vis-NIR) range of the electromagnetic spectrum. This unusual phenomenon was attributed to diffraction effects produced particularly by the anti-symmetry of the structural features that define the photonic crystal, which determine an effective variation of refractive index along the predetermined direction of propagation with different effective refractive indices.

[TSM-283] Chemisorption energy of H2 molecule on MgxNi1-x ALLOY (0.9 ≤ x ≤ 1.0) as a function of temperature (T= 0, 200, 400, 600, 700 K)

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In this work, the magnesium-nickel alloy was studied, for concentrations of magnesium x = 0.90, 0.92, ..., 1.0, at different temperatures (T= 0, 200, 400, 600, 700 K) applying Density Functional Theory (DFT). We proceed with the building of a bulk crystal structure which is cleaved in the direction of the plane (110). Then we built a supercell in order to interact hydrogen molecules on his surface. We have calculated the enthalpy of formation of the alloys and these enthalpies are used to obtain the chemisorption and repulsion of hydrogen molecule on the surface of the metallic alloy as a function of Magnesium (nickel) composition and for temperatures from 0 to 700 K. We have used the modules CASTEP and DMol3 of the molecular simulation program Materials Studio.

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Keywords: Magnesium-nickel alloy, chemisorption energy, temperature dependence.

[TSM-360] New hard phases of AlN compound

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We report a new phases of aluminum nitride based on evolutionary search, using the Particle Swarm Optimization (PSO) algorithm coupled with ab initio calculations. Our results indicate that these phases are mechanically and dynamically stable at zero pressure based on Born-Huang and phonon criteria. For the new phases, we obtain a Vickers hardness of 19.71 GPa and 21.42 GPa and are comparable to wurtzite phase of AlN compound (18 GPa). In the case of hexagonal new phase, we proposed a possible synthesis route based in hydrostatic pressure. The mechanical and electronic properties of novel phases are discussed.

[TSM-388] Single carbon nanotubes for hydrogen storage. a dft study.

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In this work, we use the molecular simulation program Materials Studio, based on Density Functional Theory (DFT), in order to realize different simulations with carbon nanotubes with a single wall. We proceed with the building carbon nanotube with the papameters m=3 , n=6, and we optimized his structure to obtain his state of minimum energy. Then we does interacting with one, two or three hydrogen molecules on his surface, optimizing their structures again. We have obtained that hydrogen is adsorbed on the surface of the nanotubes, results that does this material attractive for hydrogen storage, such as is reported by different authors. In our calculations we have used Castep and DMol3 modules of our molecular simulation program.

[TSM-448] Direct to indirect band gap of heterostructure formed by MoS2/WSe2, a first principles study.

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Van der Waals heterostructures supply novel applications due to the combination of properties of different materials. In this work, the band gap of the heterostructure that is formed by MoS2/WSe2 is reported. We found that it can be controlled by using different rotation angles between the layers forming the heterostructure. The rotation angles for this heterostructure have been found to be 0° and 16.11°, due to these rotations an effort is induced between the layers due to the mismatch of crystal structures. The heterostructure with a rotation angle of 0° presents a direct band gap of 0.7 eV, while the heterostructure with a rotation angle of 16.11° presents an indirect band gap of 0.57 eV. Structural properties of material are also reported. For the calculations an energy cutoff was set to 200 Ry a DZP basis set, using Siesta package.

[TSM-474] Thermal conductivity in silicon nanowires: a theoretical study from first principles

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In this theoretical study we propose three silicon nanowires (SiNW's) of 0.7 *nm*, 1 *nm,* and 3 *nm* of diameter and 32, 68 and 416 atoms in its unit cell respectively, with hydrogen on the surface and growth in [111] plane direction. In the first part, It was calculated an optimal structure for every system, using Density Functional Theory as a basis, with an ultrasoft potential in SIESTA code, later applying Density Functional Perturbation Theory (DFTP), dynamical matrix and vibrational modes were computed for SiNW's. In the second part, the transmittance was calculated in channels, defined inside the SiNW's, via a transfer matrix. Finally, thermal conductivity was calculated for every channel in SiNW's, applying Landauer and Kubo Formalisms and Bose-Einstein Distribution Function.

Keywords: DFT, optimal structure, DFTP, Landauer Formalism, Distribution Function.

[TSM-510] Computational simulation of a hot filament CVD process for the deposit the SiOx films

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In this work is presented a two-dimensional CFD (computational Fluid Dynamics) analysis of a Hot Filament Chemical Vapor Deposition (HFCVD) process to produce nonstoichiometric silicon oxide films (SiO_x). These materials exhibit photoluminescent properties which are required in optoelectronic applications. The model solves the continuity, momentum, energy equations in steady state by means of a commercial software. Also, a thermodynamic equilibrium analysis of the SiO_2(s) + H_2(g) reaction was carried out to know the main chemical species in the system to the formation the SiO_x films by Factsage ®. We investigate the role of fluid and heat transfer from the filaments on the substrate temperature comparing with experimental measurements with a thermocouple. A two- dimensional model in 2D with ANSYS CFD was used to simulate the temperature distribution and flow process of the hydrogen. From the simulation results, the temperature and gas velocity profiles were obtained for different flow rates (25, 50, 75, 100 sccm) and source-substrate distances (5, 6 mm). The configuration of the outlet was found significantly affect the uniformity of the fluid in the deposition area. This outlet was modified to obtain a fluid flow uniform and a large area deposited, the results was confirmed by profilometer of the films.

[TSM-520] Genetic Algorithms and Particle Swarm Optimization tools for designing High Q Photonic Crystal Cavities.

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In the present work a compassion study of Genetic Algorithms (GA) and Particle Swarm Optimization (PSO) for design cavities in photonic crystals is reported. In particular the study was focus on the L3 defect cavity, which consists on triangular lattice of holes on dielectric slab with three holes filled along the ΓJ orientation of the lattice. Shifting the holes around the cavity and/or changing the size of the holes changes the Q-factor of the cavity, therefore the problem is reduced to find the optimal set of hole displacements and hole sizes that maximizes the Q-factor The space of configuration is explored by using the rules of GA and PSO, the Q-factor for each configuration is computed using FDTD. Finally, the configurations with the highest Q factors are reported as function of either the holes position and/or hole radius size for both algorithms.

[TSM-551] First principles calculation of TiO2 doped with manganese

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The heterogeneous photocatalysis using TiO2 is a technique of degradation of organic pollutants present in wastewater effluents. The process is based on adsorption of photons with energy higher than its band gap (3.2 eV for anatase phase), since when TiO2 is irradiated higher than its bandgap energy, excited high-energy states of electron and hole pairs are generated as a result of the promotion of an electron the valence to the conduction band. The electron and hole pairs induce oxidation reactions in organic compounds. On other hand, studies have found that nanoparticles have enhanced photoactivities over their bulk-phase counterparts. In addition, depositing or incorporating transition metal dopants into the titanium dioxide particles can influence on the performance of these photocatalysts. This affects the dynamics of electron-hole recombination and interfacial charge transfer. In this work?, we calculate the structural and electronic properties of pure anatase TiO2 and Mn doped and anatase TiO2 by using the density function theory (DFT). The results indicate that the lattice is distorted and the lattice constant is reduced due to doping.

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ORAL SESSIONS

[THF-44] Corrosion Resistance of WTiSiN-Ni coatings deposited via Co-sputtering

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In this work, WTiSiN films with different additions of nickel were deposited by co-sputtering magnetron on substrates of 316L stainless steel and Ti6Al4V alloy. The analysis of the elemental chemical composition and structure of the films were carried out by X-ray dispersive energy spectroscopy (EDS) and X-ray diffraction (XRD), respectively. The corrosion resistance was evaluated by potentiodynamic test in a 3.5% NaCl electrolyte (Tafel). The morphology of the corrosive area was characterized by scanning electron microscopy (SEM) and optical microscopy 3D. In general, the results show that the coatings deposited with Ni improved the corrosion resistance of the substrates. The corrosion mechanisms of the coatings produced as a function of the amount of Ni will be discussed in this paper.

KEY WORDS: Tafel, Corrosion, coatings WTiSiN, SEM, DRX.

[THF-53] Electric and optical characterization of nano-structured COATINGS OF Zr-Si-N, W-TI-Si-N, Al-Ti-Si-N with different nickel amounts

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In this work, three different thin films Nitrides were deposited on Silicon and Glass substrates using the co-sputtering physical Vapor Deposition Process (PVD) with gradual concentrations of Nickel as follows: ZrSiN, WTiSiN, AlTiSiN. The chemical constituents were identified using Energy Disperse X-ray Spectroscopy (EDS); in order to realize the achieved phases, a structural analysis was performed using X-Ray diffraction (DRX), the amorphous hopping conductivity was confirmed by the Four point probe (FPP) technique, their optical behavior was measured using Ultra Violet-Visible Spectroscopy (UV-VIS). The effect of Nickel was found to encourage electrical improvements for the bulk of the mentioned coatings, with some traits that sticked out for each subtrate.

[THF-63] Cyclic oxidation of YSZ coatings deposited by ultrasonic spray pyrolysis technique

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In order to improve the thermal and mechanical properties of superalloys materials, the study of coatings arises as an alternative to the development of new materials. This research studies zirconium oxide coatings stabilized with yttria (YSZ) grown by the ultrasonic spray pyrolysis technique at two deposition times: 15 and 30 minutes. The coatings obtained were characterized by x-ray diffraction, scanning electron microscopy and atomic force microscopy. Subsequently, they were exposed to cyclic oxidation at high temperature in static air at 600 °C, testing its resistance to corrosion by mass loss. At environmental conditions, the coatings showed a good corrosion resistance. The longer the deposition time, the better adhesion and homogeneity of the layer. However, under aggressive conditions, as those presented in the cyclic oxidation test, degradation of the coating was present in the first exposure cycles. Finally, a deterioration of the layer was observed with the exposure time and the test conditions according to the analysis of the SEM morphology.

[THF-69] The influence of silicon and silver content on electrical properties of ZrN-Si nanostructure thin films

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In this work, the ZrN thin films with different Si and Ag contents are deposited by reactive magnetron sputtering and the influences of Si and Ag content on electrical properties are analyzed. The chemical composition of the films are studied by energy disperse spectroscopy (EDS), the microstructure was analyzed via X-ray diffraction (XRD), and the morphology was determined by scanning electron microscopy (SEM); electrical properties were analyze by four-point probe. The results show that the ZrN films are nanostructured with a fcc structure, polycrystalline and with a morphology columnar. The electrical transport will be discus in this work.

[THF-146] Low magnetization in C-doped Mn5Ge3 thin films grown on Ge(001) at high temperatures

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C-doped Mn$_5$Ge$_3$ thin films were grown on Ge(001) substrates by magnetron sputtering using the solid phase epitaxy (SPE) process, which consists on Mn and C co-deposition at room temperature followed by thermal annealing at 750 °C. Scanning electron microscopy analysis show that the growth mode obeys to a Frank-van der Merwe growth mode consisting in a continuous coverage with homogeneous thickness allover the Ge(001) substrate. Atomic force microscopy analysis revealed a low surface roughness of 4 nm, which is an important characteristic for the elaboration of multilayer devices. The low magnetization of ~ 250 kA^{-1} is one o the most important requirements for faster and lower energy consumption switching of the magnetic orientation of magnetic thin films through the spin-transfer torque process. The Mn$_5$Ge$_3$C$_{0.6}$ thin films exhibit a high T_C of 430 K, larger than 296 K reported for undoped Mn$_5$Ge$_3$ thin films. These caracteristics make Ge(001)/Mn$_5$Ge$_3$C$_{0.6}$ heteroestructures a candidate for the fabrication of functional devices, in particular C-doped Mn$_5$Ge$_3$ can be used as an efficient spin inyector into the IV group semiconductors.

[THF-180] Metal sulfide thin films: Reaction strategy and study of their physical properties

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In this work, low cost and environmentally friendly chemical deposition approaches for the fabirication of binary, ternary and quaternary metal sulfide nanocrystal thin films have been discussed. In the case of solution-processed approach for the preparation of quaternary Cu_2ZnSnS_4 films, metal chlorides and thiourea can be used as precursor sources and dissolved in dimethylsulfoxide forming precursor ink. High quality CZTS films with almost 5 mm thickness have been prepared by drop casting method followed by a post-annealing step in inert atmosphere. Structural, optical and electrical properties of the CZTS films suggest a good prospective to be used in solar cell. Among binary sulfudes Sb_2S_3 and CuS films were prepared separately by chemical bath deposition by adjusting pH and bath temperature. While, the ternary $CuSbS_2$ films were successfully developed either by single chemical bath or by termal diffusion of multi-stack Sb_2S_3-CuS layers. In the case of multi-stack configuration, the relative thickness of each binary sulfide and annealing conditions play important roles in the formation of desired crystalline phase. In all the cases, structural and electrical properties were investigated thoroughly.

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[THF-190] Modeling of silicon oxide formation in the hysteresis cycle in reactive sputtering by the Co-Sputtering Simulation Reactive mode software

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One of the biggest problems in the coatings industry is the drop in the deposition rate in reactive sputtering. By increasing reactive gas flow to obtain the desired compound, a change in the voltage at the power supply is usually observed, resulting in a decrease in the deposition rate, compared to that of the "metallic" mode, as well as an increase in the system total pressure. This phenomenon is related to the "pumping or consumption" of the reactive gas in the system. In this work, we present the possible solutions to the drop of the deposition rate using a Si target and oxygen as reactive gas, taking into account the chemisorption of the oxygen ions on the racetrack surface.

The Co-Sputtering Simulation Reactive mode software, CO-SS Rm, was developed by the authors to simulate the distribution of the deposition thickness at the substrate of target material, oxides or nitrides as a result of reactive sputtering. The software works by analyzing the sputtering yield as a function of the reactive gas amount, in addition to providing the angular distribution of compound or metallic species ejected from the target. The experimental parameters of the reactive sputtering on a 2" diameter Si (99.99%) target were: constant supplied power of 50 Watts, working pressure at 6.8 mTorr, target-substrate distance 4.5 cm, Ar and O_2 mass flow rates at 10 sccm, and from 0.2 to 3.0 sccm correspondingly. All experiments had a constant deposition time of 30 min.

The simulations carried out with CO-SS Rm took into account the various phenomena that occur in the target in order to explain the thickness decrease of the films as a function of the amount of reactive gas. The sputtering of the target include the ejection of metal atoms and the formation and ejection of silicon oxide from the racetrack surface. Hence, different processes that account for changes in the deposition rate can be considered: the diminish of the racetrack area due to the formation of monolayers of oxide on the edges of the racetrack with emission of only metal atoms; the formation and emission of silicon oxide in the racetrack, which may have a different sputtering yield respect to the metallic target, usually smaller, and the mixture of these two phenomena. The simulations were compared with silicon and silicon oxide thin films thickness measurements by means of an Optical Profilometer, while the deposit was monitored with Optical Emission Spectroscopy, OES, analyzing the emission lines of silicon, argon and oxygen.

[THF-193] Effect of deposit parameters on the microstructure of Ti-Zr-Si-N nanostructured coatings deposited through co-sputtering

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In this work, the influence of substrate temperature and discharge power in the microstructure of Ti-Zr-Si-N nanostructured coatings on 316L and Ti6Al4V steel substrates was evaluated. The coatings were deposited by co-sputtering in an atmosphere of Ar, N, varying the temperature from 300 K to 530 K at discharge powers from 130 W to 170 W at the Ti_5Si_2 target. The structural characterization and residual stresses of the coating were performed by X-ray diffraction (XRD), the morphology by scanning electron microscopy (SEM) and the chemical composition by X-ray backscatter energy (EDS). The coatings produced presented the FCC phase with a mixed orientation in planes (111) and (200). The results showed that the size of the crystallite increased with the discharge temperature from 18 to 23 nm, the average deformation percentage was 3.26 nm. The Ti / Zr ratio increased with the increase in power from 3.08 / 0.17 to 15.46 / 30.10 in atomic concentration [wt%]. The effect of the varied reservoir parameters in this investigation on the microstructure and residual stresses will be discussed in this paper.

[THF-196] Insight into structure character and electrochemical corrosion resistance of TiZrN coatings magnetron co-sputtered from both Ti and Zr targets

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TiZrN coatings were grown by magnetron co-sputtering in a dual-target facility, and their structure and electrochemical corrosion resistance were assessed. Ti and Zr contents were changed from pure TiN to pure ZrN by varying the current applied to a Ti and a Zr target. Complete Ti and Zr miscibility was observed, obtaining coatings with a single face-centered cubic (FCC) structure and lattice constant going from a=0.4230 nm (TiN) to a=0.4578 nm (ZrN) as the relative Ti to Zr content varied from fully Ti to fully Zr. The lattice constant parameter varied linearly with either Ti or Zr concentration. In the Ti-rich alloys, grazing incidence x-ray diffraction showed changes in the prevalent reflections when the grazing angle varied from 1° to 4°. On the other hand, invariable XRD patterns were observed in the Zr-rich alloys when that grazing angle varied from 1° to 4°. We attributed that to through-thickness changes of the crystallographic preferential growth direction of the crystals in Ti-rich coatings. TiN coatings displayed coarse trigonal pyramidal facets. TiZrN coatings rich in Ti displayed a morphology with very refined pyramids dispersed onto the faces of coarse pyramids, resembling a dendritic-like structure. ZrN and Zr-rich coatings displayed homogeneous rounded-tip facets. All the coatings displayed through-thickness columnar structures. According to the equivalent circuit, appraised in the tests of electrochemical impedance spectroscopy, sputtered coatings displayed assorted corrosion resistance. Some of them displayed corrosion resistance similar to that of the bulk UNS S31603 stainless steel (used as reference). The sample with the best performance in that electrochemical impedance test had a Ti/Zr ratio of 4. Although the corrosion resistance displayed a non-monotonous relationship with either Ti or Zr alloy-content, as a rule Ti-rich coating displayed improved corrosion resistance while Zr-rich coatings displayed impaired corrosion resistance. Although that electrochemical corrosion performance was a straightforward result of the Ti/Zr ratio, the potential effects of both coating's morphology and crystallite size on corrosion resistance are emphasized. Those coating's structural parameters were related to growth rate and current applied to the targets.

[THF-238] Fabrication of Tin Oxide-Antimony (ATO) thin Films by Sol-Gel/Spin-Coating

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Antimony doped tin oxide (ATO) thin films were prepared on silica glass by sol-gel/spin coating technique. The crystalline structure of tetragonal phase was observed by XRD analysis for films with 0 – 15 % Sb dopant. Transmittance between (80-90 %) were obtained for all films by UV-Vis analysis. The transmittance spectra were used to calculate the band-gap by Tauc method; the band gap calculated was 4.0 – 3.8 eV for films treated at 300–600°C, while the thermal treatment temperature increases the band gap decreases. In a semiquantitative EDS evaluation can be observed that the % Sb real increases with the temperature. Thus, there is a maximum dopant efficiency between 400-600°C. Moreover, higher temperatures promote better crystalline quality.

[THF-247] SILAR deposition of Cu2ZnSnS4 thin films: Effects of solvent composition

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The quaternary sulfide Cu_2ZnSnS_4 (CZTS) has been studied as absorber layer in thin film solar cells, due to its band gap energy, as well as large absorption coefficient, which are ideal for highly efficient solar energy conversion devices. Successive Ionic Layer Adsorption and Reaction (SILAR) is a wet chemistry technique with a lot of potential for multi-element compounds, since the reactions can be controlled in a way similar to Atomic Layer Deposition (ALD) technique. Different volumetric percentages of methanol in water were employed in order to determine the best deposition performance. Samples were characterized by X ray diffraction, scanning electron microscopy and Raman spectroscopy. The results showed that composition of the solvent played an important role on the formation of the film, as well as the incorporation of the elements. Furthermore, manipulation of solvent composition, along with other deposition conditions, allowed to obtain the direct deposition of CZTS.

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[THF-255] Deposition of NiO thin films for Applications in Electrochromic Devices

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Electronics is nowadays one of the most prominent industries in the world. Its success is due to countless technological developments that took place for the past 70 years. Still, there is an infinite number of challenges that this field is facing. One of this is the development of electrochromic devices whose applications expand from helmet visors to smart windows. These devices are based on the electrochromic effect which consists on the change of optical properties of materials upon the application of an electric field. The devices are composed of two transparent conductors on the external sides, two electrodes (anode and cathode) and one electrolyte in the middle of these, forming a sandwich arrangement. So far, these devices have not been commercialized due to several problems. For instance, the life span of these devices is, on average, 10 years which is relatively short. Another problem is that fabrication methodologies are relatively expensive. It is therefore necessary to find solutions to these problems using economic and effective materials.

Herein we discuss the fabrication of NiO thin films as cathodic electrode for electrochromic devices. In this research we grew NiO films on Si(111) substrates by rf magnetron sputtering technique and studied the effect of annealing temperature (25 ^{o}C-400 ^{o}C) on the crystalline and physical properties of the samples. The morphology was studied by scanning electron microscopy (SEM). Crystalline properties were determined by X-ray diffraction and the electrical properties were measured by the four-lead technique. We found that the higher the annealing temperature the higher the crystallinity. The morphology was granular and particle size increased as the annealing temperature was increased. Further, the current-voltage characteristics were affected by the annealing temperature. Finally, we discuss how the annealing temperature can affect the electrochromic properties of NiO electrodes if one wishes to apply this material in electrochromic devices.

[THF-329] Low temperature processing of Al2O3-GPTMS-PMMA hybrid films with applications to high-performance ZnO thin-film transistors.

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In this work we explore the synthesis of inorganic-organic Al_2O_3-GPTMS-PMMA hybrid films by a low temperature sol-gel process. The hybrid films were deposited by dip coating process and then annealed at as low as 150 ^{0} C in air. The analysis of the hybrid films was performed by UV-VIS spectroscopy, FTIR, AFM, SEM, C-V and I-V measurements. The high optical transparency and homogeneity of the hybrid films support the proper link between inorganic and organic phases with strong bonds. At microscopic level, the hybrid films have uniform, flat and smooth surface with surface roughness lower than 1 nm. The C-V and I-V measurements performed on MIM structures showed low leakage current density of the order of 10^{-7} A/cm^2 at -5 MV/cm electric field and capacitance and dielectric constant measured at 1 kHz of 20.4 pF/cm^2 and of 6.2, respectively. These thin films were applied as dielectric gate layer for room temperature sputtered (r.f) ZnO thin film transistors (TFTs) successfully. The device structure was completed with bottom gate and aluminium top contacts. From the analysis of transference curves of the TFTs with good electrical performance such as mobility 4.3 cm^2/Vs, very low threshold voltage of 1.3 V and high I_{on}/I_{off} current ratio of 10^7, at low operating voltage under 8V.

[THF-330] Fully Solution Processed CdS Thin-film Transistors with SiO2-PVP and TiO2-PVP Hybrid Gate Dielectric Layers

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A simple solution-based CdS thin-film transistors (TFTs) fabricated with inorganic-organic hybrid gate dielectrics at low temperature (200 ^{0}C). The hybrid gate dielectrics are composed of SiO_2-PVP and TiO_2-PVP and were deposited by sol-gel spin coating technique. The resultant hybrid gate dielectrics exhibited homogeneous and smooth surface morphology with very low surface RMS roughness (0.27 & 0.51 nm), excellent dielectrical properties such as low leakage current density 10^{-6} A/cm^2, good capacitance and dielectric constants of both gate dielectrics 4.8 and 4.6 at 1kHz, respectively. Furthermore, to investigate the electrical properties of the both hybrid dielectrics CdS-based TFTs were fabricated by bottom gate and top contacts configuration. The SiO_2-PVP hybrid dielectric-gated CdS TFT shows a good saturation field effect mobility of 18 Cm^2/Vs, low threshold voltage of 0.6V, low sub threshold swing of 0.25 V/dec and on/off current ratio of 10^4. On the other hand, the TiO_2-PVP -gated CdS TFTs also performed good electrical response such as 0.45 Cm^2/Vs field effect mobility, threshold voltage of 1.9 V, subthreshold swing of 1.25 V/dec and on/off current ratio 10^4 respectively.

Key words: Solution process, hybrid dielectrics, CdS, TFTs, low-temperature.

[THF-333] Effect of silicon content in microstructure of CrTiAlSiN coatings deposited by co-sputtering tecnique

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The aim of this work is the deposition and characterisation of novel CrTiAlSiN films with 4 different Si contents deposited on K20 tungsten carbide using co-sputtering method, CrTiAlN was used as reference. These coatings shows high wear resistance properties at high temperatures.

Silicon contents were obtained varying radio frequency power supply on silicon target. Morphology, semiquantitative chemical composition, microstructure and phase analysis were investigated by scanning electron microscope (SEM), energy disperse spectroscopy (EDS), X-ray diffraction (XRD), respectively. In general, all the coatings showed grains with columnar growth that tended to enlarge away from hard metal interface. Main results shows that introduction of silicon refine microstructure which is evident by grain size reduction and SEM observations.

No changes in crystallography phases in both coatings and all the analysed nitrides showed B1 NaCl crystal structure. The parameter modification observed in every case is compatible with the silicon dissolution in the cubic lattice. The crystallite size and the microstrain gradients have been obtained from the diffraction peaks broadening.

[THF-346] Mixed Metal Oxide Hybrid Gate Dielectric for High Performance In2O3 Thin-film Transistors by fully Solution-process at Low-Temperature

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More recently, fully solution processed thin-film transistors (TFTs) have attracted considerable interest owing to their low processing temperature, low-cost, large area deposition and they are potential alternatives to the current expensive vacuum-based techniques. In this work, we explored a novel mixed metal oxide hybrid gate dielectric material, $ZrHfO_2$-PMMA. The hybrid gate dielectric prepared by sol-gel method and fabricated by simple spin coating process at very low temperature (< 200 ^oC) then simultaneously followed by UV-ozone treatment for 10 min. The obtained 90-nm thick hybrid gate dielectric performs excellent electrical properties such as a low gate leakage current density (10^{-9} A/cm^2) with high gate capacitance (84 nF /cm^2) and dielectric constant (8.5) at 1 kHz respectively. In addition, the surface properties (surface roughness, hydrophobicity and surface energy) of the hybrid dielectric thin film improved by UV ozone treatment and it allowed to favourable growth of semiconductor on the hybrid gate dielectric. In order to understand the electronic properties of these hybrid dielectric films, we demonstrated them transistor applications. The bottom gate TFTs are fabricated with solution processed In_2O_3 as channel layer on top of the $ZrHfO_2$-PMMA hybrid dielectric and the resulted In_2O_3 TFT displayed high field effect saturation mobility 12.3 cm^2/V.s, low threshold voltage 1.1V, large current I_{on}/I_{off} ratio 10^6 and subthreshold slope 0.78 V/dec with an operating voltage of under 8V. This hysteresis free solution processed In_2O_3 TFT device performance is promising for future low cost flexible electronic devices.

Key words: $ZrHfO_2$-PMMA, In_2O_3, solution process, low temperature.

[THF-554] Using and interpreting core and valence band XPS for the study of material surfaces including the identification of subtle differences in surface chemistry

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The use of core and valence band X-ray photoelectron spectroscopy (XPS) for the study of material surfaces will be discussed with a focus on the methods for interpreting the data using suitable data analysis methods and calculations. Valence band XPS gives spectral features (peak positions and peak intensities) that arise from different physical principles than the core spectral region. This difference leads to the valence band region providing complimentary information to that of the core region. In many cases the valence band region can be used to detect subtle chemical differences that cannot be determined in core XPS studies. Methods for data interpretation will include a discussion of curve fitting in the core region and calculation methods in the core and valence band region. In both regions the role of the true Voigt function will be illustrated. Examples of these approaches to various systems will be discussed including the formation and study of thin (less than 100C) oxide-free phosphate films, polymer films, composite surfaces, and the identification of different oxide films (including aluminum oxides) with similar chemical composition.

THIN FILMS
(THF)
POSTER SESSIONS

[THF-18] Piezoelectric properties of polycrystalline Bi-Fe-O thin films

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Bismuth ferrite, $BiFeO_3$, is a multiferroic material widely studied for scientific and technological applications. In this work, polycrystalline thin films of the Bi-Fe-O (BFO) system with different bismuth content were deposited on indium-tin-oxide bottom electrodes using the combination of two ablation plasmas in order to correlate microstructure and ferroelectric properties. The microstructure was studied by Raman spectroscopy and X-ray diffraction. The domain structure was analyzed with piezorespose force microscopy (PFM) at the tip-sample contact resonance frequency. Switching PFM measurements were performed with the purpose to evaluate the domain reversal of the ferroelectric material, inverting the direction of the intrinsic polarization vector to obtain PFM hysteresis loops. The importance of this study is that permits to quantify the required voltage (coercive bias) that is necessary to achieve inversion in the ferroelectric material. Switching work, d_{33} coefficient, and domain stability were deduced from the hysteresis loops. Results are discussed in terms of the ferroelectric domain size and bismuth content.

[THF-25] Behavior of Ti-Zr-Si-N thin films obtained by the co-sputtering technique subjected to thermal fatigue.

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Thin films of Ti-Zr-Si-N were deposited on Ti6Al4V and stainless Steel 316L substrates using the co-sputtering reactive technique. Thermal fatigue studies were conducted in an oven in a dry environment with a total of 300 cycles, each cycle consisting of 60 minutes of cooling, 60 minutes of heating and 12 minutes of stabilization, with a temperature of 600 ° C. The behavior of the coatings of Ti-Zr-Si-N and the substrates was analyzed in relation to the temperature changes to which they were subjected and to the formation of oxides caused by the corrosive environment; It was analyzed with techniques such as: confocal laser microscopy, scanning electron microscopy, X-ray diffraction and Mossbauer spectroscopy.

[THF-39] Electrochemical and opitcal properties of bismuth based thin films syntesized by unbalanced magnetron sputtering technique

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Bismuth based compounds are good candidates to develop technologies in several fields of the materials science. Numerous production methods have been reported in literature to produce bismuth based thin films (pulsed laser deposition, radiofrequency sputtering, sol gel and metalorganic chemical vapor deposition) but not much on Unbalanced Magnetron Sputtering (UBM) in function of the parameters involved in the growth process. In this study, bismuth based thin films were grown by UBM varying the power supplied to the target and the gases mixture flux, over AISI 316L Stainless Steel and glass substrates. The microstructure of the films was analyzed by means of X-Ray diffraction and the results showed that only metallic bismuth was present in crystalline form and no evidence of compounds was found. By scanning electron microscopy the surface showed some like droplets morphologies of pure bismuth and its distribution was dependent of the growth conditions. Using ion beam techniques, the chemical composition of the films was studied finding the presence of oxygen in the films, this suggest that bismuth oxide grown in amorphous phase. The behavior of the films against corrosion processes was analyzed by electrochemical techniques. The films does not represent a high protection to the substrate itself. The optical properties were greatly influenced by the deposition conditions as revealed by UV-Vis-NIR spectroscopy. The growth conditions in the UBM sputtering technique influences the physical and chemical properties of the thin films produced.

[THF-41] Tribological properties of stainless steel coatings with silver deposited by sputtering

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The tribological properties of stainless steel coatings deposited with different silver contents by unbalanced magnetron sputtering were studied. The structure of the coatings was characterized by means of X-ray diffraction, the morphology and chemical composition were evaluated by means of scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS), respectively. The wear resistance was determined through pin on disk tests, the wear rate and coefficient of friction (COF) were determined. It was determined that the coatings deposited in inert atmosphere presented BCC structure, while the coatings deposited in the reactive atmosphere shows the BCC and FCC phases. A compact morphology was observed in coatings with a higher silver content. Also, the COF decreased with the increase of silver in the coatings deposited in the presence of nitrogen, while in an inert atmosphere the COF value increased. The wear rate was higher for the coatings with high percentages of silver, however, lower values were found for coatings deposited in the presence of nitrogen. Wear mechanism of coating deposited is discussed in this work.

Keywords: Silver, wear, stainless coatings, sputtering,

[THF-42] Optical and electrical properties of TiAlCrN thin films deposited by reactive magnetron sputtering.

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Thin films of Ti-Al-Cr-N have been synthesized onto a glass and silicon substrates by reactive magnetron sputtering of pure Cr and TiAl alloy targets. This investigation was carried out changing the Cr-target power in order control the Cr amounts in the films. The surface morphology and phase structure of the films were investigated by scanning electronic microscope (SEM) and X-ray diffraction (XRD) respectively. The electrical resistivity was measured by the four-point probe method and their optical properties were characterized by ultraviolet/visible (UV/Vis) spectroscopy. Effects of chromium content on the optical and electrical properties of TiAlCrN coatings are discussed in this work.

KEYWORD: Reactive magnetron sputtering, TiAlCrN, optical properties, resistivity

[THF-43] Nanostructured coatings of bcc and fcc stainless steels deposited by sputtering

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Due to the current demand for stainless steels and search for new materials with better properties, in this work has been deposited stainless steel films by magnetron sputtering on 316L stainless steel substrates with different Ni amounts. The thin films were deposited with a nitrogen and argon atmosphere in order to obtain FCC structure. The chemical composition analysis was performed using Energy-dispersive X-ray spectroscopy (EDS) and structural analysis was performed by X-ray diffraction (XRD). The corrosion resistance was evaluated by potenciodinamic test in a 3.5% NaCl electrolyte. The morphology of the corrosive area was characterized by scanning electron microscopy (SEM) and microscopy 3D. Overall, the results show that the coatings deposited with nitrogen atmosphere improved the corrosion resistance of the substrate. The corrosion mechanisms of the coatings produced in function of the nickel amount discussed in this work.

KEYWORD: EDS, Corrosion, stainless steel coatings, SEM.

[THF-52] Maching of VC and Nb coatings deposited via TRD

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In this work was deposited vanadium carbide (VC) and niobium carbide (NbC) coatings by thermo-reactive deposition/diffusion (TRD) on tool steel substrates. The chemical composition analysis was performed using Energy-dispersive X-ray spectroscopy (EDS) and structural analysis was performed by X-ray diffraction (XRD). The mechanical properties was evaluated by microhardness test. The morphology of the layer was characterized by scanning electron microscopy. Overall, the results show that the coatings deposited improved the durability of the substrate. The influence cutting speed, feed rate and depth of cut on various machinability characteristics be discussed in this work.

[THF-59] Study of the mechanical properties of cubic GaN grown by PAMBE

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The use of III-Nitrides semiconductors in optoelectronic and electronic devices is having a great impact at the present, the GaN semiconductor in cubic phase is one of the most important for which it seeks to improve its properties as crystal quality, strength, and durability. Using α-GaN and α-InGaN (hexagonal phase) it was possible to build a blue light emitting diode (LED).[1] In this work, by means of the PAMBE (Plasma Assisted Molecular Beam Epitaxy) technique, thin films of the GaN semiconductor were grown on MgO substrates (100).[2] The XRD results shown a dominant diffraction peak for the (002) plane of the Zinc-blended structure of GaN, and atomic force microscopy shows a mosaic morphology associated with the cubic crystalline structure. By means of the Nanoindentation technique, with a Berkovich type diamond tip operated with the continuous contact stiffness measurements (CSM) method, load-displacement curves were obtained. These curves were analyzed using the method proposed by Oliver-Pharr[3] to obtain the Hardness and Young's Modulus, which is the main interest of this research because these mechanical properties have not been studied experimentally for β-GaN (cubic phase). Elastic-plastic transition phenomena were observed in only a range of depth of the load-displacement curve during loading, these transitions are mainly due to dislocations nucleation. The values obtained from the hardness and Young's modulus were 21.1 ± 3.1 GPa and 310 ± 28.7 GPa, respectively.

Keywords: Nanoindentation, PA-MBE, Hardness, Elasticity, Gallium nitride.

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[THF-67] Corrosion resistance of graphene deposited by thermal chemical vapour deposition

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In this work was studied the influence of corrosive electrolyte on corrosion mechanisms of graphene films deposited on copper by mean of thermal chemical vapour deposition. The structure of films were analyzed by RAMAN spectroscopy and the morphology throughout optical microscopy. Corrosion resistance was evaluated by electrochemical impedance spectrocopy and potenciodinamic polarization using electrolytes of 0.5M HCl , 0,5M H2SO4 , 3,5% NaCl, 3,5% NaCl +0,5M H2SO4, Na2S2O3 (10-4mol/l) + 5%NaCl and 0,5% CH3COOH. The morphology of the corrosion track was characterized by scanning electron microscopy (SEM), atomico force microscopy (AFM) and RAMAN espectroscopy. The degradation mechanisms of the graphene produced in function of electrolyte will be discussed in this work.

[THF-70] Effect the Al and Ag dopants on the microstructure of AISI 316L-YSZ system deposited via rf-sputtering

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In this work, we present the results obtained in the deposit of nanostructured coatings of zirconium stabilized with Yttria (YSZ) and doped with aluminum, silver and aluminum plus silver. The coatings were grown from YSZ ceramic target of covered symmetrically with metallic pieces (Al, Ag) on AISI 316L steel substrates, via RF-sputtering technique. The morphology was determined by scanning electron microscopy (SEM) and the microstructure of the coatings was characterized by X-ray diffraction (XRD); the chemical composition was made through X-ray dispersive energy (EDX) analysis. The XRD analysis shows that the coatings have peaks belonging to the dopant elements, and oxides such as the Al_2O_3.

[THF-86] Characterization and synthesis of MoS2 thin-films by pulsed laser deposition controlling the mean kinetic energy of the plasma

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In recent years, molybdenum disulfide (MoS_2) has become a material of great interest for research in material science. Due to its 2-dimentional graphene-like structure and its band gap within the visible spectrum, many possible applications for electronic and optoelectronic devices could arise. In this work, thin-films of MoS_2 were deposited using Pulsed Laser Deposition (PLD) on glass substrates at room temperature and deposition pressure of $2x10^{-5}$ Torr. We used a MoS_2 target obtained by compressing high purity powders and a Nd-YAG pulsed laser with wavelength of 1064 nm. Plasmas were diagnosed by means of the time of flight technique using a Langmuir planar probe; the voltage across a 20 Ohm resistance was measured and the current was calculated in order to estimate the ion density and its Mean Kinetic Energy (MKE). The crystalline properties of the deposits were characterized using Raman spectroscopy and X-Ray Diffraction (XRD) and their optical properties by Visible-Ultraviolet (Uv-Vis) spectroscopy. Their chemical composition and stoichiometry were measured and estimated by X-ray Photoelectron Spectroscopy (XPS) and Energy Dispersion Spectroscopy (EDS) and their thickness and morphology were characterized using Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). It was observed that the crystallinity was influenced by the MKE of the plasma, having better crystallinity, bigger mean crystal size and higher thickness as MKE decreases.

[THF-104] Growth and Characterization of SmFeAsO1-xFx Films by MOCVD and Arsenic Diffusion Processes

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We report the growth of superconducting $SmFeAsO_{1-x}F_x$ thin films on CaF_2 substrates by a two-step process: 1) grown of Sm-Fe precursor films by Metal-Organic Chemical Vapor Deposition (MOCVD) and, 2) arsenic diffusion process employing a $SmFeAsO_{0.4}F_{0.2}$ pellet. The pellet is annealed in presence of the precursor films at different temperatures: 950, 980 and 1000 ^{o}C. The atomic concentration was found by Energy Dispersive Spectroscopy (EDS) for each sample, and with X-ray diffraction (XRD) crystalline phases of the samples were observed for the different annealing process. The Scanning Electron Microscopy (SEM) shows the thin film´s morphology and the resistance as a function of the temperature was obtained by the four-probe method. The Analysis show that for an annealing at 980 °C during 2 hrs it is possible to obtain a good phase of $SmFeAsO_{1-x}F_x$ and the superconducting transition occurs at ~56 K.

[THF-109] Optical properties of ZrSiN-Ag coatings deposited via DC magnetron sputtering

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ZrSiN-Ag coatings were deposited via DC magnetron sputtering in reactive phase, in order to study the effect of addiction of silver on the optical properties of ZrSiN films. The structure of the films was characterize by X-ray diffraction (XRD) and high resolution–transmission electron microscopy (HRTEM) and the morphology by scanning electron microscopy (SEM). The optical properties were characterize by UV-VIS spectroscopy and ellipsometry. The XRD results showed that nanostructured ZrSiN-Ag coatings were obtained. The ZrN film exhibited a face-centered cubic (fcc) phase with columnar structure while that the Zr-Si-N films showed a mixture of fcc and amorphous phases without columnar structure, similar to the ZrSiN-Ag films. The results of SEM showed the presence of nanoparticles of silver on the surface of the ZrSiN-Ag coatings due to the out-diffusion of silver to the surface of the coatings. The results of the optical properties showed that from 900 to 2400 nm the ZrN film has a high reflectance (74.33%) and when the silicon is added to ZrN coating the reflectance decreased (14.01%). When silver is added, the reflectance increased at 21.29% with an Ag content of 6 at. %. Additionally, the reflectance results showed the possibility of having a pattern of interference type Fabryt-Perot with the addition of silver to ZrSiN coating.

[THF-115] Tribological properties of CuxAly multilayer deposited by cosputtering

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In this work was studied the influence of Al content on wear mechanisms of Cu-Al multilayers deposited by magnetron sputtering on phosphor bronze. The chemical composition analysis was performed using energy-dispersive X-ray spectroscopy (EDS), structural analysis was performed by X-ray diffraction (XRD) and the hardness through out nanoindenter. The adhesive wear resistance and friction coefficient was evaluated by the ball-on disc test using ball of stainless steel, aluminum and zirconia. Overall, the results show that the multilayers deposited with nitrogen atmosphere improved the wear resistance of the substrate and that the wear mechanisms are produced by plastic deformation, adhesion and oxidation. The wear mechanisms of the multilayers produced in function of Al content will be discussed in this work.

KEYWORD: Wear, CuxAly multilayer, EDS, SEM, wear.

[THF-116] Effect of the Ni addition in the mechanical properties of Zr-Si-Ti-N thin films deposited by co-sputtering

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In the present work, the influence of nickel content on the structural and mechanical properties of the ZrSiTiN films was investigated. The nanostructured ZrSiTiN thin films with nickel additions were deposited onto steel AISI 4340 and AISI H13 substrates using the reactive magnetron co-sputtering technique. The structure was analyzed by x-ray diffraction and the chemical composition was identified by energy dispersive x-ray spectroscopy (EDS). The mechanical properties were studied by measurement of hardness and elastic modulus, using nanoindentation test. Nickel changed the structure of the coating from crystalline to amorphous and can improve the mechanical properties of this films due to hardening mechanisms by solid solution and the formation of a nanocomposite structure.

KEYWORD: Hardness, ZrSiTiN, EDS, nickel.

[THF-131] Diffusion of As in thin films of ZnO: N, ZnO: Ag and ZnO: Ag, N.

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In this paper we present the study on the diffusion of As in films of ZnO: N, ZnO: Ag and ZnO: Ag, N type p as a function of the post-deposit heat treatment temperature and its influence on the electrical properties, optical and structural thin films. These films were deposited by the DC co-sputtering technique from metallic targets of Zn and Ag in an atmosphere of Ar / N_2 / O_2 on substrates of Si, GaAs, and glass at room temperature. After the deposit, said films were subjected to thermal treatment at 100° C, 200° C, 300° C and 400° C, in a controlled pressure atmosphere. Finally, the films were characterized to obtain their structural, optical, and electrical properties and to find the dependence and correlation between them and the diffusion of the arsenic generated by the temperature of thermal treatment.

[THF-133] Growth and characterization of thin films of hydroxyapatite (HAp) by laser ablation technique.

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Nowadays study and innovation in biocompatible, low cost materials is very important for the medical industry. Hydroxyapatite (HAp) is a ceramic bioactive material that bears a strong resemblance to the mineral composition of natural bone, which is why it is one of the most important materials in the manufacture of prostheses and implants. In the present work, we manufacture HAp from recycled organic materials. The obtained HAp was used to deposit thin films by the method of laser ablation on substrates of Si, to then characterize them. X-ray diffracction (XRD) and X-ray scattering spectroscopy (EDS) were used for tha analysis of the microstructure and composition of the films. Surperficial morphology was analyzed with Scanning Electron Microscopy (SEM).

[THF-140] Effect of silver on electrical and optical properties of ZnO:Al/Ag/ZnO:Al thin films

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Transparent conductive oxide (TCOs) are materials that have recently been extensively investigated due to their unique properties, such as high transmittance in the visible range, low resistivity and high electrical conductivity, as a promising candidate for substitute the widely used Indium Tin Oxide (ITO) for electrodes in solar cell application and optoelectronic devices. In this study, thin films with ZnO:Al/Ag/ZnO:Al multilayer structure was deposited on glass substrates at 50 °C with different deposition times of the Ag layer by radio frequency (RF) and pulsed DC magnetron sputtering systems. The study consider the effects of deposition times of the Ag layer on the optical, electrical and structural properties of the multilayers thin films. The results indicated that thin films post deposition treatment at 300 °C for one hour improve their properties, the highest average transmittance achieved in the 400-800 nm range was 89%, the values of resistivity and conductivity improve were of the order of 10^{-4} Ω cm and 10^{3} $\Omega^{-1}cm^{-1}$. Finally, the X-ray diffraction patterns showed that as the Ag deposition time increases, the presence of the Ag (111) orientation plane is observed while the preferred orientation for the ZnO:Al is (002).

[THF-148] Effect of bias voltage on the microstructure and corrosion resistance of CrxN monolayers obtained by Arc-PVD

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Chromium nitride (CrN) films were deposited on M2 steel by arc-PVD at graded/constant bias voltages (-40 V, -80 V and -40/60/80 V). The effect of this variable in the microstructure (size grain and surface defects) of the film was studied. Corrosion resistance and the mechanical behavior was related with the modification of the microstructure. The corrosion resistance was evaluated using electrochemical impedance spectroscopy (EIS) and potentiodynamic curves (Tafel); mechanical properties by instrumented nanoindentation and scratch. It was found that the bias voltage variation affects the corrosion behavior due to the presence of defects. The formation of defects (open voids, droplets) also affects the mechanisms of failure by increasing the amount of spallation. Higher voltage increases the hardness and the modulus of elasticity due to the higher densification of the coating.

[THF-179] Evolution of crystalline phases of CuxSb1-xS2 system by thermal diffusion of chemically deposited Sb2S3-CuS multi-layers and their electrical properties

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Copper based chalcogenide ternary compounds are promising material to be used as absorber material in solar cells. In this work we explore the Cu-Sb-S system by thermal diffusion of chemical bath deposited (CBD) binary stacks of Sb_2S_3 and CuS films. The multi-stack structure was developed by double chemical bath deposited Sb_2S_3 layer of ~ 800 nm thickness followed by deposition of single CuS layer on prefabricated Sb_2S_3 film. The thickness of Sb_2S_3 layer was kept constant, while the thickness of CuS layer was varied by changing bath temperature: 40°C and room temperature (RT□24°C). For T=40°C the deposition time was 15 min and 60 min and for RT the deposition time was varied from 1h to 8h in 1 h interval. The multi-stacks of Sb_2S_3-CuS were annealed at 350°C for 30 min in N_2 atmosphere. The heat treated films were characterized by several techniques such as XRD, Raman spectroscopy, UV-visible spectroscopy, AFM, SEM and Hall effect measurements to evaluate their structural, optical and electrical properties. The formation of pure chalcostibite phase ($CuSbS_2$) as well as a mixture of famatinite (Cu_3SbS_4), tetrahedrite ($Cu_{12}Sb_4S_{13}$) and senarmonite phases (Sb_2O_3) were detected depending on the thickness ratio between Sb_2S_3 and CuS. The microstructure was studied by AFM. This showed that the surface structure became denser and homogeneous with the increment of CuS thickness. All the films showed p-type electrical conductivity. The films composed of $CuSbS_2$ exhibited a carrier concentration: 3.12×10^{17} cm^{-3}, mobility: 3.82 cm^2/Vs and resistivity: 5.22 Ωcm. On the other hand, the films composed of a mixture of $Cu_{12}Sb_4S_{13}$, Cu_3SbS_4 and Sb_2O_3 revealed that with the increase in Cu content in $Cu_xSb_{1-x}S_2$ films, the mobility was increased from 0 to 25 cm^2/Vs. On the other hand, the resistivity values were decreased from 6.23 Ωcm to 1.07 Ωcm along with the carrier concentration values from 1.34×10^{19} cm^{-3} to 2.25×10^{17} cm^{-3}. For its electrical, optical and structural properties, the films studied in this work can be used as an absorber material in a thin film solar cell.

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[THF-181] Development of Cu2ZnSnS4 films from a non-toxic soluble precrsor ink and their characterization

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In this work, we have reported a facile and cost effective way to deposit kesterite Cu_2ZnSnS_4 (CZTS) layer using a non-toxic precursor ink by drop casting method. A subsequent thermal treatment step was employed at 450 ^oC and 500 ^oC for 1 h in N_2 atmosphere to obtain the crystalline and stoichiometric CZTS films. A nominal volume of 0.4 mL of precursor ink was sufficient to cover an area of 7.5 cm^2 which results in 5 μm thickness after thermal annealing. Different techniques were used to study their structural, compositional, optical and electrical properties. An annealing temperature of 500 ^oC for 1 h produces good quality CZTS layer with tetragonal kesterite phase as evidenced by X-ray diffraction and Raman scattering analysis. The optical results suggest their good light absorption capacity in the visible spectral region and the band gap values of the films were found to vary in between 1.3 to 1.42 eV. The electrical properties obtained for the kesterite films varied with the annealing temperature. At 450 ^oC the CZTS films showed: hole concentration (n) = $1.48x10^{17}$ cm^{-3}, resistivity (ρ) = 30.17 Ωcm and carrier mobility (μ) = 10.33 cm^2/Vs. While for the 500 ^oC annealed films, the electrical properties were: n = 1.38×10^{17} cm^{-3}, ρ= 163 Ω-cm, μ= 15.24 cm^2/Vs.

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[THF-185] Corrosion behavior of stainless steel multilayers with silver deposited by Sputtering

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Stainless steel multilayers were deposited with different amounts of silver via unbalanced magnetron sputtering. The bilayers consisted in a layer deposited in inert atmosphere and a layer in atmosphere reactive with nitrogen. Corrosion resistance of the multilayers was evaluated by Potentiodynamic polarization tests and electrochemical impedance spectroscopy using a Ringer's solution as a simulated biological fluid. The multilayer coatings were characterized by means of X-ray diffraction(XRD) for determine the structure, by Scanning Electron Microscopy (SEM) was study the morphology and by energy dispersive X-ray spectroscopy (EDS) to evaluate the chemical composition. The multilayer coatings presented two phases, BCC and FCC, mainly, characteristic of stainless steel coatings deposited in inert and reactive atmospheres, respectively. The chemical composition was slightly different to the target chemical composition and the Ag increase until ~ 8 %. The multilayers shown a compact morphology with good adhesion and low rugosity. The corrosion behavior was improved in the substrate with the multilayers coatings deposited.

[THF-205] Photocatalytic degradation of organic dyes using Zn2SnO4 thin films deposited by SILAR method

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Water pollution from organic dyes has become a growing threat to our environment. In this sense, metal oxide semiconductors help to photocatalytic degradation of organic compounds in a very effective way. Within these oxides, Zn_2SnO_4 is an n-type semiconductor with a band gap of 3.6 eV and an inverse structured AB_2O_4 which is known for was high chemical sensitivity, high electrical conductivity, and low visible absorption, besides having good photocatalytic properties. Most researches have focused on the synthesis and application of Zn_2SnO_4 in powder form, but there are a few reports of this oxide as a thin film. In this work, we report the Zn_2SnO_4 thin films deposition by Successive Ionic Layer Adsorption and Reaction (SILAR) method at low temperature and their photocatalytic activity in degradation of pollutants. SILAR is a simple, cost-effective and reproducible method, by which thin films of compound semiconductors can be deposited alternately by means of the dipping substrate into the aqueous solutions of containing ions for each component. Zn_2SnO_4 thin films were characterized by X-ray powder diffraction (XRD), UV-Vis spectroscopy, scanning electron microscopy (SEM) and their photocatalytic activity was evaluated using a batch reactor. Results will be discussed.

[THF-224] Determination Structural Quality in Thin Films of BaTiO3 grown by PLD, by the photoacoustic method

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Photoacoustic technique has shown great sensitivity to detect structural changes in bulk materials and some thin films. The objective of this inquiry was to study structural phase transitions of $BaTiO_3$ thin films under different conditions of grown. The results of this technique are presented as a function of temperature for thin films of classic ferroelectric $BaTiO_3$, deposited by PLD (Pulsed Laser Deposition) method on glass and Si/Pt substrates, under different deposition conditions, to detect the structural changes suffered by the thin films, in the region of temperature of interest, to determine its structural quality. Knowing the structural changes in temperature function on ferroelectric to be measured ($BaTiO_3$), we can use a photoacoustic measurement to determine the different structures present in the films, even minority phases. And we also follow the structural changes before and after thermal treatments. We implemented photoacoustic technique using laser pulses for the thin films characterization: a Nd:YAG laser System (Ekspla, model NL303HT-10-SH) @10 Hz, and pulse-width of 5 ns; we used a Thermolyne model 21100 tube furnace for temperature control, and a tektronix TDS 5054B Oscilloscope to collect the data. So, photoacoustic technique provides us with a tool with high sensitivity, to determine the structural quality in thin films of ferroelectric materials.

Acknowledgments:

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[THF-244] ZnO:Al thin films grown by dual laser PLD

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Two sets of zinc oxide (ZnO) thin films doped with aluminum (Al) were grown by pulsed laser deposition (PLD). Films deposition was made using two lasers: i) a 248 nm KrF excimer laser (COMPex 102, Lambda Physik) with a pulse duration of 30 ns to ablate the ZnO target and ii) a Nd:YAG (Surelite I, Continuum) emitting at 1064 nm delivering pulses of 8 ns to ablate an Al target. The substrates used for the deposits were: one set on corning glass and the other on silicon (100). Each set was integrated of a control film and five doped films using different delays between lasers: 0, 5, 10, 100, 1000 μs.

The Nd:YAG laser beam was always the second emitted. The thickness of all the thin films was measured with a profilometer Dekat IIA, the average value of the thickness was 180 ± 20 nm.

By means of x – ray diffraction it was confirmed that all the thin films had crystalline structure (Wurtzite) oriented in the plane (002). Energy Dispersive X-ray spectroscopy (EDS) was used to measure the mean of dopant incorporation in the structure of the ZnO:Al thin films. Due to the well-known heterogeneity of the films grown by PLD, the dopant content was always measured in the same nine regions for all the thin films, this, to control the variability between the means of incorporation in the deposits. Through a one factor analysis of variance (ANOVA) and specific comparisons (TUKEY), it was identified (confidence of 95 %) that the delay between lasers has a significant effect on the incorporation of aluminum percentage

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[THF-250] Intercomparison of the calculation to determine the kinetics of phase transformation in thin films of Sb2Te3

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Through a Sputtering system, samples were generated in the form of thin films approximately 500 nm thick, composed of an alloy of Sb_2Te_3 in amorphous phase. To ensure the existence of said phase, the transformation of phase into solid state was propitiated by energy supplied in the form of heat, obtaining measures that register this phase transition through: Optical Reflection, Electrical Resistivity and X-ray Diffraction, obtaining clearly results of the presence of said transformation. Later, we proceeded to the acquisition of experimental data through a work cell for optical reflection and impedance spectroscopy as a function of temperature, in the same way, the electrical resistivity as a function of temperature was obtained through a system of collinear tips.

The fundamental part of the work consisted of; carry out of parallel form, calculations to determine the kinetics of phase transformation in the solid state of samples in the form of Sb_2Te_3 thin films. These calculations are based on the famous JMAYK equation, independently developed by: Kolmogorov, John & Mehl, Avrami and Yerofeevo, which describes a great variety of transformations not only of solid state, but also of complex chemical reactions. The theory for the calculation of the crystallization fraction during the phase transformation, at a constant heating rate, is made from data obtained by optical reflection and impedance spectroscopy, to later be able to make the intercomparison by both techniques. In each case the reflection change or alternating voltage applied and current measured, are proportional to micro-structural changes of the sample measured. To determine the fraction of each of these phases present in the sample, they are developed from optical and electrical data obtained, which are modeled and adjusted by an electric circuit composed of 2-RC, taking into account that the permitivity and the occupied volume corresponding to the filling fraction of each phase.

[THF-264] Wear Resistance of BCC and FCC stainless steel multilayer deposited by sputtering

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In this work was studied the wear resistance of stainless steel multilayers deposited by magnetron sputtering on stainless steel substrates. The multilayers were grown within Ar and Ar / N2 atmosphere to change the FCC and BCC structures. The chemical composition analysis was performed using Energy-dispersive X-ray spectroscopy (EDS) and structural analysis was performed by X-ray diffraction (XRD). The adhesive wear resistance and friction coefficient was evaluated by the ball-on disk test using ball of stainless steel, aluminum and zirconia. The morphology of the wear track was characterized by scanning electron microscopy (SEM) and microscopy 3D. Overall, the results show that the multilayers deposited with nitrogen atmosphere have a FCC structure, improved the wear resistance of the substrate and the wear mechanisms are produced by plastic deformation, grinding, adhesion and corrosion. The wear mechanisms of the coatings produced in function of tribological pair will be discussed in this work.

[THF-267] Ab initio study and growth of superconducting tantalum nitride thin films by pulsed laser deposition

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Since its discovery at 1911 by Kamerlingh Onnes, the superconductivity has been a promising property of specific materials that is important for scientists and engineers. Particularly, the superconducting materials have applications in lossless energy power supply, transport levitation and development of nanometric electronic devices. In this latter issue, efficient fabrication of materials with a low superconductive energy gap and an intermediate transition temperature (Tc), results essential for the development and enhancement of superconductive electronic devices in the GHz range. TaN thin films have previously showed superconductive transition temperatures of up to 10.4 K with a superconductive energy gap lower than NbN, the most commonly used material for single photon detectors in the GHz range. The Tc of tantalum nitride depends strongly of the crystallinity and stoichiometry of the thin films. In the present work, superconductive thin films of tantalum nitride were grown by using the laser ablation technique with a Nd-YAG laser on a Ta target (99.999%) varying the N2 (99.999%) partial pressure in the chamber as well as substrate temperature. X-Ray Diffraction Spectroscopy (Panalitycal X'pert Pro MRD system) and X-Ray Photoelectron Spectroscopy (XPS), with an X-ray monochromatic source and semispherical analyzer, from SPECS were obtained in order to study the crystallography and stoichiometry respectively. The R vs. T curves of the films were obtained by using four probe method. Finally, we report an ab initio study of an fcc unit cell of tantalum nitride using Quantum ESPRESSO software. We calculated the states density with the purpose of correlating them with our experimental results obtained from XPS close to the Fermi energy.

[THF-272] Simple and low-cost synthesis of metal oxide-polyvinylpyrrolidone (PVP) polymer nanocomposite for electronic applications.

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In recent days preparation of metal oxide polymer nanocomposites-based gate dielectrics have more attention due to their cost effective in the production, low temperatures processing and high reproducibility towards flexible thin film transistors, diodes and sensors applications. The preparation of polymer nanocomposite thin films typically carried out by the sol-gel technique, allows enhancing the high capacitance of gate dielectric to enable the transistors operating at low voltages. Here, we reporting a novel solution-based nanocomposite with high dielectric constant (k) prepared by silicon dioxide nanoparticles (silica NPs) and polyvinylpyrrolidone (PVP) via sol-gel route as a function of silica concentration from 5, 10, 20, 30, 40, 50 % v/v. This nanocomposite showed an excellent dielectric constant with good electrical properties due to the presence of silica NPs. The identification of functional groups present in the nanocomposite was confirmed by FTIR spectroscopy. Further analysis of nanocomposite was carried out by preparing the thin films using dip coating method and annealed at 125^{o}C. Surface morphology, size and shape of the nanocomposite was characterized by using SEM, TEM, and AFM analysis. Absorbance spectra of nanocomposite was performed by using UV-visible absorbance spectroscopy. Finally, the capacitance and leakage current parameters were measured for all the samples prepared with different concentrations of silica.

[THF-273] Photoluminescence study and structural properties of CdS thin films grown by Pulsed Laser Deposition

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Thin films of CdS were obtained using P.L.D. method, a pulsed Nd: YAG laser with a wave lenght of 1064nm was used to evaporate the surface of a solid target made of CdS powder, the growth occurs inside of a vacuum chamber with a pressure under 10^{-5} torr. The result was a set of 4 thin films of CdS growth over different substrates (glass, quartz, silicon and zaphire) with typical grain size no longer than 100nm according to SEM images. The hexagonal phase was associated to the material due to X-Ray diffractogram results. A low temperature study was performed in photoluminescence spectroscopy obtaining the temperature coefficient and the activation energies, this results match with the reported values.

[THF-285] Recrystallization study in sputtered CdTe thin films activated by CdCl2, MgCl2 and ZnCl2 solutions for photovoltaic applications

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Thin films study has allowed the development of optoelectronic devices, among them solar cells have gained importance due to politics that have favored and encouraged their adoption. Within the solar cells, those manufactured with CdTe have presented greater growth driven by First Solar Company. In this work is studied the recrystallization in sputtered CdTe thin films activated by $CdCl_2$, $MgCl_2$ and $ZnCl_2$ solutions at 375 °C and its relationship with grain growth. Sputtered CdTe thin films usually present a pronounced preferential orientation in plane (111) and small grains (ranging from 100 nm to 300 nm), which favors both the evaluation of changes in crystalline structure and grain size growth. This study shows that activating the CdTe films using different solutions has a direct impact in the films recrystallization and at the same time recrystallization influences the final grain size. This study could be applied to determine the structural grain size growth mechanisms in CdTe films, which may have an impact in lifetime of minority carriers.

[THF-291] Zinc Oxide morphogenesis and its consequent properties

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In this work the morphogenesis of sub-microstructured ZnO films is approached as a function of its synthesis parameters, through SEM and AFM studies. XRD analysis shows that texture coefficient of the surface can be controlled, allowing to stablish its relation to optical and electrical properties of the film. Amongst studies conducted there are: XPS, PL, EDS, Transmitance, Perfilometry and Hall Conductivity. Results offer a procedure to optimize potential application of ZnO in diodes and transistors. Presented synthesis technique utilizes "Spin Coating", "Chemical Bath Deposition" and Solid-state reaction.

[THF-296] P-type ZnO semiconducting thin films

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The synthesis of transparent (T=0.85) undoped and Ag-N doped ZnO thin films was done via “dip coating” technique. Obtained crystal structure was polycrystalline, corresponding to the hexagonal wurtzite phase of ZnO, with thickness varying from 220 to 346 nm for samples doped with Ag, while Ag and N co-doped films were up to 107 nm thick. Ag doping allows films to reach, for 3 %at., an Eg < 3.3 eV and a resistivity of 552 ohmcm, still showing n-type conductivity, however, when co-doping with N, p-type conductivity is achieved, although with a relatively high resistivity of 4406 ohmcm. The incorporation mechanism of N and its role in the conversion of ZnO into a p-type semiconductor is approached.

[THF-297] OPTICAL, MORPHOLOGICAL AND STRUCTURAL PROPERTIES OF CdS/ZnO BILAYER

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Solar cells based in CIGS, CZTS, and Sb2Se3 absorber layers are composed by different layers such as ZnO (buffer layer) and CdS (window layer), which are commonly stacked in substrate configuration. Optical and structural properties of the upper layers (ZnO and CdS) play an important role in solar cells (CIGS, CZTS, and Sb_2Se_3) efficiency. Particularly, high efficiency solar cells have been achieved with sputtered ZnO and chemical bath deposited CdS using low deposition temperatures (below 250°C) to avoid elements diffusion and consequently degradation. In this work, we present the optical, structural and morphological properties of ZnO/CdS bilayer changing the ZnO deposited temperature (100°C and 200°C) and the CdS deposition technique (sputtering and chemical bath deposition). In CdS sputtered samples (class A) deposition temperature was 100 °C, while in chemical bath deposited (class B) the solution temperature was approximately 75°C; In both cases, ZnO thin films were deposited on CdS by reactive RF-Sputtering at different temperatures. To compare bilayer properties, the samples were characterized by the X-Ray diffraction, UV-Vis spectroscopy, reflectance and Scanning Electron Microscopy. Class A diffraction spectra showed that CdS presented hexagonal phase, while in class B the crystalline structure of CdS changed to cubic phase; in both cases peaks corresponding to hexagonal ZnO diffraction pattern were observed. Transmittance for class B samples showed the absorption edges of the ZnO and CdS, conversely class A samples not. Furthermore, it was observed a reflectance decrease in class B samples respect to the class A. On the other hand, class A and class B samples showed significantly different morphologies.

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Keywords: ZnO, CdS, structural properties, optical properties, morphological properties.

[THF-298] Single bath electrodeposition of CuSbS2 for photovoltaic applications

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Copper antimony sulfide ($CuSbS_2$) has been proposed as an alternative to CdTe and CIGS considering its non-toxicity, relative abundance, and excellent optoelectronic properties. $CuSbS_2$ has direct band gap in the range of 1.38-1.56 eV and high absorption coefficient of 10^{-4} cm^{-1}, which are optimal for absorber layers in solar cells. In the present work, $CuSbS_2$ thin films were developed by pulse electrodeposition technique on FTO glass substrates from a single bath. The electrodeposition bath consisted of 1.5 mM $SbCl_3$, 0.4 mM $CuCl_2$ and 18 mM $Na_2S_2O_3$. The potentials were applied in pulse form with respect to saturated calomel electrode, deposition potential (V_{on}) was fixed at -0.72 V and dissolution potential (V_{off}) was varied in the range of -0.25-0.1 V. Films of approximately 700 nm were obtained after 300 cycles. As deposited films were amorphous and the films were crystallized in chalcostibite phase after annealing at 250 °C in N_2/S atmosphere for 30 minutes. The estimated band gap of the films was 1.42 eV and the films were photosensitive.

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[THF-303] Development of CuSb(SxSe1-x)2 by the selinization of electrodeposited CuSbS2 films

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In this work, we present the formation of $CuSb(S_xSe_{1-x})_2$ by the selinization of $CuSbS_2$ thin films obtained by electrodeposition technique. $CuSb(S,Se)_2$ is a ternary semiconductor, which is chemically and optically similar to high efficient absorber layer such as $CuIn(S,Se)_2$. The reported band gap of $CuSbS_2$ is 1.3- 1.6 V, which can be tuned by the incorporation of Se. Here, we electrodeposited $CuSbS_2$ from a precursor solution consisting of $SbCl_3$, CuCl and $Na_2S_2O_3$ by applying constant potentials. The deposition potentials were fixed from cyclic voltammetry measurements. A series of trial experiments with different time and temperature were carried out to fix the annealing condition. The films used in this study were annealed at 325 ^{o}C for 30 minutes at a pressure of 1 bar in the presence of 5mg of Se. The films were characterized using different characterization techniques such as XRD, Raman spectroscopy, Scanning electron microscopy and UV-Vis spectroscopy. The results showed the formation of $CuSb(S_xSe_{1-x})_2$ phase with band gap ~1.2 eV.

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[THF-305] Effect of Ge concentration on the device properties of Cu2ZnSnS4 solar cells

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In this work, we report the effect of Ge alloying on the device characteristics of kesterite solar cells. The starting materials were Cu, Zn, Sn, S, and Ge. The metal-stack Cu/Zn/Sn with different thickness of Ge (5, 10 and 15 nm) was deposited over pre-prepared glass/Mo substrate by sputtering. Device with 5 nm thick Ge layer showed an improvement of 2.7% over the reference cell without Ge (Mo/CZTS/CdS/i-ZnO/ITO). From the C-V analysis, it was observed that with respect to the reference cell there is a significant increase in the space-charge region (W_O), from ~160 nm to ~366 nm. However, a further increase in Ge layer thickness resulted in a decrease of W_O. The value of obtained for Ge-5, Ge-10, Ge-15 and reference cell were $1x10^{16}$ cm^{-3}, $1x10^{17}$ cm^{-3}, $5x10^{16}$ cm^{-3} and $9x10^{16}$ cm^{-3}, respectively, where are doping concentrations. In the case of Ge-5 a built-in potential of around V_{bi} =331 mV was observed. In order to fully understand the role of doping density on device efficiency, a numerical simulation based on SCAPS software was performed.

[THF-308] Formation of CuSbS2 thin film from thermally evaporated Sb2S3-CuS layers: effect of Cu content on the physical properties of the film

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We report the effect of Cu concentration on the structural and optoelectronic properties of $CuSb_2S_3$ thin films. First, Sb_2S_3 thin film of about 600 nm was thermally evaporated on to glass substrate under vacuum at a substrate temperature of 150 ^oC. Subsequently, CuS was deposited onto the above film without breaking the vacuum. A series of Sb_2S_3-CuS stacks were deposited by keeping Sb_2S_3 thickness constant while varying the thickness of CuS (100-300 nm). Postdeposition heat treatments at different temperatures and time durations were carried to optimize the film recrystallization process. The optimized annealing condition for the formation of $CuSbS_2$ was 350 ° C for 30 minutes in N_2/S atmosphere. Ternary films obtained from Sb_2S_3/CuS with CuS thickness below 300 nm showed mixed phases. The CuS thickness below 200 nm resulted in stibnite and chalcostibite phases and that with thickness in the range 200-250 produced stibnite and famatinite phases. However, phase-pure $CuSbS_2$ film with chalcostibite phase was identified when the CuS layer was thicker than 300 nm. The films were characterized using different techniques including XRD, SEM, Raman spectroscopy, UV-Vis, and Hall Effect.

[THF-312] Indium tin oxinitride (ITON) thin films for FPDs applications

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This work describes the study carried out about ITON thin films for its application as an active matrix for high definition flat screens. ITON thin films were deposited by reactive DC-Sputtering technique at room temperatura on glass and silicon (100) substrates in a reactive atmosphere of argon and nitrogen at different consentrations. The characterization of ITON deposited samples was performed by UV-VIS spectroscopy, fixed wavelength ellipsometry, Hall effect in Van der Pauw configuration, atomic force microscopy (AFM), scattered X-ray energy spectroscopy (EDS) and X-ray diffraction (XRD). XRD diffractograms show that deposited films are amorphous. The Surface morphology is widely affected by the presence of nitrogen in the reactive atmosphere presenting a smaller grain size for films deposited at a higher nitrogen concentration. The carrier concentration for ITON samples is also affected by nitrogen presence having values between 10^{18} and 10^{20} cm^{-3} . Furthermore, the band gap values for these samples are close to 4.0 eV and they present a high transparency in the visible región (75-88% of transparency).

[THF-314] Electric response of the arrangements GLASS/ITO/ CdS OR ZnS / CdTe USING Mo, graphite and Ag as front and rear contacts

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Nowadays it has been working on the use of second generation solar cells that allow to increase their efficiency and reduce the use of semiconductor materials, reducing its cost and weight for the solar panels. In this work the comparison between three types of contacts was made Ag, Mo and C, used as electrical contacts for solar cells of heterostructures in the cell array glass/ITO/CdS/CdTe and glass/ITO/ZnS/CdTe. Besides was realized the optimization of the process of deposition of coating CdTe semiconductor type p by sputtering. As transparent condutor oxide (TCO) was used commercial ITO (Tin-doped Indium oxide). CdS and ZnS films were deposited by chemical bath method. The first part of the work was based on the deposit of CdTe by sputtering, obtained from array "sandwich"-type films were subjected to a process of heat treatment with $CdCl_2$, to activate the CdS/CdTe or ZnS/CdTe heterojunction and to increase the size of the grain in the thin films. Second step was designing the masks for the molybdenum deposition, which were placed on glass/ITO/CdS or ZnS/ CdTe films to make the deposit through a system Intercovamex V3 using a RF source, controlling pressure, the stability of the plasma and the flow of Ar. Contacts of Ag and C were deposited using screen printing technique. Later, the cells were characterized by scanning electron microscopy scanning (SEM), transmission electron microscopy (MET), spectroscopy energy dispersive (EDS) and electrical by curves I-V. Cells getting Voc, applying 20mW/cm^2 0.200 V, I_{SC} 0.131 mA/cm^2 and Pmax 0.0122 mW/cm^2. According to the results obtained in this work, it is recommended as a contact to use graphite.

[THF-317] Non-linear optical properties of polymer thin films of a mixture of triphenylmethane dyes

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The octopolar molecule was proposed as an object of study in non-linear optics by Zyss in the 1990's due to the advantages it presents against a dipolar molecule, such as the absence of dipole moments both in the excited state and in the basal state, in addition to resolving the conflict between transparency and non-linearity, characteristics that maintain this type of molecular systems in force in the field of non-linear optics. (1) Triphenylmethane-derived dyes belonging to the octopolar-type molecules have a wide use for tissue staining but have also become the object of study in the field of non-linear optics (2). For the present study we propose the combination of two dyes of this family, malachite green and crystal violet, of which there are reports of their non-linear optical response separately. For its study, thin films were made of polymers such as polyvinyl alcohol (PVA) and methacrylate, which were later subjected to UV-vis tests. A λ_{max} = 595 nm and a peak more at λ = 425 nm were observed. Finally, the non-linear optical properties were determined using the z-scan technique, where values of n_2 = -8.05x10-11 and β = 1.08x104 were determined, respectively. This result is encouraging to be used as optical absober for applications in devices in optoelectronics.

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[THF-318] Synthesis and Characterization of SnO2@Graphene Transparent Conducting Films

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Various photovoltaic technologies have been actively studied and many more are emerging in the recent years. For most of these technologies (solar cells, LED’s, etc.), an integral part is a transparent and conductive contact, known as a TCO or transparent conducting oxide. The current market is dominated by Indium Tin Oxide (ITO), a highly conductive and highly transparent TCO, however other materials which offer an alternative do exist, such as Fluorine doped Tin Oxide (SnO_2:F) and Aluminum doped Zinc Oxide (AZO). These alternatives are viable technologies on their own, however none have surpassed the quintessential properties of ITO. In this study, we strived to achieve a low cost, highly conductive and highly transparent TCO by using SnO_2 and graphene, which is known for its amazing conductive and transparent properties. By incorporating low weight percentages of graphene in between the semiconductor lattice at the moment of synthesis with a technique derived from Spray Pyrolysis, we obtained a low cost TCO with excellent transparent and conducting properties, that were characterized by AFM, UV-VIS and Four Point Probe. The film roughness lies around 7.49-12.7 nm, while bandgap was determined to be between 4.0-4.07 eV. The material’s optical transparency goes from 86-94% in the visible spectrum and its electrical conductivity was measured to be in the range of 200-400 Ω/sq. With these results, we conclude that the obtained material is a proper candidate for use in photovoltaic applications, such as Grätzel solar cells, which will be our main focus.

[THF-322] Fabrication and characterization of CuCrO2 / Al doped ZnO heterojunction devices deposited by chemical routes

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In this work, we report on the optical, structural and electrical properties of $CuCrO_2$/ Al: ZnO heterojunction devices deposited on glass substrates by soft- chemistry routes. $CuCrO_2$ thin films were synthesized by ultrasonic spray pyrolysis, and n type Al: ZnO thin films were formed by mean of dip coating sol gel method. Different conditions of deposition (Annealing and temperature deposition) were varied in order to analyze their effect in the electrical properties of the heterojunctions. These devices exhibited a 50-70% of transparence in the visible region. $CuCrO_2$/ Al: ZnO devices showed a rectifying behavior like a p-n diode, as observed in the non- linear curves on the I-V plots, although, the final properties of devices are dependent of the electric properties of the individual components of the heterojunction. Moreover, the ideality factor calculated for $CuCrO_2$/ Al: ZnO devices are much larger than 2. Additional measurements as impedance spectroscopy, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were carried out in order to complement the electric characterization, and analyze the micro-structure of the interface of the devices.

[THF-323] Use of the hybrid technique combining Magnetron Sputtering and Pulsed Laser Deposition to prepare ZnO-Au films

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The deposition hybrid technique (MSPLD) combining magnetron sputtering (MS) of a ZnO target and the pulsed laser deposition (PLD) of Au was used to prepare composite films of ZnO-Au. The radio-frequency power applied to the ZnO target was fixed at 150 W, while the laser energy density to irradiate the Au target was varied at 1.2, 3.6 and 5.4 J cm^{-2}. Also, films of the individual materials were deposited. All deposits were carried out under an argon atmosphere (0.67 Pa) and heating the substrates at 400°C. Simultaneously, we diagnosed the plasma by optical emission spectroscopy (OES) to achieve the aim of this work, which is to study the correlation between the growth parameters, the properties of the films and the plasma species behavior. The morphology, composition, structure, thickness, transmittance and resistivity of the obtained ZnO-Au, ZnO and Au films were evaluated. The amount of gold incorporated into the ZnO-Au films increased proportionally to the laser energy, from 5.1 to 14.4 at%. The X-ray diffraction (XRD) patterns show that all the films were crystalline, the ZnO films grew with a preferred orientation in the (002) plane that was not modified with the gold addition. Also, diffraction peaks of gold were identified showing that the metal was incorporated into the films as a second phase, instead of dopant or substituent atoms into the ZnO lattice. A thickness decrement as the laser fluence increased was observed in the Au films, while the thickness of ZnO-Au films was almost unchanged. Simultaneously, the temporal evolution of the optical emission of the species in the plasmas (Au I, Au II, Ar I Zn I) was recorded at different distances from the surface of the Au target. The intensity of the emission diminished as a function of the distance, except at the nearest distance to the Au target, where the emission intensity changed for Au I and Zn I. The Au I emission intensity increased in deposits of pure Au evidencing the re-sputtering process, but it decreased during deposits by MSPLD suggesting that the re-sputtering of gold as the diminished using a background MS plasma. The intensity of the Zn I emission increased as the laser fluence raised due to the increment of the excited Zn population. The ZnO-Au thin films resulted opaque in the wavelength range 300-800 nm (Transmittance < 0.1). The gold addition reduced the resistivity of the ZnO-Au thin films in five magnitude orders respect to the ZnO film.

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[THF-343] Correlation between structural and mechanical properties for (Ti,Si,Al)N nanocomposite films

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Mechanical components presents industrial demand, which require continuous development of new coating materials and coating design concepts to obtain enhanced toughness and increased resistance to cracking. As a results, special attention is dedicated to the two-phase nanocomposites, which can offer multifunctional characteristics from the individual components. In this work, (Ti,Al,Si)N thin films have been deposited on M2 steel by dc reactive magnetron sputtering from TiAl/AlSi and TiSi targets, using nitrogen as reactive gas. A optimization procedure was carried out, varying the nitrogen flow rate and current density applied to the target, to determine the best deposition parameters to attain stable plasma conditions. Cross-section scanning electron microscopy images revealed columnar structure for low flow of Nitrogen, while increasing the gas flow rate, promote densification of the coatings. The chemical composition of the coatings was investigated by energy dispersive X-ray spectroscopy and the phase and crystal size were determined by X-ray diffraction consisted mainly of a c-(Ti,Al)N solid solution for which Si serves as a veritable grain refine, whereas the average grain size is 10-14nm. Hardness was determined by nanoindentation a low value of the Young's modulus E*between 184 y 221 Gpa, satisfying high $H/E^{*} \geq 0.1$. The main advantage of these coatings is their enhanced resistance to cracking revealed in the scratch test, plus enhanced adhesive and cohesive strength and demonstrated plastic deformation typical of soft films with critical normal force in the range of about 55-75N.

[THF-354] Growth and disorder characterization of non-stoichiometric Cu2ZnSnS4 thin films prepared using a two-step sulfurization process

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Non-stoichiometric Cu_2ZnSnS_4 (CZTS) thin films at varying Cu/(Zn+Sn) ratios were grown by sulfurizing in a two-step sulfurization process a stack of ZnS, Sn and Cu thin films. Films were sequentially deposited, by vacuum thermal evaporation, at varying thicknesses aimed to provide Cu/(Zn+Sn) ratios between ~0.65 and ~1.0. Samples compositions were determined by energy dispersive x-ray spectroscopy (EDS) revealing three different Cu-poor/Zn-rich samples and one slightly Cu-rich/Zn-poor sample. Morphology was obtained by scanning electron microscopy (SEM). SEM images allowed estimating grain sizes that change from 0.50 to 0.75 μm depending on stoichiometry. X-ray diffraction corroborating the Kesterite crystal structure of CZTS. Relevant structural parameters as the lattice parameter and average crystallite size were obtained. Crystallite sizes vary from 39 nm to 45 nm using Scherrer equation while a variation from 48 nm to 64 nm was obtained using the Williamson-Hall approximation. Depending on the Cu content estimates of lattice microstrain were also obtained. Raman spectroscopy reveals the characteristic Kesterite (KS) structure with a prominent peak shifted significantly to lower wavenumber. This behavior has been associated to partially disorder kesterite (PD-KS). This is an important finding, given the fact that it is practically undetectable using standard laboratory x-ray diffraction. The structural disorder is also related to the optical properties of the CZTS films, such as the band gap and the Urbach energy. Optical measurements confirmed a band gap between 1.39 and 1.47 eV and Urbach energy from 77 meV to 200 meV which also presents a remarkable trend that follows the Cu/(Zn+Sn) metallic ratio.

[THF-362] Optical-structural characterization of ZnO:Al films obtained by SSCVD

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This paper reports the growth of ZnO films undoped and Al-doped by SSCVD technique onto glass substrates using zinc acetate, oxygen gas and aluminum acetylacetonate, respectively, as source of Zn, oxidizing agent and source of the doping element. The samples obtained were grown at 300 ° C for 5 min, at different concentrations of doping. The optical and structural properties of these films were investigated as a function of deposition temperature and Al concentration. X-ray diffraction results show that all deposited films are polycrystalline. Las micrografías SEM muestran una superficie homogénea en todas las películas depositadas. The optical transmittance spectra showed that the Aluminium presence improves the optical transmittance in the visible.

[THF-380] Reactive magnetron sputtering of Cr-Ti oxide: Mechanical and microstructural stability at higher temperature

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Chromium-Titanium oxide thin films were deposited on steel and Si wafer substrates using reactive magnetron sputtering of Cr-Ti target. Different oxygen flow rates were used to find the optimum condition where oxide is deposited at high deposition rate. It was found that an O_2/Ar ratio of 6.6 % is the point in which surface target coverage by oxide or implantation of reactive gas species into sub-surface layer have not started yet. Beyond this ratio, deposition rate will be decreased dramatically. Films deposited using the constant O_2/Ar flow rate (6.6 %) were heat treated at different temperatures (200, 400, 500, 600 and 800 °C) for 2hr in air to evaluate the microstructural stability. X-ray diffraction (XRD) and scanning electron microscopy (SEM) as well as nanoindentation method were used for microstructural and mechanical characterization, respectively. XRD results show that as-deposited and heat treated coatings up to 500 °C, keep their amorphous structure. Beyond that, the coatings crystallize as stable phase of Cr_2O_3. Nanoindentation results demonstrate that by increasing the temperature, hardness value decreases significantly from 27.7 to 11.8 GPa for as-deposited and heat treated coatings at 600 °C, respectively.

Keywords: Cr-Ti oxide; Reactive magnetron sputtering, Microstructural stability; Nanoindentation.

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[THF-382] Effect of vacuum annealing on mechanical properties and microstructural stability of Cu-Ta coatings deposited by magnetron sputtering

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Abstract

In this study, binary Cu-Ta alloys with a Ta content of 0 to 100 % were prepared by co-magnetron sputtering. Effect of elevated temperature vacuum annealing on the morphological stability and mechanical properties of Cu–Ta films was studied. Their structural and mechanical properties were characterized by XPS, XRD, SEM, TEM and nanoindentation methods. The XRD results show that amorphous Ta is formed in the coatings with 15-67 at. % Ta along with the crystalline Cu. TEM analyses of two selected samples with 25 and 67 at. % Ta depict formation of crystalline Cu islands in an amorphous Ta matrix in both as-deposited and annealed coatings. XPS results show that annealing causes a considerable reduction of Cu_2O in the film, while content of substochiometric Ta and Ta_2O_5 oxide increase, regardless to the Ta content. A significant increase in hardness values from 0.9 for pure annealed Cu to 11.89 GPa for the samples with 98 at. % Ta, is observed.

Keywords: Cu-Ta coatings; Magnetron sputtering; Vacuum annealing; Mechanical properties.

Acknowledgments: DGAPA-PAPIIT (100116); The Royal Society (Newton Advanced Fellowship - NA160021)

[THF-383] Microstructural characterization of Cu-Ta coatings synthesized by confocal magnetron sputtering

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Abstratct:

Cu-Ta coatings with different concentration of Ta (0, 15, 25, 35, 67, 98, 100 at. %) were deposited on 1018 steel and Si wafer using confocal magnetron sputtering technique. High temperature vacuum annealing was done on all the samples at 500 °C for 2 hr. Scanning electron microscopy (SEM) and X-ray diffraction (XRD) in grazing incidence mode were used for microstructural characterization in both as-deposited and annealed coatings. SEM results show that there is a significant change in the microstructure of coating by increasing the Ta content in the film, while the microstructure is kept almost the same after annealing. XRD results indicate that Ta addition from 15 to 67 at. % causes formation of amorphous Ta along with crystalline Cu grown in a preferred orientation of the (111) planes. Films structural stability can be observed after annealing, except for sample with 25 at. % Ta, where Ta is crystallized in β-Ta structure.

Keywords: Cu-Ta coatings; Magnetron sputtering; Vacuum annealing; Microstructural stability.

Acknowledgments: DGAPA-PAPIIT (100116); The Royal Society (Newton Advanced Fellowship - NA160021)

[THF-389] Flat mirrors with multi-layered coating for outside weathering in solar concentration applications

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Solar thermal energy is a viable alternative, given the imminent scarcity of hydrocarbons as the main sources of energy production. The proposal presented in this work is based on the manufacture of flat mirrors of four layers: glass substrate, the specular layer is applied by the technique of Dynamic Chemical Deposition (DCP), the other layers are coatings against weathering and with mechanical resistance. These mirrors could be used for the conversion of solar radiation to thermal energy in parabolic trough, Fresnel or electric power production in central tower plants.

There is in CIDETEQ the technology and previous experiences of having manufactured mirrors with polycarbonate substrate with six layers. In this work, the same method is used with the variant of using only four layers. It is now proposed to use as a substrate a flat glass instead of polycarbonate, a pretreatment, a layer of silver by DCP, a protective film of silicon dioxide and a layer of mechanical protection against breakage, chipping and weathering. This work shows the characterization of each of the layers, the interaction between them and the performance of the mirror as a whole.

Advances have been made in the manufacturing process of flat mirrors with glass substrates, starting from several samples of 1.2 x 1.2 m, in which, variants have been implemented in all the stages, with acceptable results in flat mirrors of 1.4 m2. Also, prototypes of solar concentrators, heliostats, and parabolic trough have been built; using flat mirrors that can be compared with the options available in the market and other reflective materials.

[THF-396] CdS thin film indium doped prepared by chemical bath deposition method

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Semiconducting cadmium sulphide (CdS) has been demonstrated that is an excellent n-type material on optoelectronic devices. The Chemical Bath Deposition technique (CBD) by chemical bath deposition. Cadmium chloride was added as source of Cadmium, ammonia as complexing agent and indium chloride as a doping reagent was between 0.2% and 1% in steps of 0.2 %. At 70, 80 and 90°C, in a reactor that can be a beaker and the reaction can be carried out at atmospheric pressure. This study reports a simple route for coating CdS thin films onto glass-slide substrates by the CBD method, and their doped with indium. Effects of annealing at various temperatures on the optical, electrical and structural properties of nanocrystalline CdS thin films were investigated. The chemical-bath-prepared CdS thin films were obtained at 90°C on glass substrates. The band gap of the films varied in the range 2.40 to 2.46 eV. The structure was cubic phase. The CdS thin-film doped with 0.8 %w/w exhibited the highest mobility and carrier concentration.

[THF-398] RuN thin films by magnetron Sputtering

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A reactive MAgnetron Sputtering was used to obtain RuN thin films. Ar/N2 ratio with values of 60/40, 80/20, 85/15, 90/10, 95/5, and 100/0 were used to vary the nitrogen concentration. The presence of RuN before and after a sputtering etching process were obtained through a X-ray photoelectron spectroscopy, 3 peaks were identified at 397.4 ± 0.3 eV, 398.3 ± 0.3 eV, and 398.8 ± 0.3 eV binding energies in the high-resolution of N1s spectra, corresponding to hybridizations of nitrogen with transition metals, oxynitrides, and oxycarbides. X-ray diffraction analyses were performed, showing the coexistence of the RuN face-centered cubic and Ru hexagonal compact packed phases. After the etching process, the samples grown at nitrogen flow rates greater than 15% continued to show the RuN face-centered cubic phase. Atomic force microscope analyses showed that as the nitrogen concentration increased, the grain size and roughness also tended to increase.

[THF-406] TiO2-ZnO binary thin films deposited by a hybrid deposition configuration

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Binary thin films composed by zinc oxide with titanium oxide were deposited using an hybrid deposition configuration. A high purity TiO_2 target was ablated in vacuum at working pressures close to $5x10^{-5}$ Torr. During experiments the TiO_2 plasma parameters, mean ion kinetic energy and plasma density, were kept approximately constant while the equivalent total thickness of Zn deposited was varied in order to obtain different contents of zinc in the deposited films. Deposits on glass and silicon substrates using the third harmonic (355nm) of a Nd:YAG laser were obtained. Afterwards, the as-deposited films were subjected to a thermal treatment at 550°C to obtain crystalline oxides. The composition of the obtained materials was determined by EDS; it was found that the Zn contents varies from 24.1 to 42.0 at. %, corresponding to the lowest and the highest zinc thickness respectively. Raman spectroscopy showed that thin films with the lowest Zn content are formed by the rutile phase of TiO_2, whereas for Zn contents higher than 29.6 at. %, only the zinc oxide is observed. UV-Vis measurements showed a red shift of the optical band gap suggesting that Zn content can be used to tune the band gap. Surface morphology was observed by SEM revealing smooth surfaces for the samples with the lowest Zn contents and surfaces covered by submicrometric particles at higher Zn contents. The obtained thin films were tested as photocatalysts in the degradation of the malachite green dye under solar light with good photocatalytic activity.

[THF-423] Electrical and optical properties of SnO:N and SnOx thin films by DC magnetron sputtering for their use in transparent electronics

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Tin oxide has been widely used in the fabrication of transparent electronic devices because of its high conductivity and high transparency in the visible spectrum. Previous research has established that oxides such as SnO exhibit n- or p-type conductivity controlling the oxygen vacancies and maintaining optical transparency. In this work, we obtained SnO:N and SnO_x thin films by magnetron sputtering on glass varying the relative gas partial pressure (pO_2 or pN_2) from 6% to 15%, the working pressure from 1.6 to 2.5 mTorr, and using a dc power of 30 W. A heat treatment during 30 min helped to optimize the desired type of carriers in the SnO:N and SnO_x thin films. The p-type SnO:N thin film deposited at 7% pN_2 showed a band gap of ~1.9 eV, a transmittance of 79%, and mobility of 0.2 $cm^2\ V^{-1}s^{-1}$. XPS results indicated the presence of Sn^0 in the as-deposited SnO_x thin films, after the heat treatment, the Sn $3d_{5/2}$ peak shifted from 484.1 eV to 485.9 eV, suggesting the complete formation of the SnO_x. The p-type SnO_x thin film deposited at 8% pO_2 exhibited a band gap of ~2.7 eV, a transmittance of 85.5%, and mobility of 1.2 $cm^2\ V^{-1}s^{-1}$. The obtained p- and n-type SnO_x semiconductor thin films could serve to design p-n junctions for the assembly of a transparent diode.

We thank E. Aparicio, E. Murillo, I. Gradilla, and H. Castillo for their valuable technical support. This work was partially supported by DGAPA-UNAM and CONACYT under grants IN112918 and LN294452, respectively. AGF received a Scholarship from CONACyT.

[THF-425] Deposit of thin films of ZnO / CuO obtained by the dip-coating and co-evaporation technology

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This paper presents the results related to the manufacture of thin films of ZnO and CuO by the method of Dip-Coating and Co-evaporation respectively, the study of their optical, structural and morphological properties through the characterizations (UV- Vis, XRD, AFM and Raman). To obtain thin films of ZnO, the first stage of the sol-gel process is used. The methodology used was as follows; The precursors were dissolved in a stoichiometric ratio: zinc acetate and ethyl alcohol, stirred for 10 min at 60 ° C, until the compounds dissolved, then diethanolamine was added as a drip and the same temperature was continued for one hour. hour, finally, the solution was rested for its aging. The dwell time immersed in the solution was 3 min and the extraction time was 2mm / s, between layers, there was a time of 10 min of suspended runoff in the equipment clamp and an oven drying of 200 ° C ; finally, a heat treatment in the tubular furnace at 500 ° C. To obtain the thin film of CuO, it was carried out with the evaporation of the metallic copper in a vacuum environment, current ramps were used until reaching the evaporation point of the metal. The crystalline structure of the ZnO sample was analyzed by X-ray diffraction finding the Wurtzite phase, for the CuO it was analyzed with the Raman equipment resulting in a cover or cuprous oxide. The results of the Uv-Vis: showed a transmittance of 350nm with an Eg of 3.7eV and 600nm with an Eg of 2.9, the profilometry team determined that the film has a thickness of 230nm and 170nm for the ZnO and CuO respectively. And its topography was determined with AFM in both oxides.

[THF-461] Influence of the nitrogen flow rate on the electrical properties of CrN thin films

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Coatings based on transition metal nitrides such as TiN, ZrN and CrN are extensively used in industries due to their excellent properties such as hardness, wear and corrosion resistance. CrN coating has been identified as a better substitute for TiN and ZrN coatings for several applications due to its superior performance. In this work, CrN thin films were synthesized in a DC magnetron sputtering system using a mixture of Ar + N_2. The chemical composition and bonding configuration were examined using X-ray photoelectron spectroscopy (XPS). The stoichiometry variation dependence on the N_2 flow was also analyzed using Auger spectroscopy. Both, The XPS and Auger analyses were performed in situ. A gradual increase in the nitrogen concentration was observed in the coatings when the N_2 gas was increased into the reaction chamber. The electrical behavior was studied as a function of the nitrogen concentration. A lower resistivity was observed as the nitrogen concentration was increased into the sample before reaching the stoichiometric concentration; however, the resistivity increased at higher nitrogen concentrations (overstoichiometric coatings). Considering that chromium is a magnetic material, a slope change in the resistivity was observed around the Néel temperature. Furthermore, the obtained Hall coefficient showed changes in the carrier type (negative or positive) depending on the nitrogen concentration in the CrN coatings. The resistivity, conductivity and Hall coefficient for the CrN_x thin films were measured varying the temperature between 85 and 350 K.

We thank E. Aparicio, I. Gradilla and J. Díaz for their valuable technical support. This work was partially supported by DGAPA-UNAM and CONACYT under grants IN112918 and LN294452, respectively. AGF received a Scholarship from CONACyT.

[THF-466] Study of the electrochromic properties of WO3/rGO nanocomposites

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In recent years, interest in the study of the electrochromic effect in thin films of metal oxides has been shown. The electrochromic effect is present in certain materials that change its color when an electric current passes through them, this is because the electric current produces an oxide-reduction reaction that modifies the energy bands in which the material interacts with visible light. This behavior has been studied in different materials, one of the best is the WO$_3$. It has been proposed that WO$_3$ films exhibit high coloration efficiency and high absorption throughout the visible spectral region. In this work the deposition of WO$_3$/rGO films was carried out by chemical bath onto FTO substrates (8 Ohms/sq) varying the weight percentage of the rGO (0.5, 1.0, 1.5, 2 and 3 wt%) to evaluate the effect of its concentration on the structural, morphological, optical, electrical and electrochromic properties of these nanocomposites. In the XRD patterns the peaks corresponding to the orthorhombic structure of WO$_3$ were observed, the Raman spectra shows the vibration modes at 1344 cm^{-1} and 1588 cm^{-1} corresponding to vibrational modes D and G of the rGO, respectively. The band gap was calculated from the diffuse Reflectance spectra. Electrochromic tests were carried out by the use of electrochemical techniques such as cyclic voltammetry and chronoamperometry. A three electrode cell was used, with a Hg/HgO electrode and a platinum wire as reference and counter electrodes, respectively, and as working electrode, the WO$_3$ and WO$_3$/rGO film. An 0.1 M solution of LiClO$_4$ was used as the electrolyte.

[THF-476] Study of the synthesis of ZnSe thin films by chemical bath deposition (CBD)

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The ZnSe is a n-type transparent semiconductor with a band gap of 2.7eV, which has large potential for optoelectronic, and photovoltaic applications. Due to the position of its optical absorption edge (~459 nm) make of this material a promising candidate for the design of heterojunction-type solar cells. In this work, we present the synthesis of ZnSe thin films by chemical bath deposition method. Two synthesis routes were used for preparing the Znse thin films, where the effect of the hydroxide precursor (NaOH and KOH) and synthesis temperatures was assessed used. The ZnSe thin films were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD) and UV-Vis spectroscopy in order to assess the morphologic, structural and optical properties.

Keywords: ZnSe, CBD, thin film

[THF-489] Study of complexing agent effect and the reproducibility of the properties of CdS thin films synthetized by a Chemical Bath Deposition methodology.

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Thin films of CdS were synthesized by the Chemical Bath Deposition technique, to study the effect of sodium citrate as a complexing agent of the Cd^{+2} ions. The degree of reproducibility of a selected growth methodology was studied too. Three formulations of different concentrations of sodium citrate were tested, at 70 °C and at times of 15, 30, 45, 60 and 75 minutes of deposit. It was observed that the proportion of citrate in the bath has a direct influence on the characteristics of the coatings, so it was possible to identify favorable and unfavorable conditions for the chemical equilibrium of the deposit reaction and consequently for the macroscopic quality of the samples. The films obtained by a proportion of concentration citrate/cadmium 0.0025/0.0005, were yellowish greenish, perfectly homogeneous, strongly adhered to its glass substrate and with some transparency as well as specular reflection. It was shown that the complexing agent has a direct influence on the growth rate and in the homogeneity of films. Less homogeneous and thinner films at first glance, were obtained by concentration ratios citrate/cadmium of 0.0015/0.0005 M and 0.005/0.0005 M respectively. Thicknesses, optical and structural properties were studied to know the effect of these growth conditions. Optical properties of these films were studied using the UV-Vis spectrophotometer showing that have allowed direct transition and values of energy gap around 2.5 eV. Absorption spectra show the characteristic band for CdS located around 500 nm and an influence on their precise location that dependent on the concentration of citrate. Transmission spectra show that the films are highly transparent above 70% of transmittance in most of the visible spectrum. It was found that the transmittance of films decreases with increasing of the thickness. The structural properties were determined by DRX studies showing the polycrystalline and nanocrystalline nature of the films. For reproducibility studies, a select formulation was repeated 10 times. The 50 layers of CdS were characterized for a statistical analysis of the degree of dispersion of their properties. The coatings have identical macroscopic characteristics and a low standard deviation in their absorption edge data. The coefficients of variation for absorption edge between 0.12 and 0.44% is a clear evidence of the good precision of this methodology.

[THF-491] Study of better growth conditions for Chemical Bath Deposition of PbS thin films and their effects on optical, structural and electrical characteristics.

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Lead sulphide (PbS) thin films were obtained using a simplified CBD method. The methodology for synthesis used in this work contrasts with the conventional ones in two fundamental aspects, reaction temperature and reagent composition It was used room temperature conditions, which minimizes energy needs for manufacture. Triethanolamine (TEA) which is a typical component used for pH control and as a complexing agent of lead ions (Pb^{-2}) was not used in our formulations. Both, temperature and agent complexing are considered sensible factor for synthesis and controlled deposit, adhesion degree and homogeneity of any film growth by CBD. Thicknesses, optical and structural properties were studied to know the effect that growth conditions have on these properties. Were found that our films have compared properties to films synthesized by conventional and more complex formulations. The films were made onto glass slides with dimensions of 7.5 cm x 2.5 cm x 0.1 cm, at 25 °C, without TEA and deposit times from 2.5 to 6.5 hours. Were achieved metallic grey films with a thickness between 200 a 500 nm, specular reflection, certain transparency, good degree of homogeneity and reasonable adhesion to the glass substrate. It was shown that the deposit time has a direct influence on the growth rate, and that TEA is not an agent essential for the synthesis of good quality PbS films. Optical properties of these coatings were studied using the UV-Vis spectrophotometer showing that have allowed direct transition and values of energy gap around 2.12 eV. Absorption spectra show the characteristic band for the PbS located around 650 nm. Transmission spectra show that the films are virtually opaque to UV radiation, besides can transmit visible radiation in differing degrees from 10 and to 40% depending to the specific wavelength of visible light. It was found that the transmittance of films decreases with increasing of the thickness. The IR spectra show the vibrational modes characteristic of Pb-S and O-H bonds, from PbS films and $Pb(OH)_2$ nucleation centers respectively. The electrical properties were determined and DRX showed the polycrystalline and nanocrystalline nature of the films.

[THF-495] Al1-xGaxAs thin films grown on Si (100) and glass substrates

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Aluminum doped gallium arsenide ($Al_xGa_{1-x}As$) has generated an interest particular since its band gap energy can be varied between 1.42 eV for GaAs and 2.16 eV for AlAs depending on the aluminum (Al) content important for applications in optoelectronics.It's have been found that for Al content less than 4% the AlGaAs ternary alloy is a direct bandgap semiconductor, and its mismatch lattice parameter is about 1%.
In this work, we deposited $Al_xGa_{1-x}As$ layers on glass and Si (100) substrates by using magnetron sputtering technique. In order to decrease the effects of lattice mismatch parameter between the AlGaAs layer and substrates (glass or Silicon) a GaAs buffer layer about 300 micrometer thickness was previously deposited on substrate. The X-ray diffraction spectra show that the films are polycrystalline with preferential orientation (111). The Raman spectra show a behavior of two modes, corresponding to TO and LO vibrational modes of GaAs and AlAs, respectively. The band gap energy was calculated from UV-Vis spectra taken at room temperature. These results are in good agreement with the values obtained from theoretical model for an AlGaAs/GaAs/glass bilayer.

[THF-501] Slectrical and magnetic properties of GaSbMn thin films grown on Si(111)

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The development of Hall Effect magnetic field sensors with semiconductor materials III-V and III-V:Mn semi-magnetic alloys is a topic nowadays due application in different areas of physics such as spintronic. Semiconductor materials such as GaSb with a bandgap of 0.070 eV is important for a wide variety of optoelectronic applications especially in photovoltaic systems because it has optical response at wavelengths longer than silicon-based solar cells. However, when the Mn atoms is introduce in the GaSb matrix we have new opportunities in the context of spintronic, owing that in these alloys the spatial distribution of electrons and holes can be controlled easily, resulting the magnetic properties of these materials.

In this work we report electrical and magnetic properties of the GaSbMn thin films prepared by magnetron sputtering RF on silicon substrates (111) varying the growth substrate temperatures. Carrier concentrations of GaSbMn were determined from Hall Effect experiments at room temperature using the standard four-probe method. The magnetization measurements as a function of the magnetic field (-500

[THF-514] Influence of TiO2 coatings, deposited by the ultrasonic pyrolytic spray technique, on the corrosion resistance of magnesium pieces

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In this work we report the study of TiO_2 coatings on Mg substrates and their protective effect against corrosion. Mg has been widely studied to develop biodegradable implants, however, its disadvantage is the rapid degradation in physiological fluids due to corrosion. Here, the use of TiO_2 as a protective coating to modulate the corrosion resistance of the Mg pieces is proposed. The TiO_2 coating was deposited on Mg substrates using the Ultrasonic Pyrolytic Spray (SPU) technique, being a simple and inexpensive technique. Various coatings were prepared by varying experimental parameters, such as precursor flow, substrate temperature, and nozzle-substrate distance. The approximate thickness was 230 nm. The corrosion experiments were carried out using Hank's solution and Tafel curves were obtained using a potentiostat in a three-electrode configuration. The analysis of the Tafel curves showed that the magnesium substrates present a better response to the phenomenon of corrosion when the coating is deposited at low temperatures, lower than 400 ° C. The values of corrosion current (i_{corr}) show that it is possible to improve the corrosion resistance of Mg using TiO_2 coatings.

Key words. **Mg,TiO_2, corrosion, SPU.**

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ORAL SESSIONS

[TRB-82] Tribological characterization of MoS2-CNx multilayer coatings

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MoS_2 and CN_x are widely used as solid lubricants due of their wear-resistant and low coefficient of friction, therefore a multilayer arrangement with alternating layers of CNx and MoS2 were deposited to combine the monolayer properties.

In this work were deposited CN_x and MoS_2 multilayers by magnetron sputtering at 300° C on 304 stainless steel substrates and silicon wafers; Microstructure and tribological properties of multilayer coatings depend on deposition parameters like power density and distance between the target and the substrate. Both MoS_2 and CN_x were deposited with a distance of 5 cm of sputtering source and, power density of $24.68x10^3$ W/m^2 and $19.75x10^3$ W/m^2 respectively. Previous work have demonstrated that friction coefficient decrease employing as an outer layer MoS_2 over amorphous CN_x layer. This period was repeated from 1 to 5 times.

Morphology and thickness of multilayer coatings were investigated by cross section, using Scanning Electron Microscope (JEOL 7610F); the images showed a well defined multilayer arrangement and columnar structure that is characteristic of sputtered films. Thickness of coatings was around 2 to 3 microns. Tribological characterization was carrying on in a pin-on-disc type tribometer, obtaining a friction coefficient from 0.2 to 0.5. Hardness and elastic modulus of coatings were measured by nanoindentation test, obtaining elastic modulus values of 20 to 60 GPa.

[TRB-100] Microstructure and corrosion behavior of high chrome and high carbon hardfacings with Niobium additions

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Hardfacings with high chromium and high carbon are commonly known in the industry thanks to their improved strength, hardness, resistance to corrosion and abrasive wear compared to other types of hardfacings. This research studies the effect of niobium on corrosion behavior of harfacing deposited by process Shielded Metal Arc Welding (SMAW) they have been immersed into 3,5 %NaCl solution. The microstructure and the corrosion resistance was studied using optical microscopy and secondary electron microscopy (SEM / EDS) for the microstructural part and electrochemical impedance spectroscopy (EIS) for the corrosion characterization of the coatings. The corrosion tests show that the niobium additions in percentages of 4 and 6% improve the corrosion resistance of the coatings in comparison with the coating without the addition of niobium, in the microstructural analysis it was evidenced that the addition of niobium in percentages of 2,4 and 6% produce a decrease in the average size of the chromium carbides and generate the formation of niobium carbides in the matrix.

[TRB-155] Tribological performance at high temperatures of engine oil artificially degraded

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In this work, an alternative method is proposed to simulate engine oil degradation by mixing degraded oil with fresh oil to simulate a mileage. The simulated and real degraded engine oils were compared by infrared spectroscopy analysis. The dynamic viscosities of mixed oils were measured by a rheometer at 50 °C and 80 °C and a block-on-ring tribometer was used to evaluate their tribological performance under mixed lubrication regime at these two temperatures. The results showed that the simulated degradation is acceptable, the coefficient of friction decreased at higher temperature and reduced as the engine oil is close to its end of service life.

[TRB-268] Hardness and adhesion of SiOxNy thin films deposited by means of laser ablation

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Silicon oxynitride (SiO_xN_y) films are significantly attractive material because of their wide applications in optoelectronic and microelectronic devices as passivation layers because of its tunable band gap, photo luminescent, thermal stability and mechanical properties. Particularly these properties make this material ideal for solar cells applications. The main aim of the present work is to report the preparation of (SiO_xN_y) films, in order to study their hardness and adhesion that could be useful for some applications, particularly in processing of solar cells. The SiOxNy thin films were deposited using the laser ablation technique at room temperature in a pure nitrogen atmosphere. The experimental results showed the possibility of formation of different types of stoichiometry of the material when the nitrogen working pressure was varied (0.8 to 2 Pa). It was observed the formation of silicon nanocrystals embedded in an amorphous SiOxNy matrix responsible for the photoluminescent response of the samples. The Nano indentation measurements showed that in the range of pressures studied the hardness of samples is practically constant at a value of 15 GPa. The scratch tests on the films deposited at different deposition pressures (0.8 to 2 Pa) showed that the samples have good adherence to the substrate. Most of the coatings resisted a maximum load of 40 N without delamination. Raman spectroscopy and crack analyses of the scratch tests show no phase changes induced by effects of the applied load.

[TRB-304] A tribocorrosive study of tungsten nitride films

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Among the various challenges faced by the manufacture industry, degradation of machinery surfaces represents about 70% of the failure and loss. One way to combat machinery degradation is by enhancing the tribocorrosive properties of the parts that are in contact, and protective thin films are frequently used to enhance such characteristics. However, films are often designed to either reduce the mechanical wear, or to improve the corrosion resistance, but rarely are both aspects address at the same time. In the present research we focus on the use of a protective film of tungsten nitride that might provide both tribological and corrosion resistance, i.e. tribocorrosion resistance.

The tungsten nitride films were deposited at 220 °C, by RF magnetron sputtering, from a 99.99% pure W target in atmosphere of Ar and N_2. Some of the films were annealed at 400ºC for 2 hours in nitrogen to improve the crystallinity. All samples were characterized by XRD, XPS and SEM. For the initial mechanical characterization, nano-hardness and scratch test measurements were performed; giving a maximum hardness of 30 GPa and critical load, Lc2, of 17N. Finally, tribocorrosion tests were performed in an aqueous solution of citric acid, pH 4, as the electrolyte and aluminium oxide counter bodies with an applied load of 10N during reciprocating tests. After careful analysis it was shown that the tungsten nitride films had better tribocorrosion resistance than the AISI D2 steel. Therefore, such coatings are a viable option as protective films for machine processes in the manufacture industry.

[TRB-321] Application of fuzzy-based Taguchi method for the optimization of tribological performance of borided steel

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Borided steel components have a wide range of industrial applications due to their remarkable tribological, mechanical and anticorrosive properties. Boriding is being increasingly used due to its high wear resistance and low coefficient of friction. In this work, an experimental research of tribological behaviour of a borided steel under dry condition on a pin-on-disc and oscillating tribotester is carried out. The wear and friction tests are undertaken based on Taguchi's L_{27} orthogonal array accounting three main factors, namely, contact pressure, sliding speed and sliding distance. Experimental results are further examined to obtain the optimum friction and wear characteristics simultaneously utilising fuzzy logic analysis. The optimal combination is achieved at the lowest levels of all the three tribological factors. Analysis of variance is used to find the percentage contribution of each factor and their interactions on the responses. 2D surface and contour plots are used to study the variations of wear depth and coefficient of friction with the related factors. Surface morphology, diffused phases in the layer analysis, wear mechanism and layer composition analysis are done with the help of scanning electron microscopy, X-ray diffraction and energy dispersed X-ray analysis, respectively.

[TRB-328] Wear Measurements under Conditions of Different Relative Humidity

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The wear of the titanium oxi-nitride coatings made by physical vapor deposition has been studied to assess their performance and mechanical resistance. Although there are many factors involved in the wear mechanism (the applied force, the nature of the counter-body, the film thickness, etc.), it is well-know that the relative humidity surrounding the point of contact can be of great influence.

There are many ways to analyze the wear, but one of the most commonly used is the reciprocating sliding test. With this test, we can observe how the coefficient of friction change during the wear of the film and measure the wear volume and the diameter of the wear scar.

In this work we modified our standard reciprocating sliding test machine in order to control the relative humidity of the contact area between the counter-body (alumina) and the surface of the titanium based film on a stainless steel substrate. We report the variation of the wear of the nanostructured RF sputtered coatings as a function of the relative humidity. The motivation of this research is based on the fact that titanium based coatings have many applications, such as biological, aeronautics, automotive, etc., and a lot of these involve environments with very different relative humidities.

[TRB-337] Mechanical and tribological properties of AlSiN thin films with different Si content

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Aluminum silicon nitride (AlSiN) thin films are of great interest as a multifunctional coating that combines optical, mechanical and tribological properties that can be useful in different applications. Nevertheless, each of these properties can be optimized at different silicon contents. In the present work a series of AlSiN thin films with different silicon content (from 1.5 up to 20 at. %) were deposited, in order to study the hardness and adhesion behavior as a function of the silicon content, and were compared with their optical properties. The thin films were deposited using the simultaneous laser ablation of two targets (Al and Si) in a nitrogen atmosphere. The silicon content in the films was controlled via the control of the density of the plasma produced during the ablation of the silicon target. Depending on the silicon content on the films, these coatings can be produced with a band gap from 3 up to 5 eV, where the higher the silicon content produces the more transparent material. The hardness of the films can be also modulated as a function of the silicon content, achieving a maximum value of 30 GPa when the silicon content is equal to 4 at. %. The scratch tests run up to 40 N load, showed that the best adhesion of the films to the substrate (quartz or stainless steel) is obtained for the higher silicon contents.

[TRB-367] Lubricious metal oxide coatings

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The development of coatings to function as solid lubricants in applications where high temperatures (above 500 °C) are reach is of special interest for a wide range of industries. Under these environmental conditions, most of the sliding surfaces will oxidize, therefore the oxide films will dominate the friction and wear behavior of the interfaces. One possible solution is the design of coatings based on stable oxides that present low coefficient of friction and/or wear at high temperatures. Recent empirical models have shown that certain oxides, known as lubricious oxides [1, 2], have low shear strength at elevated temperatures and hence could be used as solid lubricants. In this talk, the basics of the two different empirical models proposed for the selection of such lubricious oxides are presented showing their similarities and differences. Aiming to test some of the predictions given by the empirical models, the results from the tribological properties of selected metal oxide coatings produced by magnetron sputtering are presented. We report the synthesis, structure and the wear behavior evaluated at 3 different temperatures (298, 573 and 873K) using the pin-on-disk technique.

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2. B. Prakash, J.P. Celis, Tribol. Lett. 27 (2007) 105–112.

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Keyword: Coefficient of friction, metal oxide coatings, Sputtering

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[TRB-8] Tribocorrosion and corrosion behavior of Ti-6Al-4V alloy coated with TaN/Ta layers in two simulated body fluids.

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Ti-6Al-4V ELI alloy is one of the most used materials in biomechanical industry due to its high corrosion resistance as well as its elastic modulus relatively close to that of bone tissue. This material also has excellent biocompatibility, besides its surface can be treated to promote osseointegration with host tissue. However, this alloy suffer from a low wear resistance in dry and wet conditions. This work focuses on the synthesis of hierarchical multilayer of Tantalum Nitride/Tantalum layers by magnetron sputtering on substrates of Ti-6Al-4V ELI alloy. TaN and Ta coatings are biocompatible materials, both are chemically stable, also TaN has high nanohardness, these properties make the coating of TaN/Ta resistant to simultaneous attack of corrosion and wear. Structure as well as composition of coatings were studied by XRD and EDS techniques respectively. Raman spectroscopy as Scanning Electron Microscopy were used to analyze wear track of alloy and coated samples. Hardness of hierarchically multilayer was measured based on compound hardness. Scratch technique was used to quantify adherence of multilayer on substrate. Tribocorrosion tests was made in two different simulated body fluids. One made of deionized water plus salts with same ions concentration than in human blood. Other of Fetal Bovine Serum (FBS) with a compensatory ion solution to reach ions concentration at blood. The load applied was between 0.5 to 2 N using a ball of Al2O3. Coefficient of friction, wear rate, open circuit potential, corrosion rate and total lost material were measured and its results showed a reduction of wear and corrosion rates as a consequence of TaN/Ta coating. Incorporation of proteins by means of FBS$_i$ in corrosive medium reduces coefficient of friction.

[TRB-48] Tribological Study of TiN, TiCN, AlCrN and TiCrN coatings produced by PVD (Cathodic arc) on D2 steel

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The metal mechanic industry demands new technologies and more efficient tools for all the machining processes. All this due to ecological laws, the high costs of the materials and new ways to build thing. The analysis and application of new and better cutting tools and harder coatings it's the reason for this specific research.

For this project, different coatings (AlCrN, TiN, TiCrN, TiCN) were deposited using PVD cathodic arc method over a D2 steel substract. This coated substracts went through different analysis like structural (Hardness and Scratch), chemical (EDS and XRD) and tribological tests. The chemical composition of the coatings was evaluated by energy-dispersive spectroscopy (EDS). A scanning electron microscopy (SEM) was used to analyze and see the visual results (traces of abrasion wear) of the tribological test.

As results showed after the tests were carried out, the AlCrN coating had excellent properties and the result was a tribological layer protection generated by the coating itself from the material removed during the sliding process giving it the lowest friction coefficient from them all.

Also, the AlCrN coat has a wear volume of 6.2806e-13 m^3

[TRB-49] Hardness and scratch study of TiN, TiCN, AlCrN and TiCrN coatings produced by PVD (Cathodic arc) on D2 steel.

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Industry has employed cutting tools with hard coatings for years now. Nowdays, efficiency, costs and resourses have become more important and therefore, tools and new coatings must be analysed and tested for better results.

In this project, a number of different PVD coating thin films based on TiN with inclusions of C and Cr were analyzed to choose which one was better to coat high speed cutting tools. Cathodic arc PVD process was used to coat the studied substracts. The given coatings are TiN, TiCN, TnCrN, AlCrN and these were deposited on a D2 steel substract.

Different tests were carried out to observe and analyze the behaviour of the coatings. An EDS (Energy-dispersive spectroscopy) analysis was done to obtain the Chemical composition of the coating and the percentage of the elements shown, as well as a X-Ray diffraction test (XRD) to determine the structure. Then, scratch test was applied to measure and detect thin film coating failure. Then, the coated pieces went through a Hardness Vickers test to obtain the coating hardness.

As results of the Hardness and scratch tests, The TiCN coated substract showed the best performance and Hardness level with a HV (Hardness Vickers) of 2157, followed by the AlCrN subtract with a HV of 1640 making these two the harder coatings in the test. As to say about the scratch test, AlCrN substract showed a better result being the one with a minor tangential force on it´s surface.

[TRB-64] Wear behavior of TiWSiN thin films deposited via co-sputtering

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In this work it was studied the influence of tribological pairs on wear properties of TiWSiN thin films. The films were deposited by mean of magnetron co-sputtering on high speed steel substrates. The microstructure and chemical composition of films were analyzed by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS), respectively. Wear resistance and friction coefficient were evaluated by mean of the ball-on disk test. Different ball materials were used for the test like alumina, silicon nitride, stainless steel and zirconia. The morphology of the wear track was characterized by scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS) and microscopy 3D. The wear mechanisms of TiWSiN films in function of tribological pair will be discussed in this work.

KEYWORD: EDS, Wear, TiWSiN, tribological pair.

[TRB-417] Tribological study of Hydroxyapatite/Silver coating on stainless steel AISI 316L substrate

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Modification of orthopedic prostheses by the incorporation of a biocompatible coating is attractive due to the attributes that arise from the biomaterial design of the interface. Hydroxyapatite (HA) is a favored ceramic that has served functionalities such as enhancing fixation and stabilization of the implant. In this research deposits of hydroxyapatite (HA) doped with silver (Ag) were obtained by electrodeposition technique. The electrochemical deposition method can be performed by simple apparatus compared with vacuum processes, and hence is environment-friendly. This method can be also used to control the composition, structure, and adhesion of the deposited layer with a relative ease. Hydroxyapatite/silver (HA/Ag) powder was prepared by a modified chemical precipitation method by the reaction of calcium oxide (CaO), silver nitrate ($AgNO_3$), and phosphoric acid (H_3PO_4). It was used as the cathode a platinum electrode and as anode a stainless steel AISI 316L electrode. The coatings of hydroxyapatite (HA) and silver (Ag) are widely used in biomedical applications due to their properties as biomaterials. Characterization studies of microstructure and chemical composition were performed by X-Ray Diffraction (XRD) and Fourier transformed infrared spectroscopy (FTIR). Micro-hardness was evaluated with a Vickers indenter at 50grs of load. Wear tests were carried on by a reciprocating sliding movement tribometer, employing a 10mm diameter Al_2O_3 ball, in dry conditions at 1 and 2 N normal loads to evaluate the tribological behavior. Wear tracks were analyzed by optical microscopy, to obtain volume loss (V) and wear rate (k) values; and Raman spectroscopy was performed to evaluated the presence of HA and oxidation inside the wear track. The HA/Ag coating exhibited the lowest values of volume loss (V) and wear rate (k), $8.15x10^{-3}$ mm^3 and $4.53x10^{-4}$ mm^3/Nm respectively, at 1N load. The HA/Ag coating on the substrate, showed a lower friction coefficient (u) values on the tribological tests with respect to the uncoated substrate.

[TRB-563] Green high-performance and low-friction interfaces tailored by the reactivity of novel DLC coatings and ionic liquids

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Current UN, EU and national emission legislation already restricts the use of some of today's key lubricants, for which there are no acceptable alternatives available. Without new green lubrication solutions, the performance of machinery will deteriorate, reducing operating lifetimes, shortening maintenance intervals, wasting materials, and generating higher energy losses, all leading to large-scale technical and economic consequences for the EU. GreenCOAT is about developing innovative DLC coatings tailored for chemical activity with ionic liquids, combining a unique, in-situ, ionic-liquid–DLC adsorption and a simultaneous tribological study, to establish the boundary films' adsorption kinetics, reveal their electrochemical and tribocorrosion behaviour, then perform a detailed (sub)nano-scale surface characterisation and a full-scale, green-interface validation for heavy-duty fluidpower hydraulics systems. Doped (Ag, W) and tailored DLC coatings via HiPIMS deposition for greatly improved reactivity with green IL additives. A new fundamental understanding of the tribological formation/removal of the adsorbed IL films on DLC coatings, their adsorption and chemical nature, as well as electrochemical and tribo-corrosion property will be developed. This is largely absent from the literature.

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