



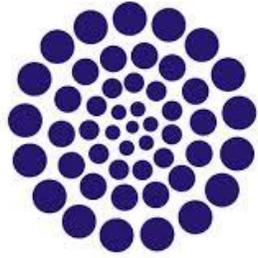
**Sociedad Mexicana de Ciencia y Tecnología
De Superficies y Materiales A.C.**

X *International Conference
on Surface, Materials and Vacuum*



September 25th-29th 2017, Cd. Juárez, Chihuahua, México

PROCEEDINGS



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X International Conference in Surfaces, Materials and Vacuum
September 25th-29th, Cd. Juarez, Chihuahua, 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 ocaion we are pleased to welcome you to participate in the X International Conference on Surface, Materials and Vacuum (ICSMV) which will held in Cd. Juarez, Chihuahua from the 25th to the 29th of September 2017.

The scientific program of the Conference is divided into plenary conferences, short courses and the different symposia with oral and poster contributions. For the X edition there will a total of 15 symposiums and one forum for science divulgation. For the X edition we keep the invited simposium of Luminescence Phenomena: Materials and Applications and the Atomic Layer deposition, the Ab-initio Calculation and Supercomputing have been reformulated as the symposium Theory and simulation of materials. From now on the Surface and Interfaces Symposium has been propose as a new forum for compiling the contributions that our members that are scattered across other symposia that could fit more properly as a surface phenomena. 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 X ICSMV
Organizing Committee SMCTSM
September 2017, Cd. Juarez, Chihuahua, México



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X INTERNATIONAL CONFERENCE IN SURFACES, MATERIALS AND VACUUM

PLENARY LECTURES



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OPENING TALK

Chirality and Optical Activity at the Nanoscale

Cecilia Noguez
Instituto de Física, UNAM, México

Chirality, the asymmetric property of non-superposable mirror images (enantiomers), is present in molecules and compounds that are essential for life. Chirality also exists in inorganic systems at the nanoscale. Chiral systems are optically active and exhibit electronic circular dichroism (CD) in the same electromagnetic window where they absorb light. CD spectroscopy is capable of measuring small differences in light extinction between right and left circularly polarized light, which makes CD a very sensitive tool to distinguish between left and right-handed enantiomers. Understanding how to control and increase the sensitivity limits of CD spectroscopies would have significant impact in pure and applied sciences; providing a powerful tool for exploring and controlling chirality-dependent phenomena, including circular dichroism, templated enantioselective-growth in stereochemistry, electronic spin filters in spintronics, among other fields. In this talk, the mechanisms that originate and control optical activity in nanoscale systems such as organic-metal hybrid NPs and twisted bilayer graphene (TBLG) are identified using a time-perturbed density functional theory. In the first case, electronic circular dichroism (CD) is studied in terms of the intrinsic chirality of the ligands, the number of ligands and the induced chirality by the arrangement of the chiral and achiral ligands in the NP. The analysis of CD allows the identification of the spectral regions where the induced chirality by the ligand array dominates over the intrinsic chirality of the adsorbed molecules, determining conditions for the control and enlargement of CD.¹ In the second case, the experimental realization of thin films with full control of the structural handedness down to the atomic scale, which is possible by stacking two graphene layers whose chiral properties are designed by an interlayer rotation angle is also investigated.²



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These results would be significant in the discussion of experimental CD spectra, which allow the development of new strategies to improve the sensitivity of chiroptical spectroscopies.

(1) Hidalgo, F.; Noguez, C. *Nanoscale* **2016**, 8, 14457.

(2) Kim, C.-J.; Sanchez-Castillo, A.; Ziegler, Z.; Ogawa, Y.; Noguez, C.; Park, J.

Nature Nanotechnology **2016**, 11, 520.



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PLENARY LECTURE I

Hardened ICs for Aerospace Applications

Jair Garcia Lemont

General Electric, Fairfield, NY, USA

This presentation is dedicated to explore the different aspects that determine the potential malfunction of the integrated circuits because of being immersed in a radioactive environment such as the space. There is also a survey on the main approaches for modeling and simulating the negative effects and be able to evaluate the robustness of circuits against radiation. Finally, there is a review of the main design techniques to be used for mitigating radiation effects at different levels of abstraction.



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PLENARY LECTURE II

Multiscale modelling of high efficiency quantum solar cells

Julio C. Rimada¹, Luis M. Hernández², Carlos I. Cabrera³ and James P. Connolly⁴

¹*PV Research Laboratory, Institute of Materials Science and Technology (IMRE), University of Havana, La Habana, Cuba.*

²*Faculty of Physics, University of Havana, Colina Universitaria, 10400 La Habana, Cuba.*

³*Academic Unit of Physics, Autonomous University of Zacatecas, Czada. Solidaridad y Paseo La Bufa S/N, 98060 Zacatecas, Zac., México.*

⁴*Laboratoire GeePs, IPVF (Institut Photovoltaïque de l'Île de France), Paris, France.*

While photovoltaic energy is achieving grid-parity around the globe, efforts to reach higher solar cell efficiencies becomes ever more difficult as they approximate the limiting efficiency. The so-called third generation concepts attempt to break this limit through a combination of novel physical processes and new materials and concepts in organic and inorganic systems. The different approaches are showed with some examples. The use of multiscale experimental and theoretical techniques to go beyond the semi-empirical understanding of these systems can lead to important achievements in the improvement of actual devices and the proposition of new designs. We show the modeling of quantum well solar cells that work in different scales, from the nanostructure to the macroscopic device characteristics. Several results of the model developed, for the different material systems and structures used will be presented, showing the different constrains of the different parameters established by the modeling in order to reach high conversion efficiencies.



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PLENARY LECTURE III

Diagnosis of Breast Cancer Using SERS in Human Saliva

Hugo Ricardo Navarro Contreras

CIACYT-Universidad Autónoma de San Luis Potosí, México.

Breast cancer is the most common type of malignancy in women and their second leading cause of cancer death. The most common method in screening and diagnostic is the mammogram. The Sialic Acid (SA), is an important pathophysiological marker and is typical to find it in high concentrations in saliva of persons with breast cancer. Due to this, SA's measurement, it appears as a form of early, effective and not invasive diagnosis of the mammary neoplasia. Surface-enhanced Raman scattering (SERS) is a phenomenon that heightens the emission Raman, proceeding from an analite that is adsorbed or be located in the proximity near to a metallic surface. In this work is demonstrated, that the use of the technique SERS, produced by silver nanoparticles, provides the high sensibility, the selectivity and specificity of SA's detection, what turns it into a viable method of diagnosis.

Acknowledgements

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Keywords: Silver nanoparticles, Surface enhanced Raman spectroscopy, breast cancer, silaic acid.



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PLENARY LECTURE IV

Quantum Molecular Machines

S. W. Hla^{1,2}

1Department of Physics & Astronomy, Ohio University, OH 45701, USA.

2Center for Nanoscale Materials, Argonne National Laboratory, IL 60439, USA

One of the goals of nanotechnology is the development of complex molecular machines that can be operated with atomic level control in a solid-state environment. Most biological molecular machines have the sizes from tens of nanometers to a few microns –a range where classical machine concepts hold. However, artificially designed molecular machines can be in the size range down to a few nanometers or less, which is in the range of quantum processes. In this talk, we will present various artificial molecular machines such as molecular motors and linear transport devices such as molecular cars operating in the quantum regime on materials surfaces. Fundamental operations of these synthetic molecular machines are investigated at one molecular machine-at-a-time in an atomically clean environment using low temperature scanning tunneling microscopy (STM), tunneling spectroscopy, and molecular manipulation schemes [1,2]. These investigations reveal how charge and energy transfer are taken place within single molecular machines as well as among the molecular machines in the molecular networks. Moreover by introducing dipole active components in the rotor arms of the molecular motors, communication among the molecules can be introduced via dipolar interaction. In addition to single molecule operations, synchronization of molecular motors can be achieved depending on the symmetry of the molecular assemblies on surfaces and the strength of applied electric field energy. Here, all the molecular motors can be rotated in a synchronized manner using 1V or higher electric field supplied from the STM tip. Below this bias, the rotor arms of the molecular motors can reorient into different directions. Careful analyses reveal that such reorientations of the molecular motors are not random, but they are coordinated to minimize the energy. Furthermore, individual molecular motors can be charged using the inelastic tunneling scheme with the STM tip. This introduces spin-active components within the molecular motors and enables us to investigate spintronic properties of individual molecular motors at the sub-molecular scale using tunneling spectroscopy. For the linear



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transport, we will present the latest development of molecular hoverboards and molecular cars for a control transport at the nanoscale.

Keywords: STM, atom/molecule manipulation, molecular machines

Presenting author's email: hla@ohio.edu

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2. U.G.E. Perera, F. Ample, H. Kersell, Y. Zhang, G. Vives, J. Echeverria, M. Grisolia, G. Rapenne, C. Joachim, and S.-W. Hla. Controlled Clockwise and Anticlockwise Rotational Switching of a Molecular Motor. *Nature Nanotechnology* 8, 46-51 (2013).



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PLENARY LECTURE V

Pulsed laser deposition of functionalized glasses

*José Gonzalo,
Instituto de Óptica, CSIC, Spain*

The spread use of photonic devices requires the combination of multiple optical active components such as switches, lasers or amplifiers, on a common planar substrate at a reduced cost and presenting low power consumption, while maintaining their compatibility with the current fiber technology. The excellent optical properties and ease of preparation of glasses makes them promising materials to achieve that goal. However, their application requires first the fabrication of high quality micron-thick thin films with good optical performance. This presentation will show that Pulsed Laser Deposition (PLD) is very attractive for this purpose. We will review our activity on the fabrication of metastable complex oxide film glasses and their nanostructuration through the incorporation of rare earth (RE) ions as functionalizing elements. We will show first how a fine tuning of the deposition parameters allows the synthesis of good quality transparent heavy metal oxide film glasses with unconventional structure and a composition well outside the bulk glass formation region, which may present a nonlinear refractive index up to 10^3 times larger than that of fused silica. Then, we will present an overview of the capability of alternate-PLD for the synthesis of nanostructured film glasses with a controlled RE concentration and a pre-designed in-depth distribution. This opens a broad range of material function and design possibilities, since the optical and photoluminescent properties of the produced nanostructures can be tailored at the nanoscale.



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PLENARY LECTURE VI

Femtosecond-resolved imaging during femtosecond laser structuring

Javier Solis, Jan Siegel

Laser Processing Group, Instituto de Optica, CSIC

The strong development over the last years of “non-linear” processing using ultrashort laser pulses has made necessary the corresponding development of tools aimed either at providing information regarding the dynamics of the process and its mechanisms or at enabling the optimization of the process in particularly complex interaction scenarios. Imaging techniques, either time-integrated or time-resolved, provide a unique tool that has been long used for the assessment of ultrafast laser-solid interactions. The presentation will provide an overview of our work regarding the use of plasma imaging techniques (“fs-resolved microscopy” in different modalities) for the assessment of the interaction of ultrashort laser pulses with dielectrics and semiconductors. We have used it in different experimental configurations equivalent to those found during fs-laser processing, ranging from surface ablation to subsurface micro-structuring, or the recently developed “ultrafast moving-spot microscopy” scheme for analyzing the dynamics of formation of laser induced periodic surface structures (LIPSS).



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PLENARY LECTURE VII

2D – 3D structural transition in sub-nanometer PtN clusters supported on CeO₂(111)

*Lauro Oliver Paz Borbón³, Andres López Martínez³, Ignacio L. Garzón³, Alvaro Posada Amarillas²,
Henrik Grönbeck¹*

¹*Competence Centre for Catalysis and Department of Physics, Chalmers University of Technology,
Sweden*

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One of the most technologically relevant application of oxide supported transition metals lies in heterogeneous catalysis. This is particularly true in emission control systems - such as the catalytic converter of automobiles - where they are usually highly dispersed and known to be oxidized under ambient conditions. One component in the automobile three-way catalytic converter is Pt/CeO₂; where Pt serves to oxidize hydrocarbons and carbon monoxide, while ceria (CeO₂) acts as an oxygen storage component. Although control at the nm-scale is desirable to open new technological possibilities, there is limited knowledge, both experimentally and theoretically, regarding the geometrical structure and stability of sub-nanometer platinum PtN/CeO₂(111) supported clusters.

In this talk, I will describe the implementation of an unbiased global optimization Basin Hopping Monte Carlo algorithm – where interatomic interactions are modelled via Density Functional Theory (DFT) methodology – to efficiently explore the potential energy surface (PES) configurations of PtN/CeO₂(111) clusters up to 10 atoms. Our calculations show a clear preference for planar 2D structures up to size Pt₈, followed by a structural transition to 3D structures at Pt₉. Our results indicate that the reducibility of CeO₂(111) surface provides a mechanism to anchor PtN clusters, where they become oxidized in a two-way charge transfer mechanism: (a) an oxidation process, where O_{surface} atoms withdraw charge from Pt atoms forming Pt-O bonds, (b) surface Ce⁴⁺ atoms are reduced to Ce³⁺. The active role of CeO₂(111) support in modifying the structural properties and eventual chemical reactivity of sub-nanometer PtN clusters is computationally demonstrated.

Keywords: DFT-based global optimization; supported Pt clusters; CeO₂ oxide support, cluster oxidation.



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PLENARY LECTURE VIII

Characterization and luminescence properties of RE (Er, Tb) and Li codoped ZnO nanostructures

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ZnO nanostructures have been extensively investigated during the last years due to their application in different optoelectronic devices. The wide direct bandgap (3.37 eV at room temperature), high exciton binding energy (60 meV) and high refraction index ($n=2.45$) make this material a good candidate to fabricate the next generation optical nanodevices. In this regard, doping ZnO nanostructures with rare earth ions is particularly significant since the optical properties of the nanostructures can be modified. Among these ions, Er³⁺ is interesting since it shows an intense intraionic transition at 0.8 eV (1.54 μm) which corresponds to minimal loss wavelength in optical communications. Furthermore, codoping semiconductor nanostructures is an efficient method to increase the intensity of this emission. In particular, Li⁺ ions have been shown to be a good candidate as activator since they slightly alter Er³⁺ symmetry which leads to a variation of probabilities of the intraionic transitions [1]

In this work, micro- and nanostructures of ZnO codoped with Er and Li and Tb and Li respectively, have been grown by a catalyst free vapor-solid method under constant N₂ flux. Nanowires and nanobelts with lengths of several microns, and thicknesses of a few hundreds of nanometers have been obtained [Fig 1(a)]. The amount of Er³⁺ Tb³⁺ incorporated into the structures has been assessed by Energy Dispersive X-ray Spectroscopy (EDX) and ranges between 2 and 6 %wt. Luminescent emission of the samples has been studied by cathodo- and photoluminescence (CL and PL). In the case of Er doped samples, as it is shown in figure 1(b), the relative intensity of the 0.8 eV (1.54 μm) emission



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band is higher in the codoped samples than in the samples where only Er³⁺ is used as dopant. The light guiding properties of the nanostructures obtained have been studied by μ PL. Figure 1c shows that the luminescence is guided along the codoped nanostructures. Spectra recorded at the exit point show that free excitons emission of ZnO is reabsorbed by the material in its path along the nanobelt while bound excitons and deep level emission bands are still present. Finally, optical resonant modes have also been observed in the nanostructures which gives rise to the possibility of using them in a wide variety of optical nanodevices



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SHORT COURSES



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SHORT COURSE A

VLSI Design and Verification

Jair Garcia Lemont

General Electric, Fairfield, NY, United States

This workshop is destined to engineers that want to develop its skills on the main standard approaches for designing VLSI Digital Systems. It is a complete development flow which comprises Architecture, Microarchitecture, RTL Coding, Analysis Pre-routing, Floor Planning, Analysis Post-routing, Testbench Elaboration and Physical Testing. At the end of this session, the engineer will have a clear idea of the scope that VLSI technology comprises.



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SHORT COURSE B

Atomic Layer Deposition (ALD) for Micro- and Nano-Electronics

Jiyoung Kim

Materials Science and Engineering, University of Texas at Dallas

The outline of the below courses includes a complete selection of topics that are normally covered during a multi-day Basic Vacuum Technology and Helium Leak Detection course/seminar. Shorter seminars consist of selected topics from these curriculums that are tailored to specific areas of interest expressed by seminar attendees. These topics are selected based on a quick survey with seminar attendees, conducted at the beginning of the seminar.

Seminar Outline

Vacuum Technology Seminar:

Introduction to Vacuum Applications and Fundamentals

- Working with numbers and temperature scales
- Understanding matter, pressure, gas properties
- Vapor pressure and outgassing
- Gas flow and conductance
- Pumping speed and throughput
- Overview of vacuum pumping methods
- Rough Vacuum Systems
 - Gauges
 - Wet and dry mechanical pumps
 - Traps and filters
 - Pump comparison



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High & Ultra High Vacuum Systems

- High Vacuum
- Gauges
- Turbo pumps/controllers and diffusion pumps
- Baffles and traps
- Cryopumps
- Pump comparison
- System configurations and operation

Vacuum Technology & Leak Detection Seminar

(Optional) - Pumping System demonstration: Rough & High vacuum system assembly and operation

- Ultra High Vacuum
- Outgassing issues
- Gauges
- Ion pumps
- Non-evaporative getter pumps
- Titanium sublimation pumps
- System configurations and operation

Vacuum Materials and Hardware

- Material selections
- Joining techniques
- Fittings, feedthroughs, and valves
- Vacuum system performance and troubleshooting
- Characterizing the system
- Most common problems with vacuum systems and typical sources



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Fundamentals of Helium Leak Detection:

Why leak test?

- Leak detection operations
- Understanding leak rate
- Leak detection methods

Leak Rate Specification Conversions

- Specification leak rate vs. std. cc/sec
- Specification pressure vs. test pressure
- The helium leak rate

Locating Leaks

- Spray and sniffer probe techniques

Measuring Leak Rate

- Leak rate testing software overview
- Hard vacuum: Inside-out testing (pressurized part)
- Hard vacuum: Outside-in testing (evacuated part)
- Bombing
- Accumulation testing

Application Specific Leak Rate Testing Examples

- Hermetically sealed parts
- Pressurized parts: accumulation method
- Pre-pressurized parts in large vacuum chamber
- Parts with pressure differential intolerance
- Small part/high sensitivity
- Long narrow tubes
- Process gas components and systems

(Optional) - Leak Detection equipment demo: basic operation of Leak



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Detector unit; leak testing of components and vacuum systems.

SHORT COURSE C

Piezoelectric characterization of ferroelectric domains by Piezoresponse Force Microscopy (PFM) using Dual AC Resonance-Tracking (DART).

A. Hurtado-Macías

Centro de Investigación en Materiales Avanzados S.C., and Laboratorio Nacional de Nanotecnología, Chihuahua, México.

The characterization of the structure and nature of ferroelectric domains in ferroelectric crystals and ceramics has been the subject of countless investigations over the past three decades. Recent research interests in ferroelectric materials are focused on their potential application as the active material in micro electromechanical systems (MEMS) such as non-volatile memories, sensors and dielectric devices. Nevertheless, in practical applications there is often concern about the potential degradation of the ferroelectric and ferroelastic properties such as the polarization, fatigue, plastic deformation and fracture. That is, the mechanical properties of the domains can influence the reliability and performance of the ferroelectric devices. Moreover, current devices have been reduced to micro scale, where its components consist only of a few domains so that the mechanical properties of each domain play a critical role in the design, manufacture and performance of devices. However, the mechanical properties of single domains need further investigations for full understanding [3]. Piezoresponse force microscopy (PFM) is used to characterize the electromechanical response of piezoelectric materials. Typically, a conductive cantilever is scanned over the sample surface in contact mode. While scanning the surface, an AC bias is applied to the tip. The electric field causes a strain 5-10nm below the surface which in turn causes a periodic deflection of the cantilever. Recently, a variation on this technique called Electrochemical Strain Microscopy (ESM) has been developed at Oak Ridge National Laboratory. This technique is sensitive to ion transport into and out of the lattice in energy storage (battery) materials such as LiCoO₂. This course describes how to run Dual AC Resonance Tracking



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Piezo Force Microscopy (DARTPFM), including using the technique to run hysteresis loops on ferroelectric materials.

SHORT COURSE D

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

Richard W. Borrett
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.



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SHORT COURSE E

Photovoltaics: from solar cells to big PV systems

Julio C. Rimada Herrera

*PV Research Laboratory Institute of Materials Science and Technology (IMRE) – Faculty of Physics
University of Havana, CUBA.*

In this short course the basics of photovoltaics energy conversion will be explained. The different technologies and materials used for fabrication of solar cells will be showed, focusing on the main technologies applied for today PV applications. The components for the installation of PV systems will be shown and their relative costs, compared with overall costs of complete systems, discussing the evolution of the PV costs and the increase of installations in the last years.



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TECHNICAL TALKS



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TECHNICAL TALK

Mo is the new Cu: See more with High Radiation

Jorge Pablo González.

Malvern PANalytical

Virtually all powder diffraction experiments in the home laboratory are done using Cu radiation. However, for certain applications more penetrating, ‘hard’ radiation is better suited. For such experiments, people often make use of synchrotron radiation, losing valuable time by waiting for beam time availability. Every Empyrean diffractometer is prepared to be used with hard radiation X-ray tubes with Mo or Ag anodes. Empyrean is certified up to 60 kV, maximizing the efficiency of the X-ray excitation. New developments on the source, optics and detector technologies have made the use of hard radiation as quick and easy as Cu, and allow for a variety of hard radiation experiments in the home lab, such as:

- Crystallography
- Short-range order measurements (pair distribution function)
- Computed Tomography
- In operando studies of batteries



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SYMPOSIA



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ADVANCED AND MULTIFUNCTIONAL CERAMICS (AMC)

**Chairmen: Jesus Heiras Aguirre (CNYN-UNAM)
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[AMC-125] Development of nanostructured alumina-based ceramic composites

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Water pollution by heavy metals represents one of the most important environmental problems. These elements enter the trophic chains and are bioaccumulated, causing several diseases and metabolic damage. As a result, the development of new materials for metal removal from aqueous media at low cost has gained interest. In this project, the fabrication of fibrous nanostructured ceramic materials by electrospinning for adsorption processes is proposed. Alumina nanofibers were obtained from different precursor solutions. According to Optic and Scanning Electron Microscopy, the mean diameters of green and calcined fibers were 900 ± 200 nm and 100 ± 20 nm, respectively. Chemical bonds and functional groups were determined by Fourier Transformed Infrared Spectroscopy (FTIR). The spectra of green fibers show the stretching vibrations of carbonyl group (C=O) at 1643 cm^{-1} , while the band at 1420 cm^{-1} corresponds to Al-OH bonds. Bands corresponding to amorphous ($648\text{-}400\text{ cm}^{-1}$), gamma (830 and 507 cm^{-1}) and delta ($729\text{-}738\text{ cm}^{-1}$) alumina polymorphs were observed in the spectra of fibers calcined at 800°C . On the other hand, the spectra of fibers sintered at 1600°C showed only the characteristic vibration bands of α -alumina phase.



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[AMC-128] Fabrication of zirconia fibers by sol-gel and electrospinning

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Zirconia is a zirconium oxide has three different forms a monoclinic, cubic and tetragonal zirconia has been applied in the industries to obtain abrasive coatings, additives, inorganic pigments and electrical components, Also as a bioceramic in the manufacture of hip, knee and dental prostheses, as well as in the manufacture of oxygen sensors and as gas adsorbent material in vacuum chambers. However in ceramic materials there is difficulty in obtaining finished products, which is why production processes are expensive, so new advanced ceramic materials based on zirconium oxide (zirconia, ZrO₂) have recently been produced to obtain better zirconia properties., However there is no specific route to obtain a fibrillar structured material, hence the need to establish a new route of synthesis and processing for obtaining zirconia membranes with high surface area. The manufacture of zirconia fibers by the electro spinning method offers an alternative for the production of ceramic materials that can be exploited in multiple applications. Precursors ZrO₂ were synthesized through the sol-gel method and then incorporated into a polymeric PVP matrix; later they were processed by electrospinning to obtain fibers with an average diameter of 91±25 nm. The ZrO₂ structure was demonstrated by Raman, DRX, IR, SEM and EDX.



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**[AMC-146] Nanostructure-Optical Properties Relationship of Sol Gel- Solvothermally Derived
Anatase TiO₂ Thin Films formed by flow coating**

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Anatase titania thin films were prepared by the flow coating process on glass substrates from chemically modified ultrafine anatase powder precursors via the use of a chelating titanium -acetate complex. The aqueous sol-gel low temperature acidic synthesis used the Ti(BuO)₄ precursor followed by solvothermal treatment resulting on chemically binding the carboxylic acid onto TiO₂ nanoparticles. Nano-powders and thin films were characterized by TEM, HRTEM, FESEM, FTIR, UVvis, and AFM. As-deposited dried films were analyzed by spectroscopic ellipsometry to determine the refractive index. Outstanding high refractive index and highly transparent thin films presumably are the result of the carboxylic acid bound anatase nanoparticles. The high value of the band gap (3.6-3.9) resulting from the extremely small average 1.9 nm aspect ratio anatase nanoparticles was found to influence the porosity of the thin films. The flow coating process allowed to produce nanostructured anatase thin films with a very low roughness and controlled porosity. Furthermore, it allowed to direct self-assembly nano-anatase into large nano-structures with crystals oriented in the direction of the flow coater.



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[AMC-311] Structural investigation of polycrystalline materials from X-ray diffraction pattern to structure solution: the EXPO program

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In the last 25 years, interest for powder solution is remarkably increased and the number of crystal structures solved by XRPD is surprisingly growing. The reasons of this progress can be found in the evolution of diffractometric instrumentation and in the development of new and efficient computational, methodological and theoretical approaches for data analysis.

Ab-initio crystal structure solution from powder diffraction data is not a straightforward process. Peak overlap, background noise and preferred orientation can all contribute to the low accuracy of integrated intensity estimates extracted from the powder diffraction pattern thus reducing the chance of success of the phasing procedures, particularly when the traditional two-step approaches are used [1].

Several methods, transformed into computing algorithms and implemented in software packages, are now available to solve crystal structures from powder data. Traditional methods working in reciprocal space like Direct or Patterson methods [1], approaches working in direct space like Simulated Annealing (SA) [2], Genetic algorithm [3] or hybrid algorithms [4-6], can be used to face different: 1) kinds of compounds, i.e., organic, inorganic, metal organic; 2) quality data; 3) structural complexities, etc.

A large variety of computer software for powder diffraction are today available and, among them, the package *EXPO* [7] plays a central role. It is a program able to carry out, all the steps of the crystal structure solution process (without linking to external programs): 1) indexation; 2) space group determination; 3) integrated intensities estimation; 4) structure solution; 5) structure completion and optimization; 6) Rietveld refinement [8].



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An overview of the main strategies implemented in the *EXPO* package will be given.

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[AMC-312]Effect of the cooling rate on the solid solution decomposition of ZnFe₂O₄ spinel

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A zinc ferrite of nominal composition ZnFe₂O₄ was synthesized from a powder mixture of pure ZnO and Fe₂O₃ by high energy ball-milling combined with subsequent calcination in air at temperatures up to 1200°C. After this heat treatment, the material was cooled to room temperature at different rates, namely water quenching and air cooling, to understand the effect of cooling rate on the structural, morphological, compositional and magnetic properties. The microstructure presented in both samples was analyzed by X Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and High Resolution Transmission Electron Microscopy (HRTEM). XRD patterns obtained with Co-K α radiation were analyzed by the Rietveld refinement method for calculation of structural parameters, like oxygen positional parameter, cation distribution, unit cell parameter and volume weighed mean crystallite size. The morphology of the microparticles obtained and the presence of nanostructures inside were determined from SEM and HRTEM micrographs, respectively. The results showed the existence of nanostructures inside the spinel crystals, suggesting that spinel solid solution decomposes during cooling to room temperature due to a cation redistribution process between the two sub-lattices of the spinel in some regions of the crystal. Finally, magnetic properties were investigated with an SQUID, by measuring hysteresis cycles at 10 and 300 K and zero field cooled (ZFC) and field cooled (FC) at 100 Oe from 10 to 300 K. The results showed that samples subject to fast cooling rate are paramagnetic at room temperature with almost negligible superparamagnetic contribution, similar to the bulk, whereas the low cooling rate gives place to a noticeable superparamagnetic contribution. This superparamagnetic contribution was associated to the spinel decomposition.



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[AMC-49] Ferroelectric Phase Transition Temperature Detected by Thermal Transport and Relative Permittivity in PZTN 53-47-x.

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Ceramics of PZT family doped with Niobium were prepared using the traditional ceramics process with reactivities of high purity to obtain $\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})_{1-5x/4}\text{Nb}_x\text{O}_3$. These were sintered in lead atmosphere at 1250°C during 100 minutes. The relative permittivity as a function of temperature were evaluated with an homemade system, using an Keysight E4990A Impedance Analyzer, a heating cell with a 1°C/min heating rate in the frequency range of 20 Hz to 5 MHz. Hysteresis loops as a function of temperature were evaluated using a Precision LC Radiant Ferroelectric Test System coupled with a Trek amplifier model 609E-6 at 1-4 kV, a heating cell with a 1°C/min heating rate. The thermal transport measurement was made using a Linseis LFA 1000 Laser Flash; at vacuum, in an interval of temperatures of 25 to 500 °C. To each temperature were carried out five valid measurements of diffusivity and the average of the same ones was obtained. Transition temperature exhibit a dependence on the dopant concentration. Additionally the crystalline structure of the samples was analyzed using XRD, also Raman Spectroscopy measurements was analyzed.



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[AMC-81] Photovoltaic characteristics of ferroelectric films with perovskite structure

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Thin films of $\text{Pb}_{0.985}\text{La}_{0.01}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$ /n-Si and $\text{Pb}_{0.975}\text{Sr}_{0.025}(\text{Zr}_{0.53}\text{Ti}_{0.47})_{0.96}\text{Cr}_{0.04}\text{O}_3$ /n-Si as solar cell were obtained by cathodic erosion method. The time deposition (20, 30 and 40 min.) on n-type silicon (/n-Si) was investigated in the photovoltaic and photoconductive contribution, as well as the efficient in these devices. The films were deposited at room temperature. The best results was for $\text{Pb}_{0.985}\text{La}_{0.01}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$ /n-Si obtained at 30 min. time deposition.



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[AMC-93] Synthesis and local piezoresponse of lithium tantalate-1.8%Fe thin films on ITO substrates

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Lithium tantalate-1.8%Fe thin films with a thickness of 220nm were deposited by the sputtering technique on indium-tin oxide substrates.

The polycrystalline phase for the lithium tantalate thin films (JCPDS card 00-029-0836), the lithium tantalate target (JCPDS card 00-029-0836), and the indium-tin-oxide substrate (JCPDS card 01-089-4598) was identified by X-ray diffraction. While the characteristic vibration modes were observed with Raman spectroscopy. On the other hand, the deposits thickness and the elemental composition were analyzed with scanning electron microscopy and with energy dispersive X- ray spectrometry respectively.

A local analysis with piezoresponse force microscopy showed a piezoelectric coefficient $d_{33}= 50$ pm/V. Curves of amplitude vs. voltage (butterfly curves), phase vs. voltage, and piezoresponse (d_{33}) vs. voltage were obtained. The observed local piezoresponse for lithium tantalate-1.8%Fe thin films is larger than macro piezoresponse measurements for the same material.



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[AMC-107] Study of the electrical properties and structural stability of the polycrystalline
RE₃Ba₅Cu₈O₁₈ superconductors (RE = Y⁺³, Sm⁺³)

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Superconductors formed in accordance to the general formula RE₃Ba₅Cu₈O₁₈ (RE=Y⁺³, Sm⁺³, Nd⁺³) feature orthorhombic crystalline structure with similar crystallographic parameters. Yttrium-based Y₃Ba₅Cu₈O₁₈ compound received the most scientific attention due to the highest critical temperature values [1-3] possible for YBCO material group. In this work, we studied the influence of replacement of yttrium atoms with Sm⁺³ in different proportions, which was possible due to similarity of their cation radii [4]. The YBa₂Cu₃O₇, Y₃Ba₅Cu₈O₁₈, (Y₂Sm)Ba₅Cu₈O₁₈, (YSm₂) and Sm₃Ba₅Cu₈O₁₈ superconducting phases were prepared using solid-state reaction method. The optimal conditions to synthesize each sample with the corresponding stoichiometry were established from the analysis of YBa₂Cu₃O₇ phase equilibrium curves. The atomic composition of the samples was defined by the energy dispersion spectroscopy (EDS). X-ray photoelectron spectroscopy (XPS) was used to estimate the stoichiometry and elementary composition of our samples. Scanning electron microscopy (SEM) was used to study surface morphology. Modification of material structural parameters was analyzed by X-ray diffraction, confirming the presence of orthorhombic phase with Pmmm symmetry in our samples. The measured dependence of resistance as a function of temperature was used to analyze how synthesis parameters influence the critical superconductive temperature T_C.

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[AMC-121] Obtention of strontium titanate fibers by electrospinning

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Strontium titanate is a ceramic derived from titanium oxide and strontium salts, with the formula SrTiO₃. The SrTiO₃ is characterized by having a body centered cubic crystalline structure that has a conformation of type ABC₃, which is known as a perovskite. This material has semiconductive properties and is therefore of interest for the development of electronic circuits. The purpose of the next project is to elaborate ceramic fibers, using the methods of sol gel and electro-spinning. For the development of the fiber, titanium tetraisopropoxide and strontium nitrate were used as precursors, maintaining a 1:1 molar ratio between titanium and strontium. Polyvinylpyrrolidone was used as the support polymer. The electro-spinning process was performed at room temperature using a voltage of 12 kV and an injection rate of one milliliter per hour. Green fibers were obtained with three different concentrations having diameters of approximately 700 nm and ceramic fibers calcined at 1400 ° C with mean diameter of 200 nm.



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[AMC-131] Fabrication of ceramic coaxial fibers of hydroxyapatite, silica and alumina

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Simple and coaxial fibers of hydroxyapatite (HA), silica (SiO₂) and alumina (Al₂O₃) were obtained by the electrospinning method. The core-shell structure of coaxial fibers was fabricated using different combinations of the three ceramics, which were HA-Al₂O₃, HA-SiO₂, and Al₂O₃-SiO₂. Parameters as voltage, needle-collector distance, and feeding rate were optimized in order to achieve a small mean diameter and smooth surface. Precursor solutions were prepared using three different concentrations of Polyvinylpyrrolidone as spinning polymer. After thermal treatment, porous ceramic materials with fibrous morphology and high surface area were obtained. The adsorption capacity of the simple fibers was determined using different dyes.



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[AMC-135] A comparison of ferroelectric properties for sol gel obtained niobium doped bismuth titanate sintered by pressureless sintering and spark plasma sintering

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Nb-doped bismuth titanate ($x = 0.0-2.0$ with a step of 0.5) samples were synthesized by chemical sol-gel method with the precursors: Bismuth nitrate pentahydrate (Alfa Aesar 98%) dissolved in acetic acid (99%) with an equilibrium molar ratio $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O} : \text{CH}_3\text{COOH} ; 1:3$, and Titanate (iv) isopropoxide (Alfa-Aesar 97+%) in the 2-methoxyethanol (Alfa-Aesar 99%) with molar ratio $\text{TiO}_4\text{C}_{12}\text{H}_{28} : \text{C}_3\text{H}_8\text{O}_2 ; 30:1$. To increase the solution stability, 10 ml of acetyl acetone (Sigma-Adrich >99%) are added. After obtaining the dry gel, it is calcined at 750°C for 18 hours. As follow, the obtained powder was grinded with mortar pestle for 10 minutes. Niobium Chloride (NbCl_5 , Alfa-Aesar 99%) is dissolved in the water before the sol gel process is started. Sintering is developed by two processes: Pressureless Sintering (PLS) and Spark Plasma Sintering (SPS). PLS pellets were made with help of die punch machine applying a load of 1400 kg and a dwelling time of 10 minutes to the powder with 2% in weight of Polyvinyl alcohol as binder. The powder compact samples are heated up at a rate of 1 °C/min until reach 300 °C for the binder removal, then fast heated up to 1000 °C with a dwelling time of 18 hours. The final relative densities for all the samples have an average around of 88%. The SPS was developed at Dr Sinter system. The powders were sintered at 1000 °C for 10 minutes at vacuum, loads of 5.2 kN, 3.5v DC, 600A and 12 pulses in ON and 2 in OFF are applied. Under the mentioned conditions the density for all samples averaged 99%. With the Niobium dopant content



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increase, the remanent and saturation polarizations increase for both PLS and SPS. The highest values are obtained for PLS. It is worthily to mention that the highest values are reported for 0.5 Nb.



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[AMC-103] Synthesis of $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ by the solution combustion method using glycine and urea as a fuel

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Lanthanum and strontium manganite presenting the perovskite type structure was synthesized, the stoichiometric ratio for this perovskite was 0.7:0.3:1. According to literature this magnetic material is under investigation for biomedical proposes. Solution combustion synthesis is an easy technique to obtain complex metal oxides such as perovskites. The synthesis of that manganite was reported by many authors using glycine and polyvinyl alcohol, however the use of urea is not reported.

The methodology was proposed to synthesize diverse samples by two routes and different calcination times, in order to obtain nanoparticles with high crystallinity and purity. However it is important to obtain these nanoparticles with a low size distribution and controllable size. The solution combustion method offers many advantages to cover these necessities.

$\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ samples were synthesized in this work, those were obtained using glycine and urea as a fuel. The characterization realized consisted in the structural analysis by XRD technique. The morphology of the samples were studied by field emission scattering electron microscopy. These samples were also characterized by infrared spectroscopy and thermogravimetric assay in order to obtain more information about the purity of the samples.

Keywords: Solution combustion synthesis, urea, $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$, biomedical application, magnetic nanoparticles.



[AMC-167] Preparation and characterization of ceramic membranes based in mullite to clarification of sugar cane juice

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Clarification of sugar cane juice is a critical step in sugar processing; clarified juice is highly dispersive and brown yellow due to impurities. Membrane technology is a promising alternative for this purpose. Therefore in this work, the synthesis of ceramic membranes based in mullite and its infiltration with SiO₂ by sol-gel process was studied. Planar ceramic membranes based in mullite were prepared from commercial available powders: mullite (58 and 63 % w/w), corn flour as pore forming (15 and 20 % w/w), kaolin talc (12 % w/w) and sodium silicate as additive (8 and 2 % w/w respectively). Mullite membranes was processed mixing the components, molding and pressing in a stainless steel container at room temperature at 75 Mpa. After that, membranes were sintered in a high temperature furnace at 1300 y 1400 °C using heat rate of 5°C/min. The infiltration membranes was realized using sol-gel process with TEOS and HCl mix (11 ml of 0.05 N HCl with 37 ml of TEOS) by immersion 3 hours. After that, membranes were sintered again at 1300 °C. The uninfiltred and infiltred membranes were analyzed by Infrared Spectroscopy to identify the characteristic groups, whereas the microstructure of the samples was evaluated by Scanning Electron Microscopy. The results of IR spectroscopy shows the characteristic bands of mullite, Si-O and Al-O (460, 750, 1100 cm⁻¹, and 560, 740, 830 cm⁻¹ respectively). In addition was identified a band between 875-900 cm⁻¹ that are typical or Si-O-Al bonds. Results obtained from SEM in the uninfiltred membranes point out heterogeneous



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closed macropores of 100 μm of pore sizes. However, the applicability of this membrane might further improve reducing the pore size $0.1 \mu\text{m} < d_p < 10 \mu\text{m}$ by the infiltration step.



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[AMC-177] Local Piezoelectrical Characterization of Ferroelectric Ceramics by Switching Spectroscopy Piezoresponse Force Microscopy

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In recent years, Switching Spectroscopy Piezoresponse Force Microscopy (SS-PFM) [1] in Dual AC Resonance Tracking (DART) mode [2] has been utilized as an effective tool to study the superficial and local domain switching behavior and piezoresponse of ferroelectric materials. This technique is fundamentally different from macroscopic piezoelectric properties of a sample, where piezoelectric behavior occurs due to the nucleation growth and interaction of multiple separated domains, while in PFM the piezoelectric response is taken from a local region by monitoring piezo-activity within a single domain. Phenomena related to domain activities such as nucleation, pinning, switching and time dependency, which occurs under a sharp tip by the application of a voltage, can be investigated.

In PFM measurements, the amplitude of the acquired signal is proportional to the effective longitudinal piezoelectric coefficient, d_{33} . Several samples were characterized using a scanning probe microscopy (MFP-3D Infinity, Asylum Research Inc., USA) under the SS-PFM mode to determine their piezoelectric properties. Piezoresponse signal and coercive voltage were obtained from BNBT, BFBT and BCZT lead-free ferroelectric ceramics samples applying a triangular waveform voltage cycle and using Ti/Ir coated Silicon tip with a nominal spring constant of 2 N/m and a resonance frequency of 70 kHz.



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Piezoelectric displacement-applied voltage (D-V) “butterfly” loops were measured and converted to piezoelectric hysteresis loops according to the law of converse piezoelectric effect to reveal the local effective piezoelectric d_{33} coefficient. Values of d_{33} were obtained for these ferroelectric ceramics. PFM images and the corresponding butterfly/hysteresis loops will be displayed and explained in the presentation.

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[AMC-181] KNN ferroelectrics lead free obtained by high energy milling

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$K0.5Na0.5NbO3$ (KNN) is a material lead-free with good ferroelectric and dielectric properties. Since Saito (2004) reported a different obtaining process and he showed that KNN is a good choice in the morphotropic phase boundary (MPB). In this investigation, we synthesized KNN ferroelectric ceramics with and without dopants as La^{3+} , Li^{1+} and Ti^{4+} individual and combined way to obtain best dielectric, ferroelectrics and thermal properties in the material. The synthesise process is by mechano-chemical activation of the combination of oxides and carbonates powders. The chemical precursors for KNN system were K_2CO_3 , Na_2CO_3 , Nb_2O_5 and the dopants were Li_2CO_3 , La_2O_3 , TiO_2 . The mechano-chemical process was in two milling stages, one of them is in 30 minutes and the other one is 60 minutes. Both stages were made in a nylamid container with zirconium balls in a relation weight: balls 1:10 and pressed in disks. Later, the milled powder is calcined at 800 °C for all the materials and sintered at 1080 °C for KNN+ Li^{1+} , 1100 °C for KNN, KNN+ La^{3+} Ti^{4+} and finally 1120 °C for KNN+ La^{3+} Li^{1+} and KNN+ La^{3+} . The XRD analysis showed that the samples crystallize in the monoclinic phase. In ferroelectric properties, we obtained the best value in polarization on the KNN undoped ($11.8 \mu C/cm^2$) but his relative permittivity value was lowest (302) than the KNN doped (> 302) and showed shifts in Curie temperature.

The thermal analysis showed a value of thermal diffusivities and specific heats that correspond with the orthorhombic-monoclinic, tetragonal-orthorhombic and cubic-tetragonal crystalline phase transition.



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[AMC-199] Effect of Nickel oxide on crystallization and mechanical properties MgO-Al₂O₃-SiO₂-MoO₃ glasses

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Crystallization is a well-recognized practical means of improving the brittleness of glass. Many glass-ceramics have been investigated, and some have been incorporated into practical materials. Glass-ceramics in the MgO–Al₂O₃–SiO₂ (MAS) system have attracted much interest on account of their superior mechanical and thermal properties, i.e., high strength and stability at high temperatures.

To investigate the effect of nucleating agents, this study investigates the crystallization behavior of an MgO–Al₂O₃–SiO₂–MoO₃ glass with high % wt molybdenum oxide and low % wt nickel oxide addition. Under a not reducing condition, crystals formed in the bulk of the super cooled liquids, whereas melting in air yielded only surface crystallization.

The purpose of using of Nickel oxide as nucleating to modify the mechanical properties, is based on the manipulation of the grain size during the solidification process.

The first crystalline phase precipitated inside the glass was α -cordierite and β -cordierite in glasses doped with nickel oxides. Nickel oxide yielded a finer microstructure of the glass-ceramic.

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[AMC-231] Synthesis of Lithium Tantalate nanofibers

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In this work, Lithium Tantalate fibers (LiTaO₃, LT) are developed by two different ways. For the first path, a powdered compound is obtained by mechanical activation using as precursors tantalum pentoxide (Ta₂O₅) and lithium carbonate (LiCO₃) for 2 hrs in a high-intensity mill. Once the LT powder is obtained, grinding is carried out with the nano-powders and acetone. The solution is then allowed to decant, and the smaller particles are removed. The suspended particles are mixed with a polymer Polycaprolactone (PCL) and are mounted in a spinning equipment. In the second method for obtaining the fibers, single fibers of LT and coaxial fibers with silica are obtained. A solution of sol-gel with lithium tantalum ethoxide as the precursor of LT and a solution of Tetraethyl Orthosilicate (Teos) as the precursor of silica for the coating of the coaxial fibers is first created. The solutions are individually mixed with polyvinylpyrrolidone (PVP) as the spinning polymer and are assembled in the spinning equipment. All samples are calcined at 700 ° C for 3 hrs to form the Lithium Tantalate phase and remove the organic traces of the polymers. The obtained fibers are analyzed and purchased with the help of SEM, Raman spectroscopy, FTIR, and XRD.



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[AMC-227] Low temperature behavior of nanostructured zinc ferrite cell parameters and magnetoresistance

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Nanostructured zinc ferrite has been prepared by solid state reaction after pressing the powders into pellets and heat-treated at 1100°C. Characterization was carried out by using X-ray diffraction, scanning electron microscopy and magnetoresistance in a range between 300 and 50 K. All diffraction peaks were indexed with the pure phase of zinc ferrite (ZnFe_2O_4) and a good contact between adjacent particles was found. Cell parameters analysis of low temperature of X-ray diffraction patterns revealed a reduction of it. And more interesting, a reduction on the rate of change of it around 150 K was determined. This behavior was in correspondence with the one found in temperature dependent electron transport measurements, which exposed a drop of electrical resistance with values going from 1100 to 55 Ω . And also, a magnetoresistance maximum was observed at this temperature. Finally, with all these results, it can be suggested that magnetoresistive effect observed is driven by a charge reordering occurring at the change in cell parameter, which is the ultimate responsible for the electrical resistance transition we found.



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[AMC-233] Characterization by XRD of ceramic refractory clays with nanoparticles of SiO₂ and Al₂O₃

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A heat treatment was carried out at 700 ° C and 850 ° C for each of the ceramic refractory clays, which are powdered. Each of them was added a percentage of nanoparticles, in order to obtain four samples in total. X-ray diffraction was performed on each sample. The purpose of adding nanoparticles of SiO₂ and Al₂O₃ To ceramic refractory clays is to be able to obtain phases of the same clays at lower temperatures than are normally obtained, since it is known that the two clays are of the aluminosilic type. With the results of the X-ray diffraction it was observed that if some phases of the aluminum oxide and the silicon oxide are obtained for a ceramic refractory clay of the type that we are analyzing. Finally we can conclude that depending on the type of clay and nanoparticle that we want to add, we can manipulate the chemical composition of the clay and thus obtain one of the many clays that exist today. This work is a part of a research for ceramic refractory clays to obtain a phase called Mullite, which is a highly refractory mineral.



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[AMC-236] Nanostructured ferrites for sensors obtained by electrospinning

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The electrospinning process in the last years has been growing up, especially, in the fabrication of the 1D nanostructured ceramics, in this work we are focused in the synthesis MnFe_2O_4 and CoFe_2O_4 both of these complex oxides are study object due to magnetic properties. For the synthesis of the complex oxides by electrospinning was necessary to use Polyvinylpyrrolidone and metallic salts of Co and Mn respectively with high purity 99.999%. After calcination, for the magnetic behavior, we used a versalab cryo free at low-temperature founding for Cobalt ferrite present $M_s = 73.162$ emu/g for Manganese Ferrite $M_s = 93.4$ emu/g. DRX confirm the crystalline structure this complex oxide belong to perovskites. The morphology of this ceramics nanofibers are polycrystalline and the range nanoparticles are 120nm that was determined using TEM.



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[AMC-247] Synthesis and Characterization of sol-gel prepared Barium Zirconate-Titanate/Barium Calcium Titanate for the Study of the Influence of Process Parameters in their Ferroelectric Properties.

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Ferroelectric properties for Barium Calcium Zirconate Titanate with compositions $(\text{Ba}_{0.85}\text{Ca}_{0.15})(\text{Ti}_{0.92}\text{Zr}_{0.08})\text{O}_3$ and $(\text{Ba}_{0.80}\text{Ca}_{0.20})(\text{Ti}_{0.88}\text{Zr}_{0.12})\text{O}_3$ were studied in the present work. The experiments were carried out by the sol-gel synthesis process. X-Ray diffraction shows that the phase BCZT was obtained without undesirable secondary phases. Raman spectroscopy reveals changes in main vibrational modes relatives with TiO_6 octahedra, due to the calcium and zirconia doping. Powder compact samples were obtained by Pressureless sintering (PLS) and Sinter Forging (SF) with relative densities about 92% and 99% respectively. The samples have regular and random sized morphology on both processes but more noticeable in SF. SF process is shorter to complete than PLS needing only 5-6 hours compared with PLS that requires 16 hours. SF allowed the formation of a homogeneous microstructure with less porosity and excellent densification useful for allowing texturization when an electric field is applied. The best samples were for SF displaying values of $P_{\text{max}}= 9.23 \mu\text{C}/\text{cm}^2$, $P_{\text{rem}}= 3.23 \mu\text{C}/\text{cm}^2$, $E_c= 0.920\text{kV}/\text{cm}$ and 270 pC/N of d_{33} .



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[AMC-259] The effect of concentrations of PVP on the morphology, phase composition, crystallinity and magnetic properties of manganese ferrite obtained by electrospinning technique

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The synthesis of the MnFe_2O_4 nanofibers was carried out by the electro-spinning technique, the precursor solution was composed of 14, 17 and 20 % Wt of polyvinylpyrrolidone (PVP), with molecular weight M_w 1, 300 K, $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and $\text{Mn}(\text{NO}_3)_2 \cdot \text{H}_2\text{O}$ in a mixture of water and alcohol. The solution was vigorously stirred for 1 h and then, it flew out through the needle at a constant flow rate of 0.3 ml/h. After collecting the fibers, these were annealed at 1100°C by 1 h in nitrogen atmosphere. The characterization was carried out by X-ray diffraction (DRX), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Vibrating Sample Magnetometry (VSM). MnFe_2O_4 pure phase was found in the nanofibers in sample with 14 %, from XRD patterns, whereas that the samples of 17 and 20 % of PVP showed Fe unreacted because of steric hindrance. Magnetic properties of calcined samples characterized by VSM were measured at room temperature to determine the magnetic interactions of the fibers, the saturation magnetization decreases from 82.24 emu/g to 61.44 emu/g with the increase of PVP. Finally, morphology, Crystallinity and fiber diameters were affected by the PVP concentration and analyzed by Scanning and Transmission Electron Microscopy.



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[AMC-271] Silver electroplating on titania-silica for signals enhancement in Raman and IR spectroscopy

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Surface enhancement raman spectroscopy (SERS) it's of great interest for its ability to detect ultra-low concentrations (nM) and for its capability to recognize the “fingerprint” of each substance, however, developed structures with a SERS effect show disadvantages like high cost, low stability and biocompatibility. The aim of this work is to develop a silica-titania-silver nanostructured support viable to be used as a signal enhancer in infrared and Raman spectroscopy.

To make the support, titanium and silicon alcoxides precursors were used in the sol-gel method, and were mixed with polyvinylpyrrolidone to later obtain a fiber membrane by electrospinning technique, this membrane was put through a thermal treatment to 800°C getting the ceramic material silica-titania, and it was analyzed by FT-IR spectroscopy. The ceramic fiber membrane was set on Indium Tin Oxide (ITO) conductor plastic, to later be doped with silver by electroplating process, varying the silver nitrate concentration in the electrolytic cell to 5, 10 and 20 mM, as well as electroplating times to 1, 2, 5 and 10 minutes, under a constant voltage of 1 V. Doped fibers were analyzed by scanning electron microscope, observing the silver deposits on the fiber matrix in a dendritic shape. According to results, it is expected that this substratum can be useful to signal enhancement on Raman and infrared spectroscopy.



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ATOMIC LAYER DEPOSITION (ALD)

**Chairmen: Pierre Giovanni Mani González: (UACJ)
Eduardo Martínez Guerra: (CIMAV-Monterrey)
Edgard López Luna: (UASLP)**



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[ALD-55] Growth and Characterization of Indium Nitride by Atomic Layer Deposition

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Atomic Layer Deposition it's a relatively new technique who allow us to make films with great structural quality at low temperatures and low cost. Indium Nitride is an interesting material due to his characteristics for applications over optoelectronics.

In this work we present the results of thin films growth of Gallium Nitride made by Atomic Layer Deposition, films were growth over Si (100), MgO (100) and GaAs (100). We propose the use of Indium Acetyl acetone and Ammonium Hydroxide as Indium and Nitrogen sources respectively.

Temperature window and times of reactions were determined and characterization by Atomic Force Microscopy, Photoluminescence, Raman and SEM was made.



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[ALD-98] Chemical depth profile of ultrathin nitrided ALD-hafnia films

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The use of high mobility materials to replace silicon in the manufacture of CMOS devices is gaining relevance, especially for THz applications.¹ However, it has been observed the migration of the atomic species from the of high mobility substrate (in particular species III-V) through the dielectric, which has been widely documented.²⁻⁴

Procedures such as nitriding of silicon oxide have helped to minimize the migration of phosphorus and boron through the dielectric.⁵ In this work, we report nitriding experiments carried out on 2 nm hafnium oxide films grown by ALD on Si (100) substrates cleaned with the RCA method. The hafnium precursor employed was tetrakis(dimethylamino)hafnium (TDMA-Hf) and water type I as an oxidant.⁶ The nitridation was carried out with a plasma remote LITMAS coupled with an ultra-high sputtering system. The plasma power was varied from 500 to 2500 W, the substrate temperature from 300 to 500 °C and the ultra-high purity (NUHP) nitrogen flow from 100 to 300 sccm.

The highest nitridation degree was achieved with a plasma power of 2500 W, a NUHP flow of 140 sccm at a working pressure of 3.2×10^{-3} torr. Although the optimal temperature was 500 °C, its dependence with this parameter can be compensated by slightly increasing the processing time. We found a region in the parametric space of the remote plasma for which the XPS signal associated with substitutional nitrogen in hafnium oxide (396.8 eV)⁷ is maximum. It was possible to achieve high nitridation ($\text{HfO}_{1.5}\text{N}_{0.48}$) most likely corresponding to a saturation level similar for silica.⁸



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[ALD-124] Refractive index and bandgap variation in Al₂O₃-ZnO ultrathin multilayers prepared by atomic layer deposition

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This research focuses on the study of the refractive index and bandgap behavior in ultrathin multilayer films of Al₂O₃-ZnO bilayers grown via atomic layer deposition (ALD) technique. Multilayer configuration stack consists in alternate layers of constant thickness Al₂O₃ (2 nm) and varying thickness ZnO films in order to obtain a total thickness of ~100 nm. A set of 10 samples based on bilayers with various 2:X thickness ratios were prepared, where X refers to the ZnO layer thickness. X is proportional to the number of cycles (N) of the ZnO precursor, varying from 1 to 100. The sample morphology was studied via Atomic Force Microscopy and the results show that the surface roughness of the multilayers varies from 0.2 to 1.2 nm, as the ZnO layer thickness increases. In all cases, the roughness values remain below 2% of the total thickness of the multilayer. Thickness and optical properties (n(l), k(l) and E_g), of each multilayer sample were studied via spectroscopic ellipsometry (SE). Cross-sectional mode scanning electron microscope images verified the multilayer total thickness and corroborated the accuracy of the optical model. The refractive index varies significantly from values close to the Al₂O₃ refractive index when the bilayer thickness is small, up to values corresponding closely to ZnO for thicker bilayers. The refractive index, as a function of bilayer thickness, varies between 1.63 and 2.3, for 1~ 370 nm, showing high sensitivity. In addition, the optical bandgap energy, E_g, determined using the Tauc model, decreases when the bilayer thickness increases, with a maximum variation of DE_g ~1.6 eV. These results reveal that the refractive index and optical



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bandgap can be modulated systematically as a function of the bilayer thickness. Such behavior is of great importance for optoelectronics applications.

Keywords: Tunable refractive index Optical bandgap modulation Ultrathin multilayers Atomic layer deposition.

Acknowledgments

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[ALD-196] Characterization and Cathodoluminescent properties of Carbon Nanotubes coated with ZnO by atomic layer deposition

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Surface engineering nanostructures through the incorporation of few atomic layers of metallic, inorganic or organic molecules on oxide surfaces, can substantially modify their properties opening to new ranges of possible applications. Furthermore, the formation of heterostructures is believed to be of importance in tailoring the physical properties of 1D nanostructures. The heterostructures with various compositions and interfaces have already demonstrated the distinctive performance in nanodevice applications. Being a wide band-gap semiconductor (3.34 eV) and a large exciton binding energy (60 meV), zinc oxide (ZnO) has been extensively investigated for electronic and optoelectronic devices, such as field emitters, photodetectors, gas sensors, and so on. Therefore, the formation of the heterojunction of ZnO and CNTs should extend the application scopes and reinforce the pristine properties of simplex ZnO and CNT materials. As a specific one-dimensional (1D) morphology, ZnO nanotubes attract extensive attention due to their high surface area, low density, biocompatibility, photocatalytic activity, turning into a promising candidate for lots of potential applications. MWCNTs were coated by atomic layer deposition (ALD) method, at 120 °C on a hotwalls ALD reactor, using Diethyl Zinc (DEZ) as precursor and deionized water as oxidant. XPS and FTIR were used to corroborate ZnO deposition. By Transmission Electron Microscopy (TEM) was confirmed the homogeneous and conformal coating of CNTs. The luminescent properties were evaluated by Cathodoluminescence (CL) and HR-XPS was used to study defects involved on emission process.



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[ALD-232] ALD coatings as oxidation barriers

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Carbon is maybe the best known material and is capable of forming several allotropes, diamond being one of the oldest known forms and carbon nanotubes the newer one. The market for industrial applications of diamond is in the order of 20 billion USD, while carbon nanotubes are currently around 2 billion market worth with a forecast of 5 billion by 2020.

However, one of the biggest problems is their low resistance to thermal oxidation. At ambient pressure, both allotropes are oxidized to CO₂ at around 600-700 C. Thus the challenge of this work is to improve the oxidation resistance of these materials. For that by means of a surface engineering approach, nano-sized coatings were deposited and TGA tested. It was found a fair degree of improvement, especially for activation energy.

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[ALD-234] High-K dielectric HfO₂ thin films obtained by ald and peald

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Optimal technological growth parameters were selected for the maximum smoothness, amorphous microstructure, low leakage current, high dielectric strength of HfO₂ thin films, required for gate applications. High quality of the layers is confirmed by their introduction to test capacitive structures. This work is a comparative study of HfO₂ thin films deposited on silicon wafers at 250°C by thermal ALD, PE-ALD (remote and direct mode) and the combination of them to get multilayers. The characteristics of HfO₂ films deposited by the atomic layer deposition (ALD) and plasma-enhanced atomic layer deposition (PEALD) method using O₂ were investigated. Plasma-enhanced atomic layer deposition was explored to produce thin HfO₂ films, where oxygen plasma acted as oxidant. Seven samples were identified such as TD, DP, RP, TD-DP-TD, TD-RP-TD, TD-RP and TD-DP for different multilayer configuration. In this notation, TD means thermal deposition, DP: direct plasm and RP: remote plasm. In this work, we explain the relationship between the growth mechanisms over the thin film properties. The electric properties of the dielectric stack based hafnium were characterized by C-V and I-V curves for each configuration. The as-deposited HfO₂ layer from thermal deposition exhibits an amorphous structure, while the HfO₂ layer from plasma processes exhibits a clearly visible polycrystalline structure. These results suggested that the stoichiometric change in the depth direction could be related to the energetic reactant in a state of plasma used in the plasma ALD process, resulting in damage to the Si surface and interactions between Hf and SiO_{2-x}. The as-deposited HfO₂ films using remote plasma have the better interfacial layer characteristics than those using direct plasma. With the combination of the ALD and PE-ALD techniques was possible to



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decrease leakage current down to 10^{-5} A/cm² and increase capacitance values up to 25. The PE-ALD films were found to have high concentrations of bridging oxygen bonds with metals (Hf–O–Hf), in contrast to the high concentrations of M–O–H in the films deposited by Atomic Layer Deposition. The lowest leakage current density was obtained for samples obtained by PE-ALD, several orders of magnitude below that of thermally grown HfO₂ films.

Keywords: Plasma Enhanced Atomic Layer Deposition, Atomic Layer Deposition, HfO₂.

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[ALD-293] Development of Integrated Logic, Memory and Sensing Technologies using ALD

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This work resumes some of the most important results that have been obtained in our research group regarding the use of atomic-layer deposition (ALD) as the main thin-film deposition technique for metal oxides with high dielectric constant. ALD has been applied for the development of logic, memory and sensing technologies in which ultra-thin metal oxides (Al_2O_3 , HfO_2 and TiO_2 with a physical thickness of $1\text{nm} \leq \text{th} \leq 10\text{nm}$), are the active part of the final devices under study. It is well known that MOSFETs based on the modulation of Schottky-Barriers for Source/Drain (SB-MOSFET) show a better performance compared to conventional planar MOSFET devices because of the many advantages given by replacing Source/Drain (S/D) diffusions by metal electrodes. Among these advantages are low parasitic S/D resistance, low-temperature processing for S/D formation, elimination of parasitic bipolar action, and inherent physical scalability to sub 10nm gate-length dimensions, which is due to the low resistance of metal and the atomically abrupt junctions formed at the metal-silicon interface. All of these advantages enable an increase in the performance of the transistors like obtaining a smaller sub-threshold slope (SS) compared to conventional MOSFET devices. Here, experimental data of Schottky-Barrier Metal-Oxide-Semiconductor Field-Effect Transistor devices (SB-MOSFET) are presented. For non-volatile emergent memory technologies, and since the invention of the memristor (an integrated device with memory-resistance properties), several materials in the form of thin dielectric films or solid electrolytes have been tested for these memory devices in order to produce reliable and reversible switching cycles of the resistive state of the oxide. Thin film-based materials able to switch from a high resistance state (HRS), to a low resistance state (LRS) and vice versa, are responsible for the “pinched hysteresis loops”, which are observed during cyclic current-voltage (I-V) measurements of these devices. Here, the resistive-switching characteristics of Metal-Insulator-Metal (MIM) devices based on ultra-thin and amorphous Al_2O_3 and/or HfO_2 (deposited by thermal ALD) are



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presented while using a maximum processing temperature for these memory devices of 300°C, ideal for Back-End-Of-Line (BEOL) processing of an integrated circuit. Finally, we present the use of metal oxides as ion-sensitive layers after directly exposing the gate oxide of a conventional MOSFET device, a metal-insulator-semiconductor capacitor or an insulator-metal structure to an electrolyte with a specific hydrogen ion concentration [H⁺]. The change of the surface charge on the insulator (based on Al₂O₃ or TiO₂) due to the adsorption of potential-determining ions causes a potential difference at the electrolyte-insulator (EI) interface. This EI potential changes the conduction characteristics of the FET's channel or the flat-band voltage of a MIS capacitor. All these integrated technologies are fully CMOS compatible, so that an ever increased functionality to these materials can be sought in order to accelerate truly advanced More-than-Moore applications.



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[ALD-294] ALD of Thin Al₂O₃ and TiO₂ Films Used as Sensitive Layers for pH Detection

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The precise measurement of pH with field-effect transistors is a well established technique that has resulted in the development of Ion-Sensitive Field-Effect Transistors (ISFET) able to measure the concentration of hydrogen ions within electrolytic solutions. Here, ultra-thin metal oxides are used as ion-sensitive layers after being deposited atop the gate of a conventional field effect transistor (FET) or metal-insulator-semiconductor (MIS) capacitor. The change of the surface charge of the insulator due to the adsorption of potential-determining ions causes a potential difference at the electrolyte-insulator interface, which changes the conduction characteristics of the FET's channel or the flat-band voltage of a MIS capacitor. This work reports the general characterization of thin aluminum oxide and titanium dioxide layers deposited by atomic-layer deposition (ALD) and the fabrication of Extended-Gate Ion-Sensitive Field-Effect Transistors (EG-ISFET) using these layers as dielectrics for pH detection. We relate the chemical changes observed in Al₂O₃ and TiO₂ to the hydration of these layers after relatively long time exposure to pH buffer solutions. Hydration of the layers' surface will produce a drift in the electrical I-V characteristics of the MOSFET devices that are used as transducers for pH detection. During continuous hydration of Al₂O₃ for instance, the aluminol (Al-OH) groups originally presented on its surface are progressively transformed to Al-(OH)₃ so that the surface density of sites reactive to protons is dramatically reduced and with this, its sensitivity for pH detection is decreased as well. This hydration phenomenon also increases the surface roughness of the Al₂O₃ while simultaneously producing an exponential decrease in the dielectric constant of the hydrated layer. All these effects, when combined to additional stressing conditions like higher temperature or bias applied, are in detriment of stable pH measurements in the long-term so that the EG-ISFET devices are useful when relatively short-time pH measurements are required. Nevertheless, highly reproducible pH



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measurements using these metal oxides are obtained after minimizing the hydration phenomenon. A clean Al₂O₃ surface is able to increase the sensitivity for pH measurement while also producing a more linear response in the measured range of pH= 4 to 10. Even though the power MOSFET device (used as EG-ISFET) requires larger threshold voltages V_{th} , the use of Al₂O₃ as pH sensing layer shows the potential that this material has regarding larger sensitivity and linearity for pH detection. This comes with the added advantages of ALD processing, which produces high-quality films with conformal characteristics and control in the thickness and stoichiometry of the oxide down to atomic level. All these features are highly desirable considering the low thermal temperatures for deposition of these thin metal oxide layers so that they can be introduced into Front-End of Line or even, Back-End of Line stages of modern integrated circuits.



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**[ALD-295] Determination of the Carrier Conduction Mechanisms in MIS Devices Based on
Ultra-Thin Al₂O₃, HfO₂ and TiO₂**

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Even though the successful introduction of high-dielectric constant (high-k) materials has enabled the continuous scaling down of advanced logic and memory devices into the nanometer regime, accurate predictions ensuring long-term operation of these devices is now more complicated due to several physical and electronic considerations: 1) precise atomic control of the high-k material in the ultra-thin regime (thickness, stoichiometry, dielectric constant, etc), 2) excessively large gate leakage current levels, 3) appearance of several conduction mechanisms able to degrade the performance and reliability of the devices, 4) interfacial defects at the high-k/silicon interface and 5) low thermodynamic stability of the high-k materials after being exposed to the inherent thermal treatments during several Front-End-Of-Line (FEOL) or Back-End-Of-Line (BEOL) stages. In order to contribute to better predictions of lifetime and/or reliability characteristics, this work reviews the conduction mechanisms in Metal-Insulator-Semiconductor (MIS) devices fabricated using ultra-thin Al₂O₃, HfO₂ and TiO₂ (less than 10 nm in thickness for each dielectric) deposited by Atomic Layer Deposition (ALD). These MIS devices were electrically characterized using standard I-V, C-V, I-V-time and I-V-temperature measurement conditions in order to determine the precise carrier conduction mechanism for each dielectric. The experimental measurements were compared with semi-empirical tunneling models like Direct tunneling (DT), Ohmic conduction (OC), Poole-Frenkel emission (PF), Trap-Assisted Tunneling (TAT) and Fowler-Nordheim tunneling (FN). After dielectric breakdown, a Schottky diode conduction model is used in order to verify the post-breakdown characteristics for each MIS device as well. Physical parameters before and after thermal annealing such as effective mass, barrier height (before



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and after breakdown), and trap energy level were extracted and then compared with simulations using SILVACO software. All values were compared with those found in literature, having great concordance. The accurate identification of self-consistent conduction models for the gate leakage current in MIS devices allows for better reliability predictions before failure of these devices and this is possible due to the high quality of the ultra-thin high-dielectric constant materials after thermal ALD.



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[ALD-296] Resonant Tunneling in MIIS Devices based on Intrinsic Quantum-Well Formation of Stacked Ultra-Thin Metal Oxides

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As a consequence of the extremely confined structures of advanced MOSFET/FinFET devices, ballistic transport is now approachable since the devices' channels are now shorter than the mean free path of electronic carriers. Well controlled ballistic transport could result in faster switching speeds and lower power consumption. However, this is difficult to obtain because of intrinsic/extrinsic phenomena: 1) random thermal fluctuations at/or above room temperature, 2) poor-quality of interfaces in the metal/dielectric/semiconductor structures, and 3) scattering events like phonon scattering or electron-electron interaction during carrier transport. The effect of resonant tunneling (RT) is widely considered for ballistic transport due to a tunneling component where electrons do not suffer scattering while their momentum is preserved. A way to promote ballistic transport is by inducing a quantum well in a highly confined structure in which electrons can tunnel through some resonant states having discrete energy levels. In this work, Metal-Insulator-Insulator-Insulator-Semiconductor (MIIS) structures composed of stacked Al₂O₃/HfO₂/Al₂O₃ (2nm/1nm/2nm in thickness) films deposited by Atomic-Layer Deposition (ALD) exploit their band-offsets to create a quantum-well with a potential energy of 1.3 eV, high enough for quantization of some energy levels and therefore, able to create resonant tunneling. After fabrication, devices were electrically characterized (I-V, C-V, I-V-T) in order to measure the carrier transport properties and correlate them with their conduction mechanisms. Experimental evidence of resonant tunneling was obtained and related to at least three distinctive Negative Differential-Resistance (NDR) zones when a positive gate bias is applied and whose peaks and valleys are related to quantization of energy levels within the conduction and valence bands of an ultra-thin HfO₂ (1 nm) intermediate layer. Because of an additional post-metallization annealing (PMA) step, inner-diffusion of atomic elements within the stacked oxides could limit the thermal budget required for these devices.



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Nevertheless, obtaining RT phenomena in these simple structures by using a highly robust processing method (ALD), paves the way to further enhancing their resonant characteristics (by lowering temperature and/or by applying an external magnetic field) and consequently, enabling a higher control of ballistic transport in extremely confined vertical structures like those found in the stacked oxides here shown.



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[ALD-56] Growth and Characterization of Gallium Nitride by Atomic Layer Deposition

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Atomic Layer Deposition it's a relatively new technique who allow us to make films with great structural quality at low temperatures and low cost. Gallium Nitride is an interesting material due to his characteristics for applications over optoelectronics.

In this work we present the results of thin films growth of Gallium Nitride made by Atomic Layer Deposition, films were growth over Si (100), MgO (100) and GaAs (100). We propose the use of Trietil Gallium and Ammonium Hydroxide as Gallium and Nitrogen sources respectively.

Temperature window and times of reactions were determined and characterization by Atomic Force Microscopy, Photoluminescence, Raman and SEM was made.



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[ALD-123] Al₂O₃-Y₂O₃ ultrathin multilayer stacks grown by atomic layer deposition as perspective for optical waveguides applications

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Nanolaminate multilayers made of Al₂O₃ and Y₂O₃ bilayer slabs were grown at 250 °C by means of thermal Atomic Layer Deposition (ALD). Several samples were prepared, where the number of ALD cycles for the Al₂O₃ slab was kept constant at 17 ALD cycles, while the number for the Y₂O₃ slabs was varied from 1 to 100. An optical model was built and adapted for each sample considering the Cauchy relationship, which was used to simulate the optical response for transparent materials. The thickness obtained from the optical model was in agreement with the thickness of cross-sectional SEM images. The optical band gap, obtained from single-effective-oscillator model, varied from 5.45 to 4.24 eV as a function of the Y₂O₃ slab thickness. The refractive index as well as the optical band gap can be modulated systematically using the Al₂O₃:Y₂O₃ ratio as control parameter. By means of simulated propagation modes it is shown that there is a multimode behavior for thickness around 200 nm at wavelengths between 300 to 1550 nm. This study reveals the possibility of using Al₂O₃-Y₂O₃ nanolaminates as the core of optical waveguides. It also shows the potential of ALD technique for fabrication of submicron waveguides useful in miniature optical circuits.

Keywords: Multilayers; atomic layer deposition; tunable refractive index; band gap modulation; optical waveguide.



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[ALD-194] A comparative study of HfO₂ thin films growth by ald, peald and the combination of both techniques

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This work is a comparative study of HfO₂ thin films deposited on silicon wafers at 250°C by thermal ALD, PE-ALD (remote and direct mode) and the combination of them to get multilayers. Seven samples were obtained and identified such as TD, DP, RP, TD-DP-TD, TD-RP-TD, TD-RP and TD-DP for different multilayer configuration. In this notation, TD means thermal deposition, DP: direct plasm and RP: remote plasm. A plasma enhanced atomic layer deposition (PEALD) process was developed to deposit high-k dielectric constant materials using alternative Tetrakis- diethylamido-hafnium and oxygen plasma exposures. The growth per cycle (GPC) showed to be dependent of the multilayer type in which growth rates were larger for simple and combined plasma methods. In this work, we explain the relationship between the growth mechanisms over the thin film properties. With the combination of the ALD and PE-ALD techniques was possible to decrease leakage current down to 10⁻⁵ A/cm² and increase capacitance values up to 25. The as-deposited films obtained with plasma were determined to be fully oxidized by the x-ray photoelectron spectroscopy (XPS). The PE-ALD films were found to have high concentrations of bridging oxygen bonds with metals (Hf–O–Hf), in contrast to the high concentrations of M–O–H in the films deposited by Atomic Layer Deposition. It was possible to determine different oxygen concentration in samples in which thermal and plasma methods were combined. The TD films showed higher dielectric constants than those obtained with plasma. These results were explained in terms of I-V, C-V and C-f measurements likely due to the enhanced ionic contribution from the M–O–M bonds, defects density and the grain size. It is believed



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that crystallization mechanisms are promoted with direct and remote plasma processes in which larger grains are formed if compared with thermal processes. The lowest leakage current density was obtained for samples obtained by PE-ALD, several orders of magnitude below that of thermally grown HfO₂ films with the same EOT.

Keywords: Plasma Enhanced Atomic Layer Deposition, HfO₂.

Aknowledgments: The authors thank to N.Pineda, L.G.Silva, E. Longoria R. for their technical support.



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[ALD-204] Modeling of surface coverage time for HfO₂ films on Si (100) substrates by ALD

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Actually atomic layer deposition (ALD) has been used for electronic devices ensemble. The high quality at the interface 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, the number of ALD cycles and the time of surface saturation. In this work is introduced a basic analytical model to estimate the surface saturation times on thin films produced by ALD procedure. Proposing that the covered 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. Finally, we contrast our model with previous experimental results in order to validate its accuracy.



[ALD-205] Effect of aperture time, number of cycles and time of coverage: Atomic Layer Deposition analysis and characterization

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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 different aperture-times of oxygen agent precursor, also the dependence with number of cycles respect to kinetic reaction, and is introduced a basic analytical model to estimate the surface saturation times on thin films produced by ALD procedure. Varying 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 covered 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, kinetic reaction and active sites with previous experimental results in order to validate its effects with the parameters of ALD characterization. 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 different aperture-times of oxygen agent precursor, also the dependence with number of cycles respect to kinetic reaction, and is introduced a basic analytical model to estimate the surface saturation times on thin films produced by



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ALD procedure. Varying 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 covered 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. 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 diferente 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. Varying 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 covered 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-206] Adsorption and dissociation of Tetrakis(dimethylamido)Titanium on Si(001) terminated OH⁻ at surface: A study of the DFT.

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In this work we have thus decided to perform systematic pseudopotential density functional theory (DFT) calculations dedicated to analyzing the adsorption properties and reaction of Tetrakis(dimethylamido)Titanium (TDMAT) on hydroxyl groups (OH⁻) terminated Silicon (Si) in the (001) crystallographic direction. Within the DFT approach using the ultrasoft pseudopotential approximation for the electron-ion interaction and a plane wave basis set for the wave functions with the use of the PWscf code. For all our considered structures, the cutoff energy for the plane wave expansion is taken to be 476 eV. A cubic supercell with a side dimension as large as 35 Å was employed in the calculations and the Γ point for the Brillouin zone integration. In all cases, we use the Perdew-Burke-Ernzerhof (PBE) pseudopotential and perform fully unconstrained structural optimizations, using the conjugate gradient method. The convergence in energy was set as 1 meV, and the structural optimization was performed until a value of less than 1 meV/Å was achieved for the remaining forces for each atom.

We report the low-energy atomic array with Si (001) reconstructed to a 2x1 structure with parallel rows of surface dimers (Si-Si bond ~ 2.4 Å), Si(001)-OH on the optimized surface was adsorbed of OH⁻ molecule in each atom of Si (Si-O bond ~ 1.7 Å and O-H bond ~ 1 Å) and finally TDMAT-OH-Si(001) the Si dimer formation site was chosen to adsorb the TDMAT over 2 hydroxyl groups. The optimized structure show the reaction between TDMAT and OH⁻ forming two amine. The amine-like nature of the reaction of TDMAT with OH⁻ suggests that the first step of this process involves the interaction of a nitrogen atom with one H⁺ and the formation of Ti-O bond (length ~ 1.4 Å).



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[ALD-223] Simulation and analysis of Al₂O₃ deposited as coating for solar cells by ALD

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The atomic layer deposition has been recognized as an exceptional deposited technique for different electronic applications. This technique is very useful in coating applications for new technologies such as solar cells grown in organic substrates, they need an efficient environment protection. Nowadays, the solar cells in organic substrates are far behind than conventional ones in two of their most important characteristics: efficiency and durability. Using an inorganic single layer coating (Al₂O₃) the permeability of the surface could be decreased; this condition could increase the resistance of the substrates in environment conditions whereby the life time of the solar cell should be higher. A deposit of single layer defect free Al₂O₃ high quality films could be reached in very low temperatures, this is ideal for thermally fragile plastic substrates. In addition, the conditions in which the coating is applied (temperature, pressure) are associated with an increase of the power conversion efficiency and higher open circuit voltage.



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[ALD-290] HfO₂-TiO₂ growth by atomic partial layer deposition. a novel technique to tune properties in a single atomic layer

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In the last few years, HfO₂ and TiO₂ have been studied as high-k dielectrics for applications in CMOS technology. A novel technique called atomic partial layer deposition (APLD), (which is a variant of atomic layer deposition, ALD) allows the possibility for the fabrication of well-controlled alloys on the single atomic layer scale with high quality and control thickness. HfO₂-TiO₂ samples were obtained by varying the precursor doses and exposure times to obtain a fractional coverage in the monolayer of Hf and Ti to tune dielectric properties. Tetrakis(dimethylamido)hafnium(IV) and Tetrakis(dimethylamido)titanium(IV) were used as precursors and H₂O as oxidant-agent. In this work, the thickness and structure of the samples were studied by x-ray reflectivity (XRR). The surface topography was studied using atomic force microscopy (AFM) along with Kelvin probe force microscopy (KPFM) for surface potential mapping with clear differences on the surface, compared with the conventional ALD nanolaminates, which confirmed the APLD growth. The films were analyzed using x-ray photoelectron spectroscopy (XPS) depth profile scans and angle resolved XPS (ARXPS) where well-defined HfO₂ and TiO₂ contributions were found for both the conventional ALD and APLD mode samples, and an additional contribution, assigned to a ternary phase Hf-Ti-O, in the APLD grown films was observed. Spectroscopic ellipsometry (SE) was used to study dielectric



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function where we found an improvement in the static dielectric constant compared to conventional ALD nanolaminates of the same materials

[ALD-298] Photocatalysis time activation of TiO_x, TiN_x y TiO_xN_y films growth by atomic layer deposition.

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This work presents an analysis of the photocatalytic time activation and efficiency in TiO_x, TiN_x y TiO_xN_y 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.



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BIOMATERIALS AND POLYMERS (BIO)

**Chairman: César Márquez Beltrán: (BUAP)
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[BIO-129] Obtention of PCL-HA-AL₂O₃ Fibers

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In this study, PCL-HA, PCL-Al₂O₃ and PCL-HA-AL₂O₃ fibers were made with the aim of obtaining a biomaterial with regenerative properties, being bioactive, with mechanical resistance; For this purpose, the formation of fibers was carried out by means of the electrospinning method. Furthermore, a porous material, flexible, with low density and high surface ratio was obtained. The parameters involved in the electrospinning process were optimized, which are voltage, distance and flow. Two different polymer/ceramic solutions of HA and Al₂O₃ were prepared, with concentration of 2% for each ceramic, and PCL 10%. A third solution with both ceramics at the same concentrations was also prepared. The electrospun fibers were homogeneous and smooth with the absence of agglomerates.



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[BIO-140] Ha and Silica-HA composites

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Synthetic materials which induce a specific biological activity are called biomaterials. A biomaterial to be considered as such must be in contact with the host tissue, and be biochemically and mechanically compatible with adjacent tissue. Calcium phosphate ceramics are widely used for dental and orthopedic reasons, because they can join tightly through chemical bonds and also promote bone regeneration. Hydroxyapatite (HA) has been researched to replace hard tissue because it's composition is similar to that of human bone. However, its biomedical use is restricted because of three characteristics: brittleness, lack of antimicrobial properties and limited contact with the host tissue. An electrospun composite of coaxial HA fibers with a SiO₂ core was proposed to counteract the inherent brittleness of HA while adding additional reactivity to the former. Precursors HA and SiO₂ were synthesized through the sol-gel method and then incorporated into a polymeric PVP matrix; later they were processed by coaxial electrospinning to obtain fibers which were characterized with techniques such as ATR-FTIR, DTA, SEM. The obtained fibers had a diameter of around 320 nm and showed a coaxial disposition with a SiO₂ core and hydroxyapatite cover. Through ATR-FTIR and SEM analysis was determined the fiber composition and the presence of characteristic chemical groups and microstructure was also observed.



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**[BIO-178] Impact of insoluble starch remnants on the behavior of corn starch/glycerol/LiCl
solid electrolyte**

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The effect of starch-insoluble remnants (i.e., ghosts) on the behavior of the solid biopolymer electrolyte remains to be studied. This work focused on this issue by considering a case-study system formed by corn starch, glycerol, and lithium chloride. The ghost content was controlled by subjecting the gelatinized dispersion to ultrasonic cavitation at various times. Ghost content reduction led to a slight decrease in conductivity. When the ghost content was reduced to almost nil, the capacitance estimated from cyclic voltammetry tests showed a decrease of about 37%. In contrast, the stability of the electrolyte, estimated by repeated potential cycles, was positively affected. Formation of free radicals and starch chain retrogradation are postulated as the mechanisms involved in the conductivity and capacitance variations in corn starch, glycerol, and lithium chloride solid biopolymer electrolyte.



[BIO-187] The Effects Of Radiation On The In Vitro Bioactivity Of Biocomposites

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The purpose of this study is to examine the effect of UV radiation on the microstructure, chemical structure and bioactivity properties of Chitosan/Extract of Mimosa Tenuiflora composites scaffolds produced by thermally induced phase separation. The composites were irradiated and observed to undergo radiation-induced degradation through chain scission. Morphology, bioactivity properties and effects on chemical and semi-crystalline structures were obtained by scanning electronic microscopy (SEM), FT-IR analysis and X-ray Diffraction. The in vitro bioactivity of the composites was investigated by incubation in simulated body fluid (SBF). The variation in porous morphology was studied and the Ca/P ratio of the samples evaluated. X-ray Diffraction was used to confirm the presence of apatite in the samples. The porosity and bioactivity produced in the samples by our experiments could be appropriate for proliferation process of cells like fibroblasts and osteoblasts.



[BIO-189] Cytotoxicity of Chitosan/Mimosa tenuiflora capsules in MDA-MB-231 cancer cells

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Breast cancer is the most common malignancy and second important cause of dead among woman. Mimosa tenuiflora it is rich in arabinogalactans, saponins and triperpenoid glycosides. Recently, arabinogalactans has reached interest of scientific community due to its potential to reduce cell proliferation and to block metastasis of liver tumor cells. Nanodiamonds are nontoxic nanoparticles for drug delivery that may enhance effects of treatments on cancer cells. For these reasons, in this work nanodiamonds and extract of Mimosa Tenuiflora were encapsulated by chitosan.

The properties of the particles were studied with Fourier transformed infrared spectroscopy (FTIR), Thermogravimetical analysis/Differential scanning calorimetry (TGA/DSC) and X-ray diffraction (XRD). The adherence of extract of Mimosa Tenuiflora was analyzed with a UV-Visible spectroscopy at a wavelength of 253 nm. Also the cytotoxicity of those capsules were evaluated using MDA-MB-231 line cell. The test revealed that the particles might be used to treat breast cancer.



[BIO-18] purification study of HCl doped polyaniline/polyvinyl alcohol blends synthesized by dispersion polymerization

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Polyaniline (PANI) has been one of the most studied conducting polymers in the past 30 years because of its interesting properties such as tunable electrical conductivity and good thermal and environmental stability. Reported synthesis methods of PANI focus on the chemical and electrochemical oxidation of the aniline monomer to obtain PANI in emeraldine phase, which has the best properties of all PANI oxidation states. In order to obtain stable colloidal dispersions of PANI emeraldine salt, recent research implies to synthesize PANI in a matrix of insulating polymers such as polyvinyl alcohol (PVA) by the chemical oxidation method, however in situ synthesis of PVA-PANI blends obtained by this method have undesired sub products such as oligomers and derivatives from the oxidant material. In this work, PVA-PANI colloidal dispersions were made by polymerization dispersion method by maintaining a 1:1 M/M relation between the monomer and the oxidant within a temperature of $-5\text{ }^{\circ}\text{C} < T < 5\text{ }^{\circ}\text{C}$. Once the PVA-PANI blend was obtained, further purification methods were applied to get rid of the undesired sub products generated by in situ polymerization. First purification method is based on a solvent system consisting of a solution of H₂O/CH₄OH (1:5) in order to obtain PVA-PANI gels by precipitation, and then making a redispersion method. The second purification consist in the use of dialysis membranes with MWCO of 12,000 Da, which is in the MW range of the PVA-PANI sub products. Purification results of PVA-PANI were characterized by ¹H RMN, FTIR, UV-Vis and TGA/DSC to analyze molecular and thermal variations from the material before and after its purification. Then, PVA-PANI



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films were obtained by spin coating the purified material in order to analyze structure and morphology by XRD and SEM characterization techniques respectively. The focus of this research is to study the properties of purified PVA-PANI blends synthesized by polymerization dispersion, in order to provide a purification method for PVA-PANI directly from the obtained colloidal dispersion.

Keywords: Polyvinyl alcohol; Biocompatibility; Polyaniline; Purification.



[BIO-22] Synthesis and characterization of Zeolite ZSM-5 modified with Ag by sol-gel method assisted by microwave for future application in tissue engineering

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Zeolites are a microporous aluminosilicates used for their bioactivity, absorbent properties and porous characteristics. ZSM-5 zeolite has a low aluminum content thus reducing toxicity and is better for biomedical applications. Therefore, the concentration of aluminum of the zeolite was varied by adding silver nitrate in the structure in different concentrations to decrease the aluminum content. Also to incorporate the properties of the silver in the structure such as the bioactivity and the antimicrobial effect. These characteristics improve the growth of P and Ca in the structure. Synthesis was performed by the sol-gel method assisted by microwave technique. Then the zeolitic material was filtered and cleaned with HCl to remove all impurities from the material. Finally, simulated physiological fluid (SBF) tests were performed on each sample for two periods of 7 and 14 days to study the growth of P and Ca in the zeolite structure.

Characterization of zeolite was made by thermal analysis techniques (TGA), scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and dispersed energy spectroscopy (EDS) to analyze the structural and chemical characteristics of zeolite, before and after their immersion in simulated physiological fluid. With these characterization techniques the growth of P and Ca in the zeolite was analyzed and indicates that there is a bioactivity in the zeolite with silver. The characteristics obtained in Ag-ZSM-5 material make them a suitable candidate for future application in biomedical engineering.



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[BIO-42] Isolation and characterization of Triticale starch films

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In this work, Triticale starch, a natural biodegradable biopolymer, was isolated, characterized and used for bag film elaboration. Starch content of the grain was 58%. The starch flour had a moisture content of $6.89 \pm 0.02\%$, protein of $1.36 \pm 0.31\%$, lipids of $0.62 \pm 0.45\%$, and amylose of $21.8 \pm 3.3\%$. Triticale starch and a biodegradable polyester (Ecoflex®) were used for extrusion-blown bag elaboration. Bag properties were compared with a commercial bag. The morphology was observed using scanning electron microscopy (SEM) and its mechanical properties were evaluated. SEM studies revealed good adhesion between polyester and starch phase for the commercial bag compared to the Triticale bag. Triticale bag had higher elongation at break and lower modulus of elasticity compared to the commercial bag as observed in the mechanical tests. For the biodegradability study, the Triticale and commercial bag had comparative weight loss after 2 months composting. Triticale can be a good source for biodegradable films elaboration.



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[BIO-58] Instrumentation amplifier in the detection of the piezoelectric effect in human tooth.

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Piezoelectric effect is a reversible process in which the materials that present the effect, generate electric charge resulting from an applied mechanical force, and generate a mechanical strain resulting from an applied electric field. The present study focused on the detection of the piezoelectricity in human tooth. The tooth was cut into small cubes of approximately 4 mm * 3 mm * 4 mm. The ADA400A Differential Preamplifier was used to detect the potential generated by the sample when a variable compressive force was applied in direction parallel face of cube the tooth. The detected potential differences were 15-30mV approximately. Applied an electric voltage of 500v on the samples, generating mechanical strain that was detected by a piezoelectric sensor.



[BIO-130] Micro-abrasion tests in a high-density polyethylene reinforced with nut fibers

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Abstract

The use of polymers in automotive and aerospace industry has been recently studied. A low weight and high wear resistance material is attractive for replacement of heavy materials used in this industry. This work shows the results of wear trials in a high-density polyethylene (HDPE) reinforced with nut natural fibers. The tribological tests were carried out using the micro-abrasion technique with a fixed ball system in order to create the wear craters on the polymer. In this case, a solution at 10% of Al₂O₃ was prepared (with a particle size around 3 μm) as the abrasive material. The reinforced HDPE was previously made at different concentrations of 2%, 4%, 6%, 8% and 10% of nut fibers. Conditions for each test were established with variation of the load and the total ball sliding distance. An optical microscope was used to determinate the crater diameter and the images obtained were analyze in a computer. Also, an analysis by X ray diffraction and Raman spectroscopy were made to supply the study and get additional information about the polymer structure. It was found that the diameter of the wear crater in low sliding distances, at the same conditions, is similar in all the different concentration of organic fibers. At higher sliding distances, it was found a variation in diameter of the wear crater dependent on the presence of fibers in the HDPE.

Keywords: polymer, HDPE / nut, wear (micro-abrasion)

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[BIO-170] Synthesis and Characterization of Magnetite Ferrofluids for Biomedical Applications

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Four Magnetite/polymer based ferrofluids were prepared by two routes. The first route was Co-precipitation by rapid injection, which we obtained an average particle size of approximately 10 nm. With the second route, synthesis co-precipitation by reflux, the average particle size was 100 nm. The spherical morphology and average particle size of nanoparticles was measured by electron transmission microscopy. The samples were suspended in Oleic Acid to form the fluids. The ferrofluids obtained were characterized in a magneto-rheological system, where we observed the system experiments important changes in the viscosity as a function of the magnetic field, shear rate and particle mean size.



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[BIO-185] Epigallocatechin-3-gallate functionalized with graphene oxide for in vitro antitumor study in human cervix cancer cells

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The results of the synthesis and characterization of epigallocatechin-3-gallate functionalized with graphene oxide are shown for the study of the anti-cancer effect in vitro in cervical cancer or human cervix cancer cell lines, CACU. Cancer is one of the great challenges for clinicians and researchers as advances in the fight against cervical cancer have been very slow, due to the time required. In order to speed up the evaluation and approval of new therapies, it is necessary to explore new paradigms such as phyto pharmaceuticals such as epigallocatechin-3-gallate, which on the one hand have demonstrated anti-cancer effects and, on the other hand, have allowed the functionalization of various nanocomposites.



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[BIO-186] Biological response of calcium phosphate for bone replacement

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The study of the biological response of calcium phosphate used for bone replacement is of vital importance to know its behavior when it is directly related to the living system. In this paper we present the elements that describe the behavior of calcium phosphate when it is used as a bone substitute in a living organism.



[BIO-188] Evaluation of in vitro bioactivity of Polycaprolactone/ Hyaluronic acid/ Multiwalled Carbon Nanotubes / Extract from Mimosa Tenuiflora composites

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Polycaprolactone/ Sodium Hyaluronate/ Multiwalled Carbon Nanotubes /Extract of Mimosa Tenuiflora (PCL/SH/MCNT/MT) composites have been produced by thermally induced phase separation method. The *in vitro* bioactivity of the composites was assessed by soaking in simulated body fluid for 7, 14, 21, and 28 days. The structure and composition of the composites were analyzed using scanning electron microscopy (SEM) coupled with energy dispersive spectroscopy (EDS), and Fourier transform infrared spectroscopy (FTIR). The results show the formation of apatite layers in the composites, which make them possible candidates for tissue engineering applications.



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[BIO-221] Solid state polymeric detectors of ionizing radiation, prepared in México

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In 1940, Frank Strain developed and patented the polymer allyl diglycol carbonate (Columbus resin formulation number 39, known as CR-39). This plastic is mainly used as low weight material in the manufacture of eyeglass lenses.

In 1978, at the University of Berkeley in California it was found that the polymer CR-39 to be an excellent detector with unique sensitivity and resolution for the recording of nuclear tracks.

The most important company from which this material was provided until 2016, in the shape of plates with appropriated dimensions to detect ionizing particles (alphas, neutrons, medium energy ions) was LandauerTM. But this company does not sell the material anymore. In place of selling the CR-39, they provide the service, increasing too much the price and wasting time.

In this work, we are reporting the methodology to prepare similar plastics to continue our investigations involving the passive detection of Radon in caves and houses, and also neutrons in hospitals whose facilities include a linear accelerator.



[BIO-225] Er:YAG laser conditioning of enamel: direct bonding of orthodontic brackets and evaluation of Shear Bond Strength.

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Phosphoric acid etching has been a standard protocol to treat tooth enamel for bonding resins and orthodontic attachments. However, decalcification is the one potential disadvantage, which leaves the enamel susceptible to caries attack. Laser ablation has been suggest as an alternative method to acid etching; but previous studies have obtained contrasting results. Based on contradictory findings concerning the use of lasers for enamel etching, the aim of this study was to investigate the shear bond strength on bovine teeth prepared for bonding with Er:YAG laser etching and compare them with phosphoric acid etching. In this experimental *in vitro* study buccal surfaces of sixty bovine teeth non-carious were mounted in self-cure acrylic resin, the buccal enamel surface was cleaned and polish with non-fluoridated pumice and rubber cup, then washed with an oil free air spray and exposed to laser energy. Group I: 15 teeth at 100 mJ pulse, 10 Hz energy, VSP, 2 watts power, 15 seconds; group II: 15 teeth at 130 mJ pulse, 10 Hz energy, VSP, 2 watts power, 15 seconds; group III at 150 mJ pulse, 10 Hz energy 2490 wavelength, VSP, 2 watts power 15 seconds; finally; group IV or control group teeth were etched with 35% phosphoric acid 20 seconds. The shear bond strength of bonded brackets with the Transbond XT adhesive system following which all the samples were stored in destiled water for 24 hours and was measured with universal testing machine. Results and Descriptive statistics. ANOVA test, of homogeneity of variances, one-way analysis of variances and Tukey test were used to analyze the data. It has been suggested the highest mean SBS values in control group while the lowest in goup I. Acording to our findings laser etching provided clinically acceptable SBS values with 130 mJ pulse, 10 Hz energy, VSP, 2 watts power, 15 seconds.



[BIO-229] Structural analysis of composite Calcium Hydroxyapatite/TiO₂ synthesized by ultrasound assisted sol-gel method

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Calcium hydroxyapatite Ca₁₀(PO₄)₆ (OH)₂, (CaHAP), is a biocrystal naturally found in coral, exoskeletons and vertebrate skeletons. It is the main component of human bones (~43-50% weight), teeth, tooth enamel, cartilage, among others, representing ~ 60-70% weight of the calcified human skeleton and 90% weight of the bone inorganic matrix. As a consequence, this is one of the most important biomaterials.

Incorporating a semiconductor (TiO₂) a calcium hydroxyapatite structure is a successful pathway to increase their physical, chemical and biological properties. The CaHAP and TiO₂ were obtained by ultrasound assisted sol-gel method, using Ca(NO₃)₂ • 4H₂O and (NH₄)₂HPO₄ as sources of calcium and phosphorus and TiOSO₄ xH₂O as sources of TiO₂. Hydroxyapatite, TiO₂ and composite CaHAP/TiO₂ powders were characterized by X-ray diffraction (XRD), X-Ray Fluorescence (XRF) and FTIR analytical techniques to evaluate the structural and compositional changes. The only phase present at pure calcium hydroxyapatite samples was the hexagonal one, while the TiO₂ was anatase phase. On the other hand, we found that the predominant phase in the composite was the hexagonal.



[BIO-258] Silver nanoparticles and their effect on the adhesion of *Streptococcus mutans* in orthodontics arches.

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Streptococcus mutans (*S. mutans*) is the microorganism associated with the development and initiation of dental caries. Adherence is one of the main factors that favors the development of this pathology. Successful treatments have been developed. However, new agents with improved physical-chemical properties must be studied. Although silver nanoparticles (NPAg) have been applied against *S. mutans*, there is no information on its effect on the adhesion of this microorganism to orthodontic additions. The aim of this study was to evaluate the effect of nanoparticles on *S. mutans* adhesion on orthodontic arch surfaces.

MATERIALS AND METHODS: NPAg of 8.2 and 21.2 nm were prepared and characterized by dynamic light scattering and transmission electron microscopy. Colony forming units per milliliter (UFC / mL) were obtained to determine adhesion activity through microbiological tests previously reported in orthodontic arches of nickel-titanium-copper (Cu-Ni-Ti), steel and nickel-titanium).

RESULTS: The two sizes of NPAg showed inhibition of *S. mutans* adhesion in orthodontic arches.

Lower sizes of NPAg showed greater activity to inhibit *S. mutans* adhesion than larger particles. On the other hand, this activity was also related according to the type of bow used. The CuNiTi arc surface showed higher adhesion compared to steel and Niti arcs.

CONCLUSIONS: NPAg have the potential to be used to control *S. mutans* adhesion on orthodontic arch surfaces. However, other evaluations should be carried out.



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CHARACTERIZATION AND METROLOGY (CHM)

Chairman: Roberto Machorro (CNYN-UNAM)



[CHM-38] **Refractive index of characterization of very thin films grown by atomic layer deposition**

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Standard concepts of refractive index are revised to conform extreme measurements of thin films. With new instrument capabilities now is possible to grow monolayers and measure its reflectance and polarization properties. To fit experimental data a refractive index smaller than the bulk material is introduced, with no explanation of the reason, up to now. In this work we propose a simple model to understand why the monolayer refractive index is smaller than the bulk.

We applied spectral ellipsometry to characterize very thin layers. They are deposited via atomic layer deposition (ALD). This technique is used for depositing thin films with precise control of thickness down to atomic scale and the possibility to deposit several materials, including different oxides. ALD is a powerful tool to fabricate ultra thin, highly uniform and conformal material layers. We also work with nanolaminates, which are thin films composed of layers of different materials, characterized by having alternated individual layers of nanometer thickness. Aluminium and Yttrium oxide multilayer were coated on a silicon wafer by ALD.

The aim of this work is to provide a plausible explanation to the refractive index for very thin materials. Do the optical refractive index has a meaning at this level? Our thickness measurements correlate very well with those of transmission electron microscopy (TEM). Effective medium approximation is used to fit ellipsometric parameters, from which the evolution of refractive index relative to Al_2O_3/Y_2O_3 layers is obtained as a function of thickness, then the gap of the multilayer is drawn.

Acknowledgments

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[CHM-180] Comparison between Al and Ag for the construction of low thermal emissivity filters deposited by magnetron sputtering technique

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Low-e coatings or low thermal emissivity filters, are used in industry for windows that do not let pass the heat. This type of windows are used in the housing market and self-sustainable buildings. They are characterized by high transmission of visible light (about 80%), but a low thermal emissivity of about 20% in the infrared (IR). Currently, this type of windows is too expensive due to the use of silver (Ag) in its construction. One of the disadvantages of Ag is that it darkens on contact with the environment, therefore the necessity of using a double glass vacuum assembly to protect it. In this work the use of aluminum (Al), as a replacement of silver in Low-E coatings, is proposed. An advantage of using the Al is its cheaper price, but keeping the behavior of the silver: having approximately the same values of transmittance in the visible and the IR regions. Besides Al hardness is greater when exposed to the environment. Comparison between Low-e made of Al and Ag are shown using 3 layers in their construction, including their optical characterization.



[CHM-195] The Physical Origin of the Shirley Background in Photoemission Spectra

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The current paradigm for describing the background in photoemission spectra is inelastic-losses of the emitted photoelectrons. We have shown that extrinsic scattering can explain only a small fraction of the background signal near the photoemission peak [1] and that the current theories dealing with both intrinsic and extrinsic scattering cannot reproduce the experimental signal [2,3]. The latter can be modeled as a sum of component due to inelastic losses plus a step-shaped contribution known as the Shirley background. This implies that the physical origin of the Shirley signal is not inelastic losses. We studied the behavior of the background of the Cr 3*p* photoemission spectrum for photon energies around the Cr 2*p* and Cr 2*s* edges. It was found a strong modulation of the intensity of the Cr 3*p* Shirley background signal around the Cr 2*p* threshold. This strongly suggests that the physical origin of the Shirley part of the background of the Cr 3*p* spectrum is not related to inelastic scattering, but to channeling [4,5] between the 2*p* and 3*p* levels.

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[CHM-230] Development and characterization of a temperature sensor based on fibers of
ABO₃ compounds

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Lithium Niobate (LN) and Lithium Tantalate (LT), both ferroelectric ceramic materials, are used to develop nano fibers for sensing applications. The fibers are manufactured using conventional and coaxial electrospinning with silica on the outside. For the spinning solutions, the sol-gel is created for each type of material, using the ceramic precursors lithium niobium ethoxide and lithium tantalum ethoxide, as well as a sol-gel of Tetraethyl Orthosilicate (Teos) as silica precursor for coating. The sol-gel solutions are mixed with the polyvinylpyrrolidone polymer (PVP) to facilitate electro-spinning. The mixtures are assembled in electrospinning equipment in simple and coaxial configuration obtaining LN, LT, LN / Teos and LT / Teos fibers. The obtained fibers are subjected to a calcination process for 2hr at 800 ° C. Characterization by scanning electron microscopy, Raman spectroscopy, and X-ray diffraction are performed on each sample. Sintered fibers are subjected to temperature changes to evaluate their response.



[CHM-250] Aging spectral markers of tequila observed by Raman spectroscopy

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Raman spectroscopy (RS) is a resonance technique of high resolution that provides in a few seconds chemical and structural information of almost any organic or inorganic material or compound, allowing its identification. The spectral trace of its narrow and highly resolved bands of the sample under test provide specific information of the compounds for the chemical analysis, and has great potential for multicomponent identification. RS also offers important advantages as an analytical tool. For example it is fast and non-destructive and requires little preparation of samples, making it very versatile. For example, while employed as an analytical tool to assess the quality of alcoholic beverages through RS, it has been possible to determine, among other things, the actual concentration of ethyl alcohol. For liquor samples, the concentration of ethanol in colorless and odorless alcoholic beverages has been determined. In this work, we studied the aging spectral markers of three kinds of tequilas: blanco, reposado and añejo. These tequilas belongs to the same production house "El Charro". This factor is of great importance since most of the studies reported so far have analyzed tequilas from different production houses, brands and types of liqueurs, which makes difficult the interpretation of the results and conduces to a high uncertainty of the data. Conversely, our study is focused on tequilas elaborated in the same place with controlled factors, e.g. the type of water used for the elaboration, the origin of raw materials like agaves, sugar, barrels, among others. For the RS experiments the 532 and 785nm excitation lines were used in normal incidence. We were able to distinguish the aging state of tequilas by using the fluorescence of Raman spectra. In addition, a method based on the profile of the OH (water) region of the Raman spectra was developed to qualitatively study the ethanol content in tequila samples.

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[CHM-6] Mechanical analysis of a hard boron coating on a chrome molybdenum steel

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A boron coating is studied with a thermochemical treatment at temperatures of 1273 and 1223 K with an exposure time of 0.5 and 2 h; the adhesion of the layer is analyzed by the Rockwell C technique prescribed by the German standard VDI 3198 and obtained a qualitative classification; the maximum Hertz pressures are estimated by finite element analysis; the growth rate and the morphology of the FeB/Fe₂B layer are shown by optical microscopy; the presence of FeB/Fe₂B phases was determined by X-ray diffraction (XRD). The Scanning Electron Microscopy (SEM) technique shows the distribution of the alloying elements in the layer FeB/Fe₂B/substrate formed on the surface of the AISI 4140 steel. The elastic modulus and hardness were obtained with nanoindentation tests in the biphasic layer. The histogram determines the growth trend per phase for each condition of the thermochemical treatment. This research aims to characterize the morphology, growth tendency, adhesive and mechanical behavior of the boride coating formed on AISI 4140 steel by means of the dehydrated box paste technique.



[CHM-61] Synthesis and characterization of CNT-TiO₂ nanotubes via ALD for the degradation of azo dye amaranth.

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Among the metal-oxides, Titanium oxide has photo-physicochemical properties that are important in a wide range of technological applications, including environmental and energy-related fields. This material is widely investigated for wastewater and air cleaning, mainly because of its strong oxidizing abilities for the decomposition of organic pollutants, but also because it is non-toxic, environmentally friendly, and chemically stable. Keeping that in mind, the purpose of the present work is to combine the characteristics of CNT with TiO₂ to engineer enhanced materials for photocatalytic applications. Here we present a transmission electron microscopy (TEM) characterization together with a detailed XRD, TGA and XPS measurements for the characterization of the resulting nanostructures. Finally, The CNT-TiO₂ were evaluated as photocatalytic material in the degradation of the alimentary azo dye amaranth.

Acknowledgments

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[CHM-62] Studies on the optical and structural properties of quartz of mines.

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Different types of quartz were obtained on distinct sources in the state of Zacatecas in order to determinate their optical and structural properties, and so their diverse impurities inside, which can vary upon the region they were extracted. Sample analysis was carried out by X ray diffraction technique, IR and UV-Vis spectroscopy. SiO₂ compounds were present in the samples as expected; Calcites compounds and impurities of transition metals and alkaline earth elements also were found. Geological studies were made using optical petrography which is in concordance with X ray diffraction analysis, in which, silica and metal oxidations appear. Finally, structural characterization showed the hexagonal phase of SiO₂ and cubic CaCO₃. In the cases were fluorite compound has appeared, this compound presented a cubic structure.



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[CHM-78] Evaluation of hard coating in steel farming

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In this paper evaluate the hard surface formed in a tooling for the agricultural industry, with a hard coating; through the process of boriding by dehydrated paste at temperatures of 900, 925 and 950 C, with residence times of 1, 2, 3, 4 h. The morphological characterization of the present phases were determined by optical microscopy (MO); also scanning electron microscopy (EDS). The FeB/Fe₂B layers obtained on the surface of the material are determined by the technique XRD, Hardness and fracture toughness is evaluated using the Vickers microindentation technique. Using the law of parabolic growth the mobility of boron was included potential influence of boron, treatment time, and temperature and time incubation in hard layers. With the present show the growth of iron boride and mechanical characteristics for possible applications in the agricultura



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[CHM-127] Micro-abrasion tests in hard coatings

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Abstract

The hard coatings in the industry have been studied over time, due its multiples properties that it presents. It's possible to use in different applications, as: cutting tools, medical and food applications, etc. This work shows the results of wear trials in hard coatings, such as: titanium nitride (TiN), titanium aluminum nitride (TiAlN), titanium chromium nitride (TiCrN), titanium boro nitride (TiBN), deposited in a substratum of M2 steel by PVD technique (using cathodic arc). The tribological tests were carried out using the micro-abrasion technique with a fixed ball system in order to create the wear craters on the coatings. In this case, a solution at 10% of Al₂O₃ was prepared (with a particle size around 3µm) as the abrasive material. Conditions for each test were established with variation of the load and the total ball sliding distance. An optical microscope was used to determinate the crater diameter and the images obtained were analyze in a computer. Also, an analysis by X ray diffraction, Raman spectroscopy, and mechanical and optical profilometry were made to supply the study and get additional information about the coatings. It was found that the diameter of the wear crater at low slip distances, under the same conditions, is different in all coatings. On the other hand, it was found that micro abrasive wear resistance was better in the film of TiN and was showed a lower micro abrasive wear resistance in the film of TiBN.

Keywords: hard coatings, TiN, TiAlN, TiCrN, TiBN, wear (micro-abrasion)

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[CHM-242] Monitoring and determination of cleaning level of the target before deposition in a reactive DC magnetron sputtering

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In this work we present an efficient target-cleaning approach that can be used to estimate the target healthiness in a DC magnetron sputtering deposition. The method is based on the monitoring of the plasma in real-time by means of optical emission spectroscopy (OES) during a traditional cleaning phase in an Ar atmosphere. SiOxNy thin films were grown on silicon wafers for different deposition configurations of Ar, O, and N fluxes, producing thin films ranging from those of SiO₂ till Si₃N₄. The stoichiometry of the resulting films was measured by in-situ spectroscopic-ellipsometry. From this monitoring it is demonstrated that the intensities of emission lines from Ar are sufficient indicators of the target cleanliness, allowing estimating the time when the target is ready to start deposition. Hence, this approach can be suited for an industrial environment since could avoid wasting time and, on the other hand, improve target lifetime due to efficient erosion of the target during the cleaning phase.



[CHM-268] Physicochemical investigation of co-deposited Mg and Ti oxides onto Mg substrates.

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Magnesium has been extensively studied to develop biodegradable implants, however, its main disadvantage is the fast degradation in the physiological fluid because of electrochemical corrosion. To improve Mg corrosion resistance modification of the surface has been proposed. In this work, we report the physicochemical properties of TiO₂-MgO thin films deposited onto Mg substrates with the aim of reduce its degradation in the Hank's solution. TiO₂-MgO thin films were deposited by the reactive RF-sputtering technique from Mg and Ti metallic targets. Samples with different TiO₂/MgO rates were prepared by varying the sputtering power. XRD analysis showed that coatings with a high content of MgO present a cubic crystalline structure, while a decrease on the crystallinity was found as the TiO₂ content is increased; finally, coatings with the highest content of TiO₂ are amorphous. XPS analysis showed the formation of Ti-O and Mg-O bonds; whose ratio varies with the sputtering power applied to the Mg and Ti targets. SEM micrographs showed that films are smooth without pinholes or cracks; this characteristic makes the films suitable for corrosion protection. Tafel curves showed the variation of the corrosion current as function of the MgO/TiO₂ rate. This work has been supported by CONACYT under PDCPN-2015 program (grant 28).

Keywords: Magnesium, MgO-TiO₂, corrosion protection.



[CHM-279] Detailed analysis of the photoemission spectra of copper films with coexistent Cu¹⁺, Cu²⁺ and Cu³⁺ oxidation states

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A precise assessment of the composition of Co¹, Fe² and Zn³ oxides has been reported through peak fitting of their 2p photoemission spectra. In those reports, it was shown the need to employ reported modeling methods⁴ and to consider both branches ($j=3/2$ and $j=1/2$) during the fitting procedure to correctly assess the peak intensities.

In this work, metallic copper films were obtained by sublimation in ultra-high vacuum (5.5×10^{-8} Torr) on RCA-cleaned Si(100) substrates. The copper films were heat treated in an ultra-high purity oxygen atmosphere at 200 °C from 1 to 10 min, and then characterized by angle resolved X-ray photoelectron spectroscopy using a monochromatic Al K α source ($h\nu = 1486.7$ eV) and a pass energy of 10 eV.

From the spectrum of 4 min two chemical copper species were observed, both Cu¹⁺ (932.5 eV) and Cu²⁺ (933.5 eV), together with their satellites (Cu¹⁺: 946.5 eV, Cu²⁺: 941.1 eV, and Cu²⁺: 943.9 eV) were clearly identified.⁵ The spectrum also contained other peaks at 934.7 eV and 942.4 eV. The calculation of composition using multi-layer model (MLM)⁶ indicates that correspond to Cu³⁺. The angular dependence prove that these oxide species are evenly distributed in the bulk. .

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Luminescence Phenomena: Materials and Applications (LPM)

Chairmen: **Ciro Falcony: (Cinvestav-IPN)**
Giancarlo C. Righini: (Centro Fermi)



[LPM-36] Charge transfer influence in the photoluminescence of lead-free Ba_{1-x}Ca_xTi_{0.9}Zr_{0.1}O₃ electro-ceramics

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The present work shows an important high violet-blue emission observed in the Ba_{1-x}Ca_xTi_{0.9}Zr_{0.1}O₃ nanoparticles (BCZT-Np) where $x = 0.1, 0.125, 0.15$. This result suggests that the charge transfer effects (CT) play an important role in these nanoparticles. The BCZT-Np were prepared by using the sol-gel glycol route. The structural and optical properties of BCZT-Np were determined by X-ray diffraction (XRD), Raman, diffuse reflectance Ultraviolet-Visible spectroscopy (UV-Vis), energy loss electron spectroscopy by transmission electron microscopy (EELS-TEM) in scanning mode and photoluminescence (PL) analysis. The Rietveld analysis for the XRD patterns and the normal phonon modes resolved by Raman confirm that powders heat treated at 700 °C for 1 h show a perovskite-type structure with tetragonal phase (P4mm space group). Kubelka-Munk model and the Tauc method suggest an indirect electronic transition for BCZT-Np. The optical energy band gap values (E_g) measured by UV-Vis varies from 3.13 to 3.18 eV. These results are in agreement with the E_g values obtained by the energy loss function in the analysis of valence EELS region (0-50 eV). An intense photoluminescence centered at 489 nm (blue emission) was observed in the BCZT-Np. This behavior could be associated to the presence of charge transfer effects between Ti 3d states with O 2p states. The interpretation of Ti L_{2,3} edge in the core-EELS region (452-470 eV) was performed in combination with multiplet calculation (based on a modified Hartree-Fock method). The crystal field theory and the charge transfer parameters were included in order to reproduce the experimental results. The PL results



open the possibility to extend the potential application of this lead-free BCZT electro-ceramic for light-emitting devices.

[LPM-43] Rare earth doping of thin film oxides for white light emission: from RGB to wideband

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The development of white-like emitters and phosphors for light emitting devices (LEDs) has ranged in a wide variety of materials, from bulk-like powders, massive glasses or thick coatings to nanostructures such as nanocrystals, quantum dots or engineered thin films; each of these offer technological and/or scientific advantages, but still focusing the research on features like the color rendering and luminous efficiency.

In this matter, we approach some of these issues by studying simpler oxide structures (Al_2O_3), and by means of the pulsed laser deposition (PLD) technique we've produced thin films combining the ablation processes onto different targets, the alternating process allows us to generate multilayered nanostructures with high control of the rare earth dopants and its concentration and distribution on the thin film. Among the mentioned systems we put special focus on the tri-chromic phosphor Eu:Tb:Tm (RGB) and the sole dopant of Eu^{2+} and its wideband-like emission in the visible range.



[LPM-100] Synthesis and characterization of Er³⁺-doped tin dioxide glass-ceramics produced by sol-gel route

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Glass-ceramics are nanocomposite systems that exhibit specific morphological, structural and spectroscopic properties with potential groundbreaking applications for integrated photonic devices, thanks to their optical transparency and the possibility of doping with several kinds of rare earth ions. Among different glass modifiers, SnO₂ shows great advantages, such as the reduction of nonradiative contributions to the relaxation mechanism, thus allowing higher fluorescence efficiency.

Silica-tin dioxide glass-ceramics [xSnO₂-(100-x)SiO₂, with x = 10, 20, and 30 mol %] doped with different concentrations of Er³⁺ (0, 1, 2, and 3 mol %) were fabricated by the sol-gel process in different geometrical systems: pillars and planar waveguides. The precursors, SnCl₂·2H₂O and Er(NO₃)₃·5H₂O, were dissolved in ethanol and added to the starting solution that had been prepared by mixing tetraethyl orthosilicate (TEOS), ethanol, de-ionized water, and hydrochloric acid.

The effects of the heat-treatment temperature, the SnO₂ and Er³⁺ concentrations, and the fabrication protocol on the structure and distribution of erbium ions in glass-ceramic were investigated by X-ray diffraction, m-line analysis, transmittance and time resolved luminescence spectroscopy. Obtained films were crack-free, with a transmittance of around 90% over the 250 nm – 3.0 μm spectral region. The waveguides exhibited an attenuation coefficient of 0.74 dB/cm at 1542 nm. The local environment



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of the Er^{3+} ion in SnO_2 nanocrystal was investigated by numerical simulations. The important role of SnO_2 nanocrystals as Er^{3+} luminescence sensitizers was also experimentally confirmed.

This research is performed in the framework of the COST MP1401 project “Advanced Fibre Laser and Coherent Source as tools for Society, Manufacturing and Lifescience” and the MAECI bilateral project “Plasmonics for a better efficiency of solar cells” between Italy and South Africa. T. N. L. Tran acknowledges the scholarship of the Ministry of Education and Training, Vietnam International Education Development.



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[LPM-302] Fiber-optic lasers and their applications

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Fiber-optic lasers are lasers in which the active gain medium is an optical fiber doped with rare-earth elements such as Erbium (Er), Ytterbium (Yb), Thulium (TM), Holmium (Ho), and so on. The principal cavities to develop this kind of lasers are the linear and the ring cavities. With these two cavities we can generate continuous wave and pulsed lasers. To generate pulsed lasers we have two principal techniques: the Mode-locking and Q-Switching techniques (passive or active). Modelocked fiber lasers are capable of producing high-quality short or ultrashort optical pulses, and are essential optical sources for a great variety of photonic applications. For applications in the ultrashort pulse regime passive mode-locking is the preferable technique. Actively Q-switched fiber lasers have been investigated extensively due their applications in remote sensing, medicine, and terahertz generation, an so on. This technique is usually achieved to improve pulses stability and higher pulse energies. In recent years, fiber lasers operating in the 1550 nm wavelength region are widely studied because of their properties such as high gain, eye-safe laser emission, and single-mode operation, among others. Since Er/Yb double clad fiber (EYDCF) came out, different approaches of fiber lasers were reported in order to reach high efficiency and high power emission. Fiber lasers using Tmdoped fiber (TDF) as a gain medium offer the possibility of obtaining laser emission in a wavelength region from ~1.8 to 2.1 μm . The features of this spectral window includes high transparency, eye safe emission, and high absorption in air and many human/animal tissues, making TDF lasers attractive for applications involving free-space/atmosphere light propagation and medical laser surgery, and have been of increasing interest for potential applications in different research areas such as optical instrumentation, light detection and ranging (LIDAR), communications and material processing. In this work we make a review of our work in the area of fiber-optic lasers.

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[LPM-16] Study of thin films based on oligophenylenes deposited by spray-pyrolysis technique

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In recent years, *pi*-conjugated organic molecules have been of great interest due to their unique electrical properties that make them able to act as active materials in photodiodes, molecular sensors and photovoltaic cells. The oligophenylenes have attained considerable attention due the smallest ones (terphenyl, quaterphenyl, quinquephenyl) are not only able to radiate a high-energy light on the blue region of the spectrum, but also to display a rich thermotropic polymorphism. We report here the deposition of oligophenylenes to study their properties. In previous studies, it has been reported changes on surface characteristics of thin films based on oligophenylenes deposited by other techniques. Thin films were deposited by spray-pyrolysis technique on glass substrates varying parameters as temperature, angle and distance of deposition. Then were studied by AFM, UV-Vis and PL spectroscopy. The changes on the properties depended of the deposition condition. It is expected to see improvements as PL intensity and rugosity of the thin film with the parameters variables in the technique used. The oligophenylenes here studied could be candidates for optoelectronics application devices.



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[LPM-27] Study of deposition of terfenylene molecules by spin coating – spray pyrolysis process to improve superficial rugosity and optic properties.

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Organic thin films have significant impact on Flexible Electronics. These have a wide scope of application within this area of study. Thin films offer a compact and versatile design in devices such as transistors, biosensors or OLEDs. In addition, low cost and high reproducibility, the synthesis process of materials requires low energy consumption which makes them a potential candidate for their application on an industrial scale. One of the problems in thin films is the behavior of the material used for their deposit. It has been observed that the optical properties of the material decrease as the number of molecular packing increases on a thin film. In this work, we reported the deposition of thin films based on terfenylene using two deposition techniques. The films were deposited by Spin Coating-Spray Pyrolysis, by varying temperature and deposition time, as well as the structure multilayer. In order to know the chemical, optical and microstructural properties the films were characterized by Fourier Transform Infrared Spectroscopy, Visible Ultraviolet, Photoluminescence, Scanning Electron Microscopy, and Atomic Force Microscopy respectively. The characteristics obtained in thin films make them a suitable candidate for optoelectronics and flexible device applications.



[LPM-79] Layered Gd-based upconversion phosphors and its incorporation into PMMA films.

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Up-conversion (UC) luminescence in Li-Gd₂O₃ powder doped with Ho³⁺ and Yb³⁺, and its incorporation into polymethyl methacrylate (PMMA) films are studied under continuous wave excitation at 980 nm. Powder samples were prepared by the simple evaporation technique. They were structurally characterized using x-ray diffraction and electron microscopy techniques; SEM measurements reveal that phosphors have a layered shape. A study of UC emission from Ho³⁺ was performed. The effect of Yb³⁺ co-doping presence makes possible the holmium green emission in the UC luminescence model, meanwhile lithium presence could increase the Ho³⁺ light emission due to a notable change into Li-Gd₂O₃ structure. On the other hand, PMMA films were synthesized by spin coating technique, they have excellent transparency (around 99 %T) even when they have a high phosphor content. Green light emission was achieved in phosphors under UC luminescence model by excitation at 980 nm, CIE coordinates of phosphors are at the middle of the “green area” (0.3, 0.6), these luminescent properties are transferred to PMMA films.



[LPM-87] NIR and visible upconversion luminescence under 1.5 μm excitation of $\text{Y}_2\text{O}_3:\text{Er}^{3+}$, Yb^{3+} , Li^+ nanostructured powders

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Generation of VIS and NIR upconversion luminescence within the first and second biological optical windows in Y_2O_3 co-doped with Er^{3+} , Yb^{3+} and Li^+ phosphors excited with 1532 nm light is reported. The upconversion emissions at the green and red light emission region (at 530-570nm and 640-700nm) correspond to transitions from the $^4S_{3/2}$ and ($^4F_{9/2} + ^4I_{9/2}$) to ground state $^4I_{15/2}$ of electronic energy levels of the Er^{3+} ions respectively. The near-infrared emissions at 900-1100 nm region correspond to inter-electronic energy levels transitions from $^4I_{11/2}$ to $^4I_{15/2}$ of Er^{3+} ions and from $^2F_{5/2}$ to $^2F_{7/2}$ of Yb^{3+} ions. The role of Li^+ ions is to enhance the luminescence emission of these phosphors around 9, 7 and 11 times in the regions green, red and NR-IR, respectively in comparison with only-erbium doped samples. The luminescence spectra of these phosphors remain unchanged when dispersed in deionized water, cholesterol and in bovine serum.



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[LPM-208] Synthesis of Eu³⁺: Y₂O₃ phosphors using benzyl alcohol route by microwave-assisted technique

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In this work it is shown the synthesis of Eu³⁺:Y₂O₃ powders using the “alcohol benzyl” route by microwave-assisted solvothermal technique. Different concentrations of (Eu³⁺) as an activator ion and annealing temperatures in the range from 270 °C to 1000 °C were considered during the synthesis. Yttrium nitrate was used as precursor of the host lattice and Europium Chloride was used as source of Eu³⁺. Techniques such as Photoluminescence (PL), X-ray diffraction (XRD), Fourier Transform Infrared spectroscopy (FTIR), Energy Dispersive Spectroscopy (EDS), Scanning Electron Microscopy (SEM) and Transmission electron microscopy (TEM), were used to get the characteristics of the powders. Photoluminescence spectra of the as-synthesized samples showed the characteristics emission bands due to Eu³⁺: ⁵D₀ → ⁷F₁ (593nm), ⁵D₀ → ⁷F₂ (611nm) ⁵D₀ → ⁷F₃ (651nm). The FTIR and RS showed C-C bonds located at (1400cm⁻¹), O-H (3500cm⁻¹), and O-Y (380, 1600 cm⁻¹). The EDS showed the 3:2 (O/Y) stoichiometry. In addition, XRD results and TEM showed the lamellar phase of Benzyl Eu³⁺: Y₂O₃ at low temperature. Upon an annealing treatment of the powders, the Y₂O₃ cubic phase was obtained. SEM micrographs showed a flower like morphology even when the powders were annealed at high temperatures.

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[LPM-256] Lu₂O₃-Eu₂O₃ ceramic powders and luminescent properties

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A luminescent material is that material which possesses the ability to convert the types of energy into electromagnetic radiation, the radiation emitted by the material belongs to the range of the visible spectrum, luminescent materials have broad applications ranging from the production of solid state lasers, Display monitors, up to white light diodes.

The methods of production are several, however, the simplest and most successful, is the sol-gel method.

In this work, different systems of ceramic powders have been synthesized. The concentrations of those of Lu₂O₃ / Eu₂O₃ were 80/20, 70/30, 60/40, 50/50 40/60, 30/70 and 20/80 mol% respectively, with the aim of studying the properties of the different systems on the luminescence and the intensity of the emission, the obtained xerogélicos ceramic were analyzed structurally, morphologically and spectroscopically.

Photoluminescence spectroscopy showed in all systems an emission around 615nm which is an emission of the Eu characteristic, on the other hand, it was found that the 80/20 system presents the emission of the mayor within the proposed systems. The XRD showed that the structure is present in all the systems is cubic and a series of displacements can be seen as they change the concentrations of Eu that were used in the synthesis

Keywords: luminiscence, photoluminescence, powders, ceramics, sol-gel



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[LPM-288] Thermo- and photoluminescence properties of doped Ce, Tb Strontium
Pyrophosphate

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Strontium pyrophosphate ($\text{Sr}_2\text{P}_2\text{O}_7$) activated with Ce, Tb ions synthesized by evaporation method was studied using thermo and photoluminescence. $\text{Sr}_2\text{P}_2\text{O}_7$: Ce showed three broad transitions at 310, 328 and 347 nm wavelength corresponding to the transitions $5d^1 \rightarrow 4f^1$ of Ce^{3+} . Broad emissions located at 460, 491, 543, 583, 595 and 620 nm associated with the transitions $^5\text{D}_4 \rightarrow ^7\text{F}_J$ (J=3,4,5 and 6) were observed in $\text{Sr}_2\text{P}_2\text{O}_7$:Tb powders. $\text{Sr}_2\text{P}_2\text{O}_7$: Ce,Tb exhibited the same transitions related with the emissions of the Ce^{3+} and Tb^{3+} ions. All samples showed remarkable CIE chromaticity coordinates. Thermoluminescence (TL) glow peaks around 85 and 155 °C was observed in $\text{Sr}_2\text{P}_2\text{O}_7$: Ce, $\text{Sr}_2\text{P}_2\text{O}_7$:Tb and $\text{Sr}_2\text{P}_2\text{O}_7$:Ce,Tb samples irradiated with beta particles from ^{90}Sr source. The beta TL response was emitted by $\text{Sr}_2\text{P}_2\text{O}_7$:Ce $^{3+}$ samples. The phosphors presented well thermal and optical emissions indicating its possible application in beta radiation dosimetry and lighting field.



[LPM-310] Layered nanophosphors: Enhanced luminescence by intercalation of organic ligands

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Y₂O₃:Eu³⁺ based materials are well-known red downshifting phosphors which excitation depends directly of the O2p to Eu4f charge transfer (CT) band and higher lying levels at $\lambda > 250\text{nm}$ [i], leading to small optical absorption cross-section with high energy requirements. Recent research efforts have been focused in the broadening of the absorption band of rare earth (RE) based phosphors towards longer (more accessible) wavelengths[ii],[iii],[iv],[v]. One attractive approach consists in improving the luminescence of these materials by organic ligands at the particle surfaces. This effect is known as “antenna effect” arising when light is strongly absorbed by organic ligand and much of the energy is then transferred to RE ions that emit efficiently. Thanks to organic molecule, the obtained system can provide a good optical absorption even in region out of RE absorption resonance[vi]. For this purpose, the structural anisotropy of layered materials with rich interlayer chemistry and the unique behavior of swelling and exfoliation into the basic building block: individual layers. Specifically,

the ions between the layers can be quantitatively exchanged with others even at ambient conditions with the host structure well conserved, which can lead to measured changes in geometrical, chemical, and electronic environments of either guest or host, and thus enable materials to be tailored to meet specific requirements

In this work we report the synthesis of layered nanophosphors carried out by a simple evaporation method followed by thermal annealing at temperatures up to 1100 °C, are described for a europium doping concentration of 4.3 at.%. The intense luminescence emission spectra of these samples are associated with the characteristic intra-electronic energy levels of Eu ion transitions. The dominant



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emission peak is at 611 nm, corresponding to the 5D₀ to 7F₂ transition, and the dominant excitation peak is at 245 nm. Upon the addition of TTA two effects occur: a broad band from 300 nm to 415 nm peaking at ~390 nm attributed to the absorption of TTA appeared and the band from the O²⁻ to Eu³⁺ charge transfer (CT) decreases. It is found that the the integrated excitation cross-section (ECS, area under the excitation spectra) of the neat L-Y₂O₃:Eu is enhanced by 100% upon addition of 300 wt% TTA. Bellow 300 wt% the amount of antennas are insufficient and some Eu³⁺ ions cannot be sensitized. When the concentration of antennas is >300 wt%, concentration quenching of the organic molecules occurs and thus luminescence intensity decreases dramatically.

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MICROELECTRONICS AND MEMS (MEM)

Chairman: Wilfrido Calleja (INAOE)

Norberto Hernandez Como, (Centro de Nanotecnología, IPN)

Horacio Estrada, (CIDESI)



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[MEM-75] Development of Fabrication Process of Comb-Drive Electrostatic Actuator MEMS to Study the Strain Mechanism in Two-Dimensional Transitional Metal Dichalcogenides

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Currently, the integrated circuit manufacturers have successfully managed to miniaturized silicon based transistors allowing for higher performance electronic devices. However, they have reached the power dissipation density limit, which is a trade-off between the capacitance switching, supply voltage, and switching frequency. As a result of this energy efficiency limit, Nano/Micro-Electro-Mechanical Systems (N/MEMS) devices were proposed as an ideal alternative switching device for low power electronics. Although, as promising as these devices look, there are still many present challenges that exist. For example, low contact reliability and limited endurance. Recent studies of two-dimensional layered materials such as graphene and transitional metal dichalcogenides (TMDs) such as MoS₂ and WSe₂ have shown very promising electronic properties. One interesting phenomenon of TMDs is that their electronic characteristics change as a function of strain. For example, in MoS₂, a phase transition from semiconducting to conducting state occurs around 11% uniaxial tensile strain. Therefore, new designs of Silicon Germanium (SiGe) and Silicon on Insulator (SOI) comb-drive electrostatic actuator MEMS have been proposed as a novel way to strain TMDs. However, a systematic MEMS fabrication process is needed to achieve repeatable uniform tensile strain. In this work, we have developed a two-mask process including deposition and etching recipes for SiGe and SOI for quad, hexa and octa comb-drive configurations.



[MEM-120] Highly Stable IGZO Thin-Film Transistors on Softening Polymer Substrate

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In recent years, flexible electronics have attracted great interest in biomedical field, where semiconductor devices such as thin-film transistors (TFTs) on polymer substrates can facilitate complex circuits into soft packages as healthcare applications. Biomedical devices have taken advantage of microfabrication processes to build components on top of flexible substrates for addressing and mapping electrical signals. However, the practical realization of these technologies remains elusive due to the lack of mechanical resilience of the electronic component when being bent. Therefore, further research in flexible electronics requires mechanically stable devices such as capacitors, transistors, as well as diodes. Previously, shape memory polymers (SMP) have been used as softening and flexible substrate for medical implantable devices. The SMP substrates have the property to keep a shape after being deformed, as well as to return to their original form when an external stimulus is applied. In this work, a thiol-ene/acrylate based SMP is presented as mechanical substrate to develop TFTs based on indium-gallium-zinc-oxide (IGZO) semiconductor. The SMP was spin-coated and fully polymerized on top of a glass carrier. Then, the IGZO TFTs were fabricated using gold (Au) as contacts on top of the SMP. Atomic layer deposition was used for the deposition of hafnium oxide as gate dielectric at 100°C. RF sputtering was used for the IGZ deposition. The resulting devices show a stable electrical performance after a thermal annealing process at 250 °C. The IGZO TFTs on SMP exhibit an average mobility of $>15 \text{ cm}^2/\text{V}\cdot\text{s}$. Also, the electrical performance of the TFTs on SMPs was studied after mechanical bending tests with radii of curvature of 5 mm for 104 cycles (over 4-hour). Logic inverter circuits using IGZO TFTs on SMPs denote the ability to add complex circuitry flexible electronic applications.



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[MEM-182] Electric VLSI and MEMS Design System

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The Electric VLSI Design System is an open source EDA of Static Free Software that traditionally can handle many forms of circuits design as Custom IC Layout, Schematic Capture (Digital and Analog), Hardware Description Languages (VHDL and Verilog). In this work, we propose the development of a new module for Micro-Electro-Mechanical-System (MEMS) design and modeling. This new tool provides the creation of MEMS 3D model from the layout using Java 3D and Oracle JMF libraries for MEMS 3D animation. An automatic Layout generation with parameterized cells has been developed to simplify the design of complex structures. The main contributions of this work are to provide a free CAD platform for MEMS with freedom to create domestic technologies and design rules to enable the manufacturability of MEMS devices in our institutional fab labs.

The Microtechnology and Embedded Systems group of the Computer Research Center (MICROSE-CIC) at the Instituto Politécnico Nacional, develop the MEMS Design System taking the Electric VLSI Design System as a baseline. This project is open source and accessible to any university, school or group interested in the use and development of tools for the MEMS design flow.

Our MEMS tool uses a multi-level surface micromachining technology and currently incorporates several common structures such as cantilevers, IDE, comb drives, springs and Chevron thermal actuators.



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[MEM-262] Development of MOEMS accelerometer built on SOI

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We developed an accelerometer sensor consisting of a Micro-Opto-Electro-Mechanical System (**MOEMS**) device built with SOI technology and which sensor is mounted on a two element metal package assembly for optical coupling to an optical fiber. The **MOEMS** structure consist of a 450 μ m thick (**SOI** handle) mass structure coupled and centered to four 60 μ m thick (**SOI** device) springs. The sensor has two planar and metalized sections in the center mass which can be both used as mirrors for optical interrogation. For the current design, we use one side of the mirror for optical interrogation. The sensor assembly (the **MOEMS** sensor and optical fiber attached to the metal package) was mounted on a certified acceleration controller and shaker system for professional motion characterization, and was tested from 0.01Gs to 5Gs. For the characterization of this sensor, we also developed a **LabVIEW** experimental interface to measure phase and amplitude performance of sensor by using optical interferometry. Also, given that the sensing element is built on Silicon and does not use its electrical capabilities for this design, the sensor withstands high electromagnetic ambient conditions during its optical feedback. In this presentation we present the design and fabrication steps of the micromachined devices, optical characterization setup, along with their characterization results, amplitude and phase shift up to 3KHz range, as well as the localization of the resonant frequency for the different designs we have developed. The results show that these devices have potential for vibration monitoring applications including for these under high electromagnetic conditions, such as power generation machines, big motors, transformers, as well as integration into electrical condition-monitoring equipment.



[MEM-276] SOI Micro Test System for Strain and Mechanical Parameters Determination

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In this work we present the design of a micro system used to probe the deformation of a material in a film when is stretched by the force produced in an electrostatic actuator. The device is designed to be fabricated on a SOI wafer, and is formed by an electrostatic actuator, parallel plate capacitor and the material under test.

The structure is defined in the device layer of the SOI wafer with a thickness of 80 μm . The device layer is machined using Bosch process. This proposal is designed to measure the deformation of a material in order to determinate its mechanical properties, because during the microfabrication process the deposited materials acquire different characteristics. For this reason we propose to use an electrostatic actuator-based system to produce a controlled deformation in the test material. The change of the length in the material is related with the capacitance variation in a parallel plate capacitor.

This mechanism can be used with different materials in order to determine their mechanical properties such as maximum deformation and yield stress. Some materials that can be used are metals and several polymers, the compatibility of the materials depend on the fabrication process, a required characteristic is that the material has to be elastic.



[MEM-84] Simulated Novel Comb-Drive MEMS Actuators Intended for Mechanical Strain of
2D-Layered MoS₂

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Since the 1960's, the integrated circuit community has successfully continued Moore's Law by effective scaling of silicon based transistors that has allowed higher integration densities. However, as scaling technology has improved, passive power density dominates and has become a major power consumption problem. New alternatives must be investigated in order to overcome the aforementioned limitation. Nano/micro-electro-mechanical system (N/MEMS) devices offer excellent on/off ratios with very steep subthreshold swing. However, there are certain issues such as the adhesive force between the contacts. Furthermore, two dimensional transition-metal dichalcogenides (TMDCs) materials have been studied due to their intrinsic properties, such as their relatively high strength and modifiable bandgap as a result of mechanical strain. In some TMDCs it has been shown theoretically that mechanical strain allows for the material to alternate between a state of semiconducting to conducting with applied uniaxial tensile strain. For example in MoS₂, this transition occurs around 11% tensile strain. However, there are currently no MEMS designs that are meant to exploit the benefits of the TMDCs tunable conductivity. In this work, we designed and simulated a novel MEMS quad, hexa, and octa comb-drive actuator with high electrostatic forces, which can enable us to mechanically strain a two-dimensional layer of MoS₂. Moreover, these MEMS comb-drive actuators will allow us to study strain behavior of free-standing TMDCs monolayers.



[MEM-110] Design of a wireless TMCPS sensor to measure blood pressure in the left ventricle

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Today biomedical technology represents a strategic field of study because it is projected as an area with very high potential to solve various health problems. In this context, electromechanical devices (MEMS) for medical applications (BioMEMS) have given way to the development of sensors and actuators defined on fully flexible and stable substrates that in combination with blocks of CI's allow the recording of electrical and biological signals, providing support to portable analysis and therapy schemes, revolutionizing medical diagnosis and treatment modalities. In this work, the design of an array of touch mode capacitive pressure sensors (TMCPS) aimed at measuring blood pressure in the left ventricle (LV) wirelessly is presented. The principle of operation is based on the relation between the changes of capacitance as a function of the applied pressure, associated with the changes of an electric variable reflected in the external device. The array of sensors was designed to operate in a pressure range of 5 to 300 mmHg, so that each of the sensors covers a different range of operation, therefore, the main component of output capacitance is the sum of the capacitances related to the contact area of the diaphragms. Among the main features of this device we can mention: biocompatibility when using polyimide as protective film, wide range of operation, device size according to the anatomical restrictions of the VI (2x2cm), radiation distance of 3.5cm to 13.56MHz and mechanical flexibility when using polyimide as flexible substrate material.



[MEM-209] Discharge characteristics and capacity of textile electrochemical batteries

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Batteries are essential for powering portable electronic devices. In a battery, the energy is stored in chemical form and then it is converted to electrical energy by connecting the battery to an external load. In this work, we fabricated an electrochemical battery using cotton fabrics and aluminum and silver electrodes. Each fabric is impregnated with silver nitrate (AgNO_3) and aluminum chloride (AlCl_3) solutions, to serve as dry electrolytes, and one fabric is impregnated with sodium nitrate (NaNO_3) solution to serve as a salt bridge. The battery is then activated with some microliters of deionized water. The battery voltage was 1.3 V. The discharge characteristics were obtained by discharging each battery with a constant current of 1 mA. The discharge cycle stops when the battery voltage reached 0.9 V. We tested three batteries at different water concentration (80, 160, and 240 ul). The battery activated with 160 ul turned out to be the one with the highest capacity of around 3 mAh. To the best of our knowledge, there is no previous report about the capacity of this type of battery. This study demonstrated that low water concentration (80 ul) is not enough to maintain the reaction for long times, but also that high water concentration (240 ul) affects the battery operation by reducing its performance. The fabricated batteries are intended to be used in smart textiles, wearable and flexible electronics.



[MEM-210] Fabrication of a microfluidic device for surface plasmon resonance sensor

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In this work, we integrate the surface plasmon resonance (SPR) sensing technology with microfluidics. This integration offers the advantages of small volumes and rapid processing while maintaining improved reproducibility. The fabrication of the microfluidic device was done with polydimethylsiloxane (PDMS, sylgard 184) and a mold made of 100 um thick SU-8 photoresist. The volume in the microfluidic channel was calculated to be around 1.6 ul. Instead of a high-cost lithography mask, we used screen printing and a UV-LED lamp to transfer the pattern to the SU-8. The final shape to the PDMS microfluidic device was obtained with a 3D printed mold. Then, the device was bonded to a glass with Cr/Au using an UV/ozone chamber. The microfluidic device was tested with a NanoSPR 6 equipment using different concentrations of sucrose from 0.04 to 0.2 g/ml. We obtained a linear behavior in the detection of the index refraction at different sucrose concentrations. The fabrication method was a simple, inexpensive, and scalable technique. The application of this microfluidic device can be extended by changing the solution and also by functionalizing its surface for further fabrication of lab-on-a-chip devices.



[MEM-260] Test structures for characterization and modeling of inter-metallic connections (vias) in resonant oscillators using a nanoscale CMOS technology

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Resonant Rotary Traveling Wave Oscillator (RTWO) is an innovative approach used for multigigahertz-rate signal generation in communication systems and clock signal generation/distribution in high-performance microprocessors. These oscillators are made with metal lines (copper or aluminum) only, taking advantage of the distributed Inductive-Capacitive (LC) nature of the interconnection lines in Complementary Metal-Oxide-Semiconductor (CMOS) processes for integrated systems (ICs). However, the technological advances have allowed to have a higher density of integration within a IC; this results in an increment in the number of metal levels and making larger the dimensions of vertical interconnections (commonly named vias) between the different levels of interconnect, and therefore the distance that the signals must travel. Moreover, these vertical interconnects present different discontinuities (for example, different widths in the structure) through them according to the number of metal levels of the used technology. All these effects, along with the operation of the oscillator in frequencies at the order of GHz, and even THz, are causing degradation in the integrity of the signal of the RTWOs.

Accordingly, in this work test structures for characterization and modeling of vias, using a UMC 130 nm Mixed-Mode, Single-Polysilicon, 6-metals, P-substrate, RFCMOS technology, are presented. The structures were made of aluminum in Metal-6 level, and all them consist of a microstrip interconnects. The analysis and quantifying of undesirable effects introduced by vias are presented. The method of the design and analysis include simulations using advanced simulation tools: a 3D electromagnetic program (EMPro) for the extraction of electrical properties of the interconnect lines (Resistance, Capacitance, Inductance and Conductance), Mentor Graphics suite for the geometric pattern (layout) generation of the test structures, and Hspice for the electrical simulation.



Keywords: Devices, integrated circuits, MEMS.

[MEM-273] Design and fabrication of a planar micro antenna for radio frequency communication

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Radio frequency identification (RFID) is an evolving technology whose development and application possibilities are difficult to calculate. Despite the reliability of RFID technology, there are several factors that influence negatively on its performance, the main factors can be summarized to: transmit power, size of the radiating elements (antennas), directivity, the working frequency and even the environment.

Antennas play a vital role in RFID systems, so its optimization is a paramount for the development of this technology. In this work we present the design and fabrication of a planar micro antenna altogether with a variable capacitor to work as a wireless analog sensor that can be used for many applications, such as reading capacitive-based pressure sensors, energy harvesting and medical applications among others. The micro antenna has a spiral pattern, the number of turns was fixed in 10, the turn width and the separation between turns were varied from 5 μm to 10 μm , and the external diameter of the antenna was varied from 400 μm to 8 mm.

The micro antenna design was validated by multiphysics simulation in order to obtain some operating values and electric parameters, compatible microfabrication techniques were selected for the system manufacture, an external reading circuit was implemented in order to proof the reading capabilities of the micro antennas and the capacitor at two central operating frequencies 125 kHz and 13.56 MHz.



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[MEM-274] TFT fabrication with non conventional materials and logic circuit applications.

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The semiconductor industry has been rapidly growing since half of the last century, increasing production rates, reducing the size of the devices and increasing their capabilities while mass producing them, reducing costs, since the transistor invention in 1947. In those devices, silicon became the elected material given its high fusion point and a natural oxide layer preventing leakage currents. The thin film transistor TFT, on the other hand, is ideal for low density circuits applied in a large area applications, such as liquid crystal displays. Since the first TFT fabricated in 1962, new processes and materials were proposed and used to further improve the device quality by achieving high carrier mobilities, transparency or mechanical properties, depending on the application.

In this work, we present the design and fabrication of thin film transistors (TFT) for applications in logic circuits using zinc oxide (ZnO), a 30 nm layer deposited by RF sputtering, which makes it an ideal material for several applications given its high mobility values. An Indium-Tin Oxide (ITO) coated glass is used as gate electrode and substrate respectively and an aluminum oxide layer, deposited by ALD, used as gate insulator layer following a staggered bottom-gate configuration guaranteeing the quality of the semiconductor-insulator contact. Gold is used as source and drain electrodes forming ohmic contacts with the semiconductor layer, thus, the device relies on the majority carrier concentration variation for its operation. Finally, the entire structure consists of various devices in which the transistor geometries vary with values of $L=10, 20, 40, 80, 160 \mu\text{m}$ and the relation $W/L=5, 10, 20$.



[MEM-277] Design of a 1-DOF Positioning System Using Bulk and Surface Micromachining

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In this work, we present the design of a 1-DOF (degree of freedom) positioning system using a combination of two of the most used methods in MEMS fabrication, bulk and surface micromachining. In the proposed system, bulk micromachining is used to take advantage of the thick device layer ($> 40 \mu\text{m}$) of a SOI wafer to make a pair of comb-drive actuators that produce a force of $4.2 \mu\text{N}$ each. On the top of the device layer of the SOI wafer, a thinner polysilicon layer ($< 3 \mu\text{m}$) is obtained using surface micromachining. This layer is used to form: the springs that are needed to reset the actuator, the shafts that transfer the force to a positioning element, and the final stage whose position is controlled. In this way, the spring constant obtained for the flexing elements is smaller than if they were constructed using the device layer of the SOI wafer, and do not add big parasitic loads to the actuators. The general design of the system is based in the rack and pinion mechanism. The comb-drive actuators control the position of a geared element that functions as the pinion. The final stage consists of a square element attached to a rack gear. The interaction between these two elements results in the free positioning of the final stage in one dimension. The proposed design can achieve a displacement of almost $500 \mu\text{m}$ with steps of $12.56 \mu\text{m}$. The resolution of the system and the size of the actuators can be improved by adding a gear train for the transmission of the movement, but this element is not analyzed in this work. The system can be used in a lab-on-chip to store a cell sample, and to discretely choose each cell to be analyzed or processed by another system, like a cell membrane strength test.



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NANOSTRUCTURES (NSN)

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



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[NSN-71] Analytical and Simulation Study of Conduction Modulation of MoS₂ via Strain Using Electrostatic Comb-Drive Actuators

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There has been remarkable progress on the exploration of two-dimensional layered materials, such as graphene and transitional metal dichalcogenides (TMDCs) and the results are fascinating. A single layer of TMDC consists of three atomic layers in which the transition metal is covalently bonded by two chalcogens in a sandwich-like structure. The weak van der Waals interactions between adjacent planes permit isolation of single layers from the bulk, using mechanical or chemical exfoliation methods. Monolayers of TMDCs have very distinct electrical properties from their bulk counterparts, primarily due to the confinement of charge carriers in two dimensions. An interesting property of some TMDCs is that their bandgaps ($>1\text{eV}$) are highly sensitive to strain. For example, MoS₂ has a direct bandgap of $\sim 1.9\text{ eV}$ and has a strain sensitivity of $-0.077\text{ eV}/\%\text{strain}$ which enables a large range of electrical conductivity from semiconducting to conducting. Current experimental techniques to strain 2D layered materials include atomic force microscopy (AFM) and nano-indentation. However, these methods are not able to track changes in electrical conductivity with applied uniaxial tensile strain. Moreover, the effects of strain beyond $\sim 2\%$ on the optical and electrical properties of MoS₂ have not been fully investigated. In this work, a quad, hexa, and octa electrostatic comb-drive actuators were used to simulate strain up to six percent in MoS₂. These were further analyzed using analytical equations to predict the conductivity behavior of MoS₂ under uniaxial strain.



[NSN-82] Geometric Quantification of Chirality in Ligand-Protected Metal Clusters

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Chirality has been found as a novel and relevant property in nanomaterials like ligand-protected metal clusters and metal nanorods. This property not only would be important in related research areas like asymmetric catalysis or chiroptical phenomena, but also generates fundamental questions on the existence of chirality at the nanoscale. In particular, x-ray total structure determination, electron diffraction studies, NMR and circular dichroism spectra, as well as theoretical calculations of gold clusters protected with thiolate or phosphine ligands have confirmed the existence of chiral structures in the size range of 18-144 Au atoms. In this work, we perform a comparative analysis of the degree or amount of chirality existing in the known chiral ligand-protected gold clusters, through the geometric quantification of chirality using the Hausdorff chirality measure (HCM). The results indicate that indeed, the calculated HCM values are consistent with the current knowledge on the different sources of chirality: achiral cores and chiral arrangements of ligands in, for example, Au₁₀₂(SR)₄₄ and Au₃₈(SR)₂₄, or intrinsically chiral cores, like in Au₂₀ protected with phosphine ligands. On the other hand, our calculations also indicate that the chiral *I*-Au₁₄₄X₆₀ has an intermediate index of chirality between the achiral carbonyl phosphane-protected Pd₁₄₅ cluster, and the recently synthesized and crystalized chiral Au₁₃₃(SR)₅₂ one. Additional insights, as well as limitations, in using HCM to geometrically quantify chirality in bare and ligand-protected clusters are discussed.



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[NSN-157] STM and AFM techniques on the study of the density of states, electrical properties and magnetic domains in Mn-doped GaN and ZnO

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The scanning tunneling spectroscopy (STS) technique, in the scanning tunnel microscope (STM), is used to probe the local density of states (LDOS) in metals and semiconductors. This technique is useful to determinate energy-level states generated by impurities and point defects in semiconductors, besides its conductivity type and surface band-gap (SBG). In this work, we present results of the use of this technique for the characterization of the defect-related electronic states in GaN, GaN:Mn, ZnO and ZnO:Mn grown by different methods. STS measurements from GaN:Si (0001)/sapphire films grown by HVPE show SBG of 3.5 eV, and interesting this sample revealed a conductivity-type inversion (from n to p-type) after an annealing treatment in H₂ at 700 °C that we attributed to the formation of gallium vacancy (V_{Ga}) acceptor defects. Mn-doped GaN films synthesized by MBE exhibited a dependence of the resistivity with the Mn concentration, which promoted the formation of numerous screw dislocations and defects type pits. AFM measurements, in the conductive mode, revealed electric charge accumulated in regions around of these defects. Besides, AFM in magnetic mode confirmed the generation of magnetic domains by the incorporation of Mn. STS measurements from monocrystalline ZnO (0001), exhibiting a SBG of 3.5 eV and the presence of a donor state at 1 eV under the conduction band, attributed to oxygen vacancies (V_O). Similar results were observed in undoped ZnO nanorods, attributing the donor state to oxygen vacancies. ZnO and ZnO:Mn films grown by atomic layer deposition (ALD) technique showed the same value for the SBG, although with several donor defect-related states with activation energies between 1.2 and 0.4 eV.



[NSN-244] Porphyrin system building a scandium based metal–organic framework: Synthesis and characterization

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There has been extensive research in recent years into the synthesis and applications of metal-organic frameworks (MOFs), which are analogous to zeolites because both are ordered porous solids with defined, repeating crystalline structures [1,2]. However, the surface areas of MOFs are very high and they can be prepared with pore sizes much greater than can be achieved with zeolites. The MOFs materials are generated by the association of metal ions and organic ligands, which assemble 3D structures. MOFs have potential uses in gas storage and separation, catalysis, drug delivery, biomedical imaging and electrochemical applications[2,3,4]. The use of large organic molecules is of current interest in the assembly of MOFs because of its well-defined geometry. The porphyrins are conjugated tetrapyrrolic macrocycles with structures that possess rigid planar geometry, and high photochemical stability. All these properties made them attractive candidates for their use as a ligand in the synthesis of MOFs [5]. Among the many trivalent metals used in the synthesis of MOFs, it has been shown that scandium gives a range of stable MOFs materials [6]. Here, the macrocycle *meso* tetrakis(4-carboxyphenyl)porphyrin [TCPP] as linker has been investigated to synthesize a scandium based metal-organic framework. The TCPP has 4 CO₂-groups that bonded to Sc³⁺ cation. Different molar ratios (Sc/TCPP), solvent, temperature and time of reaction were explored. Structural identification of the solid was performed by means of X-ray powder diffraction. Characterisation by SEM microscopy was performed on the samples and these materials exhibited morphology like long fibres (or wires) and crystals. The fibres are so long that it was not possible to determine their length. However, for the solid which involved water in the synthesis crystals were 20 - 30 μm in length and 0.5 -1.5 width. Adsorption studies of gas adsorption for N₂ at 77 K gave a uptake of 12 mmol g⁻¹ with a BET surface area of 784 m²g⁻¹.

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[NSN-251] Molecular beam epitaxy of InAs nanowires on GaAs(221): strain distribution and surface ordering

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Semiconductor nanotechnology is one of the areas that undoubtedly have had utmost impact in our daily life. Throughout the advances in this area, a plenty of devices such as mobile phones, personal computers, TVs, medical diagnosis support systems, among many others has been improved. In order to satisfy the current and near future technological issues, materials researchers have been focused in refining the synthesis of semiconductor nanostructures. As a particular example, the InAs quantum dots (QDs) are one of the most studied nanostructures. The self-assemblage of InAs QDs on GaAs(100) by molecular beam epitaxy (MBE) is usually obtained by employing the Stranski–Krastanov growth mode. This method is mainly driven by strain originated because of the epilayer-substrate lattice constant misfit, which produces a stochastic distribution of nanostructures on the GaAs(100) surface. Surface order can be propitiated with the use of high-index substrates, also allowing for the synthesis of one-dimensional InAs systems, like quantum nanowires (NWRs). The NWRs 1D arrangement involves also different mechanisms of strain distribution, quantum confinement effects, and surface anisotropy. In this work, we report the synthesis of InAs NWRs by MBE on GaAs(221). Highly ordered one-dimensional InAs arrays are obtained. We employed Raman spectroscopy and an autocorrelation function analysis of the atomic force microscopy images to evaluate the arrays. For the most ordered surface NWRs (lowest correlation length) the Raman spectra exhibits small downward wavelength shifts of the GaAs resonance modes. As it is known, the wavelength shift in Raman spectra is modified by confinement effects, which causes a wavenumber redshift; and by strain effects, where compressive



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strain induces a blue shift of optical phonon modes. Since confinement effects are not expected for GaAs, our observations indicated that the Raman shifts are associated to the InAs/GaAs interface strain, that for instance account for the GaAs tensile strain related with the InAs NWRs surface ordering.

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[NSN-269] Molybdenum and Tungsten based Transition Metal Dichalcogenides (TMDs):
Growth and characterization.

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Several two-dimensional (2D) materials have been demonstrated in the last years. Their growth and characterization have seen rapid progress. About 10 years ago the first 2D material, graphene, was reported, and soon other materials like hexagonal boron nitride (hBN) and transition metal dichalcogenides followed. Tungsten and molybdenum based TMDs are true semiconductors with very particular properties useful for optoelectronic, electronic and valleytronic applications. Moreover, recent developments on TMDs heterostructures and alloys have open the door for a new and exciting research opportunities.

The aim of this talk is to show the efforts and results on the growth, characterization of a particular family of TMDs. First, the growth of single and multilayers of Ws₂, MoS₂ and WSe₂ crystals using chemical vapor deposition will be discussed. Traditional optical and morphological techniques like Raman, Photoluminescence (PL), Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM) are used to characterize the crystals. Subsequently, electrostatic and thermal properties of MoS₂ and Ws₂ monolayers are investigated by means of Kelvin Probe Force Microscopy (KPFM) and Scanning Thermal Microscopy (SThM). Finally, the growth of MoxS₂-Wx-1s₂ single and bilayers alloys will be presented as well as the evolution of their optical transitions (excitons, trions and defects) in terms of the excitation power dependence of photoluminescence.



[NSN-278] TL and OSL properties in Eu -doped long persistent nanophosphors

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We report on the thermally and optically stimulated luminescence properties of $\text{Sr}_4\text{Al}_{14}\text{O}_{25}:\text{Eu}/\text{Dy}:\text{B}_{0.4}$ and $\text{Sr}_4\text{Al}_{14}\text{O}_{25}:\text{Eu}/\text{Nd}:\text{B}_{0.4}$ long persistent phosphors synthesized by the combustion method using urea ($\text{CH}_4\text{N}_2\text{O}$) as fuel. The highly exothermic redox reaction between the metal nitrates and organic fuel is in excess more convenient than using solid reaction method. After exposure to low dose beta radiation the phosphors exhibit ultra-long strong afterglow with a typical multiple exponential decay curve, which is attributed to the thermal activation of holes from a trap distribution followed by the emission of $4f^65d \rightarrow 4f^7$ transition of Eu^{2+} ion. We investigate the thermoluminescence (TL), optically stimulated luminescence (OSL) and afterglow (AG) properties in powder samples of $\text{Sr}_4\text{Al}_{14}\text{O}_{25}:\text{Eu}/\text{Dy}:\text{B}_{0.4}$ and $\text{Sr}_4\text{Al}_{14}\text{O}_{25}:\text{Eu}/\text{Nd}:\text{B}_{0.4}$ exposed to beta radiation using a Risø TL/OSL-DA-20 reader. The TL glow curve of $\text{Sr}_4\text{Al}_{14}\text{O}_{25}:\text{Eu}/\text{Dy}:\text{B}_{0.4}$ consist of two broad peaks located around 125°C and a lower intensity peak at 325°C, while the TL of $\text{Sr}_4\text{Al}_{14}\text{O}_{25}:\text{Eu}/\text{Nd}:\text{B}_{0.4}$ exhibits a main peak at 225°C and low intensity one around 100 °C. The samples exhibit green persistent luminescence or afterglow (AG) due to thermal emptying of trapped charge carriers at low temperature trapping levels. The integrated TL as a function of dose shows a linear behavior for doses below 1.0 Gy and saturates for doses higher than 30 Gy. A strong OSL signal is observed in previously irradiated samples after stimulation with 870 nm IR light with a similar dose behavior. In conclusion both phosphors were successfully synthesized by the combustion method and exhibit strong persistent luminescence features as well as integrated TL/OSL linear low dose behavior.

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[NSN-4] Fabrication of a ZnO nanostructures-based mis diode through chemical routes

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Because its physical properties, ZnO is considered a potential semiconductor compound for fabricating electronic and optoelectronic functional devices. In this regard, several growth techniques have been developed in order to meet the requirements of commercial devices based in this material. On the pathway for improving the performance of the current devices, low-dimensional ZnO structures seem a promising alternative.

Here, we report the fabrication of a metal-insulator-semiconductor (MIS) structure based on ZnO nanostructures grown on the surface of an anodized aluminum substrate ($\text{Al}_2\text{O}_3/\text{Al}$). While the semiconductor layer was obtained through a low-temperature hydrothermal route, the insulator-metal interface was fabricated by anodizing the surface of an aluminum foil (previously electropolished). Finally, the MIS structure was annealed at 300 °C in order to ensure solid-contact at the interfaces. The obtained MIS architecture was characterized by scanning electron microscopy/focus ion beam (SEM/FIB), energy dispersive spectroscopy X-ray (EDS), x-ray diffraction (XRD), micro-Raman spectroscopy (μRS), cathodoluminescence (CL) and electrical measurements (I-V, C-V). The formation of a sandwich-like structure was confirmed by SEM/FIB techniques. The EDS analysis suggests formation of three different phases: ZnO, Al_2O_3 and Al phase; the XRD results confirms the latter. It is shown that the obtained semiconductor layer is constituted by interconnected leaf-like ZnO nanostructures with average thickness of ~ 50-100 nm. According with the Raman spectrum, these ZnO nanostructures are crystalline, although native defects are present as the broad visible-band centered at 533 nm in CL spectrum reveals. Finally, the characteristic response of a metal-oxide-semiconductor junction is observed in the acquired I-V and C-V curves, demonstrating that it is possible to fabricate a ZnO nanostructures-based MIS diode using chemical routes.



[NSN-20] CuS thin films doped with CuS nanoparticles for semiconductor devices applications

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Semiconductor nanocrystals are of great interests for both fundamental research and industrial development. This is due to their unique size-dependent optical and electronic properties and their exciting utilization in the fields of light-emitting diode, electrochemical cells, laser, hydrogen producing catalyst and biological label.

In this work, we present the synthesis and characterization of copper sulfide (CuS) nanoparticles suitable for semiconductor applications using a simple and manufacturable process. The solution based process was synthesized at room temperature using copper nitrate chloride and a thiourea as source of copper and sulfur, respectively. The effect of the concentration of glycine as a surface stabilizer or surfactant for growth control of CuS nanoparticles was studied. Also the aging time of the nanoparticles was studied.

Optical properties of CuS were analyzed by UV-Vis spectroscopy; functional groups were identified by Fourier transform infrared spectroscopy (FTIR) and the surface morphology by scanning electron microscopy (SEM). The particle size for CuS nanoparticles were less than 500 nm. A decrease in band gap was observed inversely to the glycine concentration and proportionally with the aging time.

Keywords: CuS, semiconductor, nanoparticles



[NSN-24] Quantum Wire's electronic distribution under an external electric field whitin the Yukawa approximation.

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The development of growth techniques such as Molecular Beam Epitaxy or Metal-organic Chemical Vapor Deposition have allowed the synthesis of high-quality semiconductor quantum wires (QWRs). QWRs possess unique one-dimensional (1D) quantum confinement properties and have emerged as promising structures for the next generation of electronic and optoelectronic devices. In addition, the strong 1D confinement of electrical carriers, photons and phonons makes the QWRs very attractive laboratory systems for probing 1D Physics of great interest both experimentally and theoretically. Even so, the problem of many electrons interacting into a QWRs is very complicated problem.

In this work, we present a study of a system of many electrons into a circular $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QWR which are interacting between them under a Yukawa-like potential (YP) and under the effect of an external electric field. Our model contains parameters such as the Al concentration (by using the Varshni model), the substrate orientation (implicit in the effective mass), the dopant level (associated to the screening parameter κ in the YP), the cross section geometry of the QWR (circular) and the magnitud of the external electric field. To fit the model to experimental values, we consider concentrations of 10^6 - 10^{22} e^-/cm^3 , the (631) Miller orientation of the GaAs substrate, an Al concentration of $x=0.23$, and a conduction band offset of $V=206$ meV. By using the Yukawa model and these parameters, we have calculated the electronic density distributions into circular QWRs for different electronic concentration and external electric field strength. For the calculation, the ground and first excited state along the QWR were considered.

Our results show carrier displacement due to the external electric field. When the conditions are set to form a Wigner molecule different scenarios are observed which are dependent on the strength of the external field.



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[NSN-25] Nanowired Y-junction electronic distribution within the Yukawa approximation.

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Among a number of available growth techniques to achieve the challenging task of precisely control the self-assembling of semiconductor nanostructures, Molecular Beam Epitaxy and the use of high-index substrates is specially adequate to produce structures such as quantum wires (QWRs). Recently in our working group, we have reported the synthesis of nanoscale nanowired Y-junctions (junction of two nanowires) in a controlled manner, which could have important applications in nanoelectronics and 1D electronic transport research.

In this work, we present a study of a two square $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QWRs system forming the Y-junction. In the model, we consider many electrons which interact through a Yukawa-like potential (YP). To contrast the model with experimental values, we consider electronic concentrations of 10^6 - 10^{22} e^-/cm^3 , a (631) Miller orientation of the GaAs substrate, an Al concentration of $x=0.23$, and a conduction band offset of $V=206$ meV. By using the Yukawa model and these parameters, we have calculated the electronic density distributions into the QWRs Y-junction for different electronic concentrations, QWR lengths and cross sectional size.

Our results show the optimal conditions to form a Wigner molecule in the cross section of two coupled QWRs and its dependence with the dimensions of the Y-Junction.



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[NSN-34] Use of organic materials for the synthesis of hidroxyapatite(HAp)

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Hydroxyapatite (HAp) is the major mineral constituent of vertebrate bones and teeth. In this research project the biodegradation of the sea shells, coral and egg waste have been used effectively to produce hydroxyapatite nanostructure by using two methods, microwave irradiation and solid state. The conversion of the organics materials into HAp is produced by the formation of calcium hydroxide. The preheated calcium hydroxide is converted to hydroxyapatite by a chemical exchange reaction with diammonium phosphate under hydrothermal conditions or under microwave radiation. All the HAp were characterized by X-ray powder diffraction (XRD) method, Fourier transform infrared (FT-IR) spectroscopy, Raman spectroscopy and Energy Dispersive X-ray Spectrometry (EDS). The product obtained, which contains carbonated HAp has numerous potential applications, such as material for biomedical applications in prothesis implants, it can be used as a medium for heavy metal absorption and absorbing and decomposing CO.



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[NSN-44] Morphology of SiO₂ Surfaces Bombarded with 1.0-MeV Si ions

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This work studies pattern formation in SiO₂ substrates by means of ion implantation at high energies. In particular, we performed 1.0-MeV Si ion implantation on SiO₂ substrates at 70° angle with respect to the surface normal. These ion implantations experiments are performed at high currents from a 3 MV Pelletron accelerator of the Instituto de Física, UNAM, at room temperature conditions. In the case mentioned, surface morphological changes are studied with respect to ion implantation fluence. The atomic damage is described in terms of macroscopic effects observed by surface analysis techniques, such as scanning electron microscopy (SEM) and atomic force microscopy (AFM). The formation of surface ripples is interpreted using continuum model approaches. These include recently proposed models of interface and surface growth, taking into account a thin layer of heavy-damaged region of the target material. The authors acknowledge the technical support of M. Galindo, K. López, F. Jaimes, M. Escobar and J.G. Morales. This work was financially supported by DGAPA-UNAM under PAPIIT IN111717.



[NSN-45] Anisotropic of pattern formation for Au+ ion implantation in rutile

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The work presents the study of rutile <100> surface modification by Au+ ion implantation. Rutile single crystals <100> were implanted with 1.0 MeV Au+ ions with a beam incident angle 60°, using the Instituto de Física 3 MV Pelletron accelerator at UNAM. The SRIM calculation predicts an average range of 70 nm. For a fluence of $2.5 \times 10^{17} \text{ cm}^{-2}$ the calculated number of displacements per atom (dpa) at the peak is 3100; the sputtering yield is 58. The implantated samples were analyzed with SEM, AFM and Fourier analysis. Periodic profiles of the order of nm were observed. The profile depends on the sample orientation. Two mutually perpendicular orientations were chosen. In the first a predominant roughness is seen; in the other a wave pattern is observed. A model calculation of ion collection in presence of sputtering predicts a saturation value near of the surface of the single crystal, this aspect would aid in the formation of the waves. The authors acknowledge the technical support of M. Galindo, K. López, F. Jaimes, M. Escobar and J.G. Morales. This work was financially supported by DGAPA-UNAM under PAPIIT IN111717.



[NSN-52] Optical and structural properties of $\text{MO}_x\text{-1S}_2\text{-W}_x\text{S}_2$ SINGLE Layer alloys

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Two dimensional materials (2D) have become one of the most exciting fields of material science research. The possibility to achieve and engineer Van der Waals heterostructures and alloys have opened the door for new and exciting research opportunities especially for the development of ultra-thin high efficiency and tunable optoelectronic devices.

In this work we present the optical and structural characterization of 2D single bilayer $\text{Mo}_x\text{-1S}_2\text{-W}_x\text{S}_2$ single layer alloy. The structure was synthesized on a single step APCVD growth using a mixture of MoO_3 and WO_3 solid precursors at 1000°C. Micro-Raman spectra recorded at different points of the structures reveals the presence of in-plane and out-plane vibrational modes of both materials. Raman maps revealed the distribution of each material along the crystals.

Photoluminescence (PL) spectra performed on $\text{MoS}_2\text{-WS}_2$ monolayer alloy exhibits two broad peaks centered at 1.84 and 1.60 eV, however in the case for the bilayer, we observed a redshift of one contribution from 1.60 to 1.51 eV. In order to understand the recombination mechanisms, we studied the intensity dependence of these contributions. In addition, in order to identify each spectral feature, the data was fitted using Lorentzian functions. Based on the power dependence law (1), the results indicate that the $\text{MoS}_2\text{-WS}_2$ alloys (monolayer and bilayer) PL spectra is composed by multiple contributions such as excitons, trions and defects. Moreover, the peak related to the presence of WS_2 A exciton was found at 1.88 eV and a contribution at low energies (~1.6 eV) suggests a strain induced by the substitution of tungsten atoms in MoS_2 crystals (2,3). Finally, we present LDA calculations in order to show how the band diagrams and the lattice strain are affected with the incorporation of W in the lattice.



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[NSN-57] Synthesis of silver nanoparticles from Neem leaves using microemulsion

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Silver nanoparticles (AgNPs) were synthesized by reverse micelle microemulsion method, using aqueous extract of Neem (*Azadirachta Indica*) leaves and silver salt. The plant extract acts both as reducing agent as well as capping agent. The compounds responsible for reduction of silver ions are flavanones and terpenoids. Various techniques were used to characterize the synthesized nanoparticles: XRD, TEM and optical absorption. The synthesized AgNPs exhibits lowest energy absorption band at 470 nm. The effects of the precursors' concentration and the molar ratios of oil to surfactant on the particle size and size distribution were investigated. The silver colloid has favorable stability and can be preserved for a long time without precipitation. Based on the obtained results, it can be concluded that natural compounds obtained from plants can be efficiently used in the production of AgNPs and could have applications in various fields such as antibacterial material, biomedical and nanotechnology, among others.



[NSN-64] Adsorption study in aqueous medium of arsenate by Goethite nanorods

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Arsenic is one of the most widespread inorganic pollutants worldwide and represents a significant potential risk to human health and the biosphere. It is well known that arsenic is highly toxic and carcinogenic; at present, there are reports of diverse countries with arsenic concentrations in drinking water higher than those proposed by the World Health Organization (10 µg/L). Nanomaterials and nanotechnologies inspire new possible solutions to major environmental issues nowadays. It has been reported that adsorption strategies using iron oxyhydroxide as goethite are very efficient for the removal of arsenic in drinking waters, the adsorption mechanism is not yet clear. In order to shed light on this subject, we attempt to study the interactions between arsenic species and α -FeOOH nanorods in an aqueous medium. Goethite nanorods were prepared using a precipitation method with $\text{FeCl}_3 \cdot x\text{H}_2\text{O}$ as a metal source and KOH aqueous solution as precipitating agent. As-synthesized nanorods were put in contact with $\text{As}_2\text{O}_5 \cdot x\text{H}_2\text{O}$ solutions at room temperature at pH 4 and 7. Goethite particles were characterized by DRX, TEM, FT-IR and XPS. Results showed that goethite nanoparticles had 30 nm wide and 410 nm long, and a narrow size distribution. The presence of arsenic on particles surface was confirmed, which is more remarkable when pH= 4 conditions are employed. On the other hand, after adsorption experiment, it was evidenced from FTIR and XPS that once arsenic species interact with the nanoparticles, they form bidentate binuclear complex and doubly protonated monodentate of As(V) at pH= 4 and 7, respectively, and Simply protonated monodentate complex of As(III) after As(V) reduction, by X-ray from XPS technique, in both conditions. The developed methodology could be implemented in the water treatment industries, reducing the costs of the processes and making them more environmentally friendly.



[NSN-68] Chemical bath deposition of CdS thin films doped with photo luminescent nanoparticles.

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In this work CdS thin films were deposited by chemical bath on glass substrates. CdCl₂, NH₄OH, NH₄Cl and SC(NH₂)₂ were used as precursor compounds for the synthesis of the thin films. The films were doped with different photo luminescent nanoparticles such as carbon, functionalized carbon nanotubes, gold and silver nanoparticles. Luminescent nanoparticles were synthesized separately by different chemical methods. For the doping process, nanoparticle solutions were added to the chemical bath by varying the volume of the solution of the particles. The results are discussed according to the type of particles and the volume added to the chemical bath.

The films were structurally characterized using the techniques of X-ray diffraction and Raman spectroscopy. The optical characterization was carried out by UV-Vis spectroscopy. The chemical composition as well as the atomic percentage content of impurities were obtained by energy dispersive X-ray spectroscopy. Scanning electron microscopy was used to study the surface morphology of films.



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[NSN-77] Synthesis and characterization of gold nanoshells for therapeutic medicine

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Gold nanoshells have gained attention recently due to their versatile optical properties. In particular, their spectrally selective extinction has been exploited for experimental medical applications, functional coatings and contrast enhancement for analytical techniques. Here we discuss the production of gold nanoshells and the formation of gold nanorings by using of SiO₂ nanosphere template. Hollow Au/SiO₂ nanoshells can be converted to nanorings upon addition of excess KAuCl₄. Nanorings present a distinct particle geometry, with optical properties exhibiting characteristics of both nanorods and nanoshells. The gold nanoparticles, which are in the size range 10–50 nm, are used due that have a plasmon resonance with incoming radiation causing them to both absorb and scatter light. This effect can be harnessed to either destroy tissue by local heating or release payload molecules of therapeutic importance. Gold nanoparticles can also be conjugated to biologically active moieties, providing possibilities for targeting to particular tissues. Then the exploitation of the plasmon resonance of gold nanoparticles is very interesting in photo-thermal therapeutic medicine.



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[NSN-89] Nanocolumnar CdS thin films grown by Glancing Angle Deposition from a Sublimate Vapor Effusion source

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The glancing angle Deposition (GLAD) technique was used to grow cadmium sulfide (CdS) thin films on glass and indium tin oxide (ITO) coated glass substrates from a sublimate vapor effusion source. The samples were prepared under different incident deposition flux angles (α) of 0° , 20° and 80° , while both the substrate and the source were under rotation. The temperature of the source was 923.15 K. Scanning electron microscopy images showed that the GLAD method combined with the source produced dense nanocolumnar shaped structures with height and diameters of ~ 200 and ~ 30 nm respectively. The deposited films showed a hexagonal structure with preferential (002) plane orientation and crystallites sizes between ~ 25 nm and ~ 35 nm. A maximum solar weighted transmission of $\sim 92\%$ was obtained for the sample prepared at $\alpha = 80^\circ$, with a substrate/source rotation velocity ratio of 55/20 in the wavelength region of 400-900 nm. The average band gap energy of the films was ~ 2.42 eV. Refractive indexes between ~ 1.4 and ~ 2.4 at a 550 nm the wavelength were also obtained.



[NSN-94] Synthesis and characterization of protein - metallic nanoparticles loaded PLGA.

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Nowadays, numerous nanotechnology devices have been generate great attention in medical field because of their potential uses in the diagnostic and treatment of diseases. For instance, nanoparticles, fabricated with organic, inorganic or hybrid materials, have been widely used as bioactive-molecules nanocarriers for treat a particular disease, since because of the nanoparticle matrix could be protected the active compound from cellular clearance increasing the blood circulation times and local therapeutic action. Therapeutic proteins can play an important role in the treatment and prevention of several human diseases. However, the protein low physicochemical stability restrict its bioactive action. Therefore, it is important to development a nanosystem able to entrap the therapeutic protein, enhancing the protein stability and therapeutic efficacy. In this work, the encapsulation of a water-soluble protein in poly(lactic-co-glycolic acid) (PLGA) nanoparticles is investigated. PLGA nanoparticles were prepared by a double emulsification-solvent evaporation technique. We used recombinant human lysozyme (rHL) as a model therapeutic protein and gold nanoparticles. Lysozyme is a bacteriolytic enzyme that is widely distributed in various tissues and body fluids, including the liver, articular cartilage, plasma, saliva, tears and milk. Lysozymes play an important role in host defense by preferentially hydrolyzing the β -1,4-glycosidic linkages between the N-acetylmuramic acid and N-acetylglucosamine groups present in the peptidoglycan cell wall of Gram-positive bacteria. The hydrodynamic diameter, zeta potentials and polydispersion index were evaluated in each preparation.



[NSN-96] An study of ZnO nanoparticles with unusual crystalline phase, grown by a self assembly process within a SiO₂ matrix using reactive rf sputtering

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Nanocrystals of ZnO were embedded within a SiO₂ matrix by a sequential deposit using reactive R.F. sputtering. The ZnO nanoparticles (NP's) were obtained by depositing a very thin layer (around 20 nm) of Zn on the bottom of the valleys of a first SiO₂ rough surface and then covered by another SiO₂ layer. The compression produced by the SiO₂ matrix on the ZnO NP's brings about a phase transition to an unidentified crystalline phase of ZnO. The structure was determined by means of X ray diffraction patterns. The ZnO + SiO₂ composite shows a transmittance higher than 80 % for wavelengths > 450 nm. Optical absorption allows to reveal the character and value of the optical band gap. Vibrational modes of the material were determined by Raman spectroscopy.



[NSN-116] Gold Catalysts Supported on CeO₂-Al₂O₃ for Sulfur Oxidation

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Gold catalyst with mixed supports CeO₂/Al₂O₃ have been synthesized by an ultrafast and environmentally friendly microwave autoclave method. Morphology, particle size and chemical composition of the catalyst were characterized by means of XRD, AFM, TEM, XPS, UV-Vis spectroscopy and particle size analyzer. The catalyst of particle size 10-15 nm exhibit a high and stable activity towards the oxidation of aromatic sulfur; the catalytic ability was compared by varying oxidation agents, temperatures and pH range of the oxidation reaction.

Keywords: gold nanoparticle catalyst, Sulfur oxidation, mixed supports of ceria-alumina



[NSN-119] Green synthesis for FLG using Ultrasonic Exfoliation and *Opuntia ficus-indica* extract

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Abstract: The green synthesis promotes the partial or total substitution of potentially harmful chemicals for the environment by more friendly ones, also is very concerned about the energy consumption. In this green synthesis approach, commercial graphite was mixed with *Ofi* (*Opuntia ficus-indica* extract). The mixture was sonicated in ultrasonic bath by short times at room temperature. The nanostructures were characterized by Raman spectroscopy, XRD, XPS, AFM and TEM. Raman spectroscopy was used for the study of vibrational properties. The intensity ratio between the G and 2D bands in the Raman spectrum, followed by the deconvolution of the 2D band, suggests the presence of graphene of 4 and 5 layers. The diffractogram showed a strong decrease in the intensity of the plane (002) that corresponds to an interplanar distance of 0.34 nm, characteristic of the graphite structure. The reason C/O measured by XPS showed oxidation degrees adequately compared with the reports on few layers graphene. The roughness of the layers in the AFM images revealed small elevations of 1 nm in height and close to 100 nm in length. Structural and morphological properties of the sample were studied by transmission electron microscopy (TEM). Two, three, four and five-layers graphene structures were detected. These results suggest a way for FLG synthesis through environmentally friendly route without acids and strong chemical oxidants use.

Keywords: Green synthesis, Few Layers Graphene, Sonication, *Opuntia ficus-indica*.



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[NSN-126] Creation of CuAl-C nanoparticles using discharge arc immersed in liquid

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Metal nanoparticles and their oxides have a considerable number of present and future applications in the military, medical and industrial, but few studies have been conducted on toxicological effects of exposure of metal nanoparticles in vitro. The preparation of metal nanoparticles is of great interest because of their optical, electrical and catalytic, etc. These properties depend on the size, shape and dispersion of nanoparticles, which can be controlled using the method of synthesis. Within the parameters that influence the morphology of nanoparticles are the choice of reducing agent relative amounts and concentrations of reagents, temperature and duration of the reaction. Metal nanoparticles have properties different from bulk materials synthesized from the same atoms.

Aluminum nanoparticles have been proposed as drug delivery systems, specifically by encapsulating the drugs with nano sized particles of aluminum to increase solubility, thus avoiding clearance mechanisms and allowing for site-specific targeting of drugs to cells. Copper nanoparticles have unique optical, catalytic and chemical properties specific to the nano level. Several ways of protecting the nanoparticles from oxidation have been proposed. For example, graphitic coatings have been used to stabilize metallic nanoparticles and to minimize their size in conductive and magnetic fluids.



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In this work we present the creation of nanoparticles of Al-C, Cu-C and CuAl-C using the technique of discharge arc immersed in distilled water. We sought to determine the optimum conditions for the growth of nanoparticles varying system parameters such as current (50-300A).



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[NSN-141] Synthesis of bronze-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 from 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, bronze 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. For example, graphitic coatings have been used to stabilize metallic nanoparticles.

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



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[NSN-142] Metalorganic precursors in the preparation of alpha-alumina nanofibers by electrospinning

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The obtainment of stable nano-alumina structures of alpha-alumina allows its application in components resistant to high temperatures as supports for catalysts, insulators and reinforcements due to their chemical inertia, low thermal conductivity and high resistance. In this work the effect of the use of different concentrations of two metalorganic precursors, aluminum isopropoxide and aluminum formate, in the preparation of alpha-alumina nanofibers was studied. The nanofibers were obtained by combining the sol-gel and electrospinning techniques. For the preparation of sol-gel, molar ratios of 0.5, 1, and 1.5 of precursor in water were used. Subsequently, the fibers were characterized by SEM having an average size of 70.82 ± 26.68 nm and 69.07 ± 45.10 nm using aluminum isopropoxide and aluminum formate with a molar ratio of 0.5.



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[NSN-145] Synthesis of iron particles

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The principal route for obtain metal nanoparticles is the chemical synthesis. The main objective of the next research is optimization of chemical processes for the synthesis of iron nanoparticles. In the synthesis of iron nanoparticles, we used 5 concentrations of iron (III) clorhide, with differents amounts of Polivinilpirrolidone, in the reduction we used gallic acid, aiming to optimize a route that gives us stable and non-oxidizable iron particles. As preliminary results, particles with an approximate size of 130 nm were obtained for a concentration of 0.001 M FeCl₃, for the concentration of 0.01 M a size of 45 nm, the concentration of 0.02 M the particle diameters are in the 7 nm, for the concentration of 0.03 M the approximate diameters are of 41 nm, and finally in the concentration of 0.05 M the particles did not present nanometric size as they precipitate in the medium.



[NSN-147] Pt₃Fe/C bimetallic alloy nanoparticles as electrocatalysts with improved activity for the ORR

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The synthesis of two nano catalyst (octahedral and octapods) of Pt₃Fe for oxygen reduction reaction (ORR) in acid media is presented. Catalysts were prepared through chemical reduction with the properly amount of oleylamine, oleic acid, and precursor salts (Pt(acac)₂ and Fe(acac)₃). In one of the two synthesis we use dibenzyl ether and tungsten hexacarbonyl (W(CO)₆) as solvent and reducing agent respectively. Subsequent, both catalysts were dispersing in a carbon matrix (Vulcan Carbon) previously thermally treated. The presence of the alloy Pt₃Fe in the catalysts was proved by XRD. TEM micrographs shown the morphology of the nanoparticles with an average 7-9 for octahedral and 12-14 nm for octapods. The electrochemical performance of Pt₃Fe/C was evaluated by cyclic voltammetry, CO stripping and rotating disk electrode in HClO₄ as electrolyte. Octapods of Pt₃Fe/C nano nanocatalyst showed the best catalytic activity in terms of 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 octapods nanocatalyst, which could be used as a cathode electrode in a PEM fuel cell.



[NSN-150] Synthesis and characterization of NiCu nanoparticles decorated with Pt for ORR.

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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 is present. 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 with Pt. The metallic core inherits the crystal structure of its composing elements, i.e., the face-centered-cubic (FCC) structure. The diffraction peaks 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 decorated 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 311 mA/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. Therefore, this finding suggests a methodology for producing a carbon supported octahedral nanocatalyst, which could be used as a cathode electrode in a PEM fuel cell.

Keywords: NiCu alloy; octapods, octahedral nanoparticles; ORR catalyst; fuel cells.



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[NSN-151] Use of nanoparticles of silicon dioxide in the stabilization of a silty sandy soil

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1. Summary

Some materials used in construction such as silty sand (SM) have difficulties to be compacted due to the limited range to absorb water, in this context different stabilizers are used in the market, however, recently, nanotechnology has also reached this field, where the particle size seems play an important role in the stabilization process depending on its nature. Although there are previous studies related to, stabilization of soils with nanomaterials, the mechanisms of have not been explained yet. This study presents results of the stabilization of silty sand from a material bank in the region of Querétaro with different percentages of hydrophobic and hydrophilic silicon dioxide nanomaterials in order to explain how these nanoparticles influence physical behavior such as cohesion and mechanical properties such as shear strength. The physical characterization was carried out using the soil classification system (SUCS), standar compactation test, method A. The mechanical characterization was carried out by means of the non-consolidated triaxial assay; chemical and microstructural characterization carried out by scanning electron microscopy (SEM), infrared spectroscopy (FTIR) and X-ray diffraction (XDR). The soil was mixed by the direct incorporation of the nanoparticles in powder and manual kneading. From the results, it is concluded that there is an increase in the shear strength and in the plastic behavior for the soil mixed with hydrophilic nanoparticles due to the attraction of water due to the nature of this particles and its surfaces area.

Keywords: Silty sand, cohesion, plastic behavior, nanomaterials, stabilization.



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[NSN-155] Syntheses of graphene by sonication and ultrasonic bath

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Graphene is one the simplest form of carbon and definitely the thinnest material ever produced. It has one-atom-thick planar sheets of sp² bonded carbon atoms densely packed in a honeycomb crystal lattice. The interest in graphene is for its exceptional properties (chemical, mechanical, thermal and electrical) that it present, it permit to be used in fabrication of different optoelectronic devices. In this work graphene is obtained from graphite through sonication with the help of solvent N,N-dimethylformamide, where graphene can be separated from graphite with the help of centrifugation, and other method was by ultrasonic bath for a long time in a aqueous medium of graphene oxide. The stable aqueous dispersions of graphene were confirmed by measuring the Raman spectra in the regions of G and 2D bands and the XRD pattern shown the presente characteristic peak of graphene.



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[NSN-161] “Growth and Characterization of CdS nanostructures and Bi nanoparticles”

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CdS nanostructures, as nanowires (NW's) or nanobelts, are expected to have important applications at the nanoscale, in applications comprising sensors^[i], 3rd generation solar cells^[iii], photodetectors^[iii] and lasers^[iv]. In particular, it is expected that NWs of CdS, an important n-type II-VI semiconductor typically used as window material in thin film solar cells^[v], would greatly raise the contact area with the absorber material in these devices. Moreover, reflection losses and photo-excited carrier mean free paths could be reduced with a consequent increase in efficiency.

In this work, CdS nanostructures were prepared with bismuth nanoparticles with sizes between 30 and 80 nm as a catalytic agent onto CdS layers grown on glass as substrates. The CdS nanowires and substrate layers were obtained using a sputtering growth system with three magnetrons. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) allowed observing the morphology, size and distribution of the bismuth nanoparticles and the obtained nanostructures that were also studied by energy-dispersive x-ray spectroscopy (EDS). The structure of CdS was identified by means of x-ray diffraction (XRD).

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[NSN-172] Synthesis of titanium dioxide nanofibbers by electrospinning technique: applied voltage effect

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In this work presents the controlled synthesis of titanium dioxide nanofibbers by electrospinning technique. By varying the voltage was possible to control the diameter and formation of the fibbers within the nanometer scale. Titanium isopropoxide was used as the precursor solution and polyvinylpyrrolidone was used as a guide for carrying out titanium dioxide nanofibbers in an electrospinning device. Continuous stables homogeneous fibbers and nanometric diameters were obtained at 15 kV with an average diameter of 90 nm that was measured by Scanning Electron Microscopy. The titanium/polyvinylpyrrolidone fibbers were subjected to a heat treatment at 550°C to control the crystal structure of the nanofibbers, which were found to be anatase crystalline phase that was determined by X-ray diffraction and confirmed by Raman spectroscopy. These analyses corroborate the presence of titanium dioxide nanofibbers that showed a non-linear relationship between diameter and distance of work

In this work presents the controlled synthesis of titanium dioxide nanofibbers by electrospinning technique. By varying the voltage was possible to control the diameter and formation of the fibbers within the nanometer scale. Titanium isopropoxide was used as the precursor solution and polyvinylpyrrolidone was used as a guide for carrying out titanium dioxide nanofibbers in an electrospinning device. Continuous stables homogeneous fibbers and nanometric diameters were obtained at 15 kV with an average diameter of 90 nm that was measured by Scanning Electron Microscopy. The titanium/polyvinylpyrrolidone fibbers were subjected to a heat treatment at 550°C to control the crystal structure of the nanofibbers, which were found to be anatase crystalline phase that was determined by X-ray diffraction and confirmed by Raman spectroscopy. These analyses



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corroborate the presence of titanium dioxide nanofibbers that showed a non-linear relationship between diameter and distance of work

[NSN-179] Microwave assisted chemical bath deposition and thermal annealing of CdS thin films.

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In this work CdS thin films were deposited on glass substrates following two procedures. On one of the procedures the films were deposited by chemical bath assisted with microwave radiation while in the other procedure the already deposited films by conventional chemical bath were thermally treated. CdCl₂, NH₄OH, NH₄CL and SC(NH₂)₂ were used as precursor compounds for the synthesis of the thin films. The substrates submerged in the precursor solution were exposed to microwaves for 5 seconds and 1 minute in 5 s intervals and let them sit for 1 to 6 days. The results were analysed as a function of immersion time of the substrates in the solutions. The thermally treated films were deposited by conventional chemical bath. This films were treated for 1 to 3 hours. The films were structurally characterized using the techniques of X-ray diffraction and Raman spectroscopy. The optical characterization was carried out by UV-Vis spectroscopy. The chemical composition was obtained by energy dispersive X-ray spectroscopy. Scanning electron microscopy was used to study the surface morphology of films. The authors thank Sergio Oliva for his technical support.



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[NSN-191] Study of Ag decorated ZnTiO₃ for photocatalytic applications

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At present, the hydric resources pollution is a topic of great interest to the scientific community. The water pollution, mainly by the industrial sector, has caused that much of the environment is affected by its toxic residues that mostly contain dangerous organic compounds to the environment and human consumption. To address this problem, in recent years different water treatment methods have been implemented, in order to reach the total water purification. Heterogeneous photocatalysis is one of the advanced methods of environmental decontamination, based in the use of a semiconductor (catalyst) and sunlight. In this work, a study of the structural, optical and morphological proprieties of Ag decorated ZnTiO₃ powder is presented. ZnTiO₃ powder was prepared by the combustion method. The structural, optical, chemical and morphological properties of the Ag decorated ZnTiO₃ powder were studied by the XRD, UV-Vis, XPS and SEM characterization techniques. The photocatalytic tests, under UV light radiation (254 nm), were made using rhodamine B.

Acknowledgments

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[NSN-198] N doped TiO₂ prepared by hydrothermal method for the organic pollutants photodegradation

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The development of semiconductor materials with properties suitable for photocatalytic applications follows being a challenge for the scientific community. Changes on the structural, optical, morphological and electrical properties are some of the attempts to improve its efficiency. TiO₂ is a semiconductor material widely studied due to its characteristics as non-toxicity, good chemical stability, strong mechanical properties, low cost, and excellent photocatalytic performance. However, its photocatalytic activity needs to be improved in order to expand its absorption sunlight range. In this work, N doped TiO₂ powder was prepared by the hydrothermal method, in order to improve its photocatalytic activity for the dye photo-degradations. Studies about X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), UV-Vis spectroscopy and x-ray spectroscopy (XPS) were developed in order to assess the photocatalytic behavior of the N doped TiO₂ powder with respect to the processing conditions.

Acknowledgments

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[NSN-207] Synthesis and Characterization of Cobalt Sulfide and Chromium Sulfide
Nanoparticles

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This work focuses on the study of two kinds of binary chalcogenides: cobalt sulfide and chromium sulfide nanoparticles. It has been reported potential applications of cobalt sulfide in photoconductors, radiation detectors, thin film transistors, light emitting diodes, photoelectric cells, anodes for Li-ion batteries, catalysts for hydrodesulphurization and dehydrodearomatization, among others. As for chromium sulfide, it has been reported applications as energy solar materials and biological applications. Among the methods to synthesize these materials, it has been reported chemical bath deposition, chemical vapor deposition, electrochemical deposition and hydrothermal and solvothermal methods. The method to synthesize our nanoparticles is chemical aggregation where we use metallic ions of cobalt and chromium and sulfide ions. Results presented are based in the following characterizations techniques: UV-VIS, TEM, SEM, XPS. Data to study optical properties were obtained with the UV-VIS technique. Absorption was obtained to find the band gaps of our chalcogenides. They are 3.06 for CrS, 3.09 for Cr₂S₃ and 2.62 for CoS. The TEM technique permitted us to obtain micrographs of three types of images: panoramic, medium and high-resolution. From HRTEM micrographs, we made an image process to find the von Laue diffraction pattern. From here, we calculate the interplanar distances and the Miller indexes associated to them. Surface morphology obtained by the SEM technique shows us we have distinct forms (triangular and circular) and sizes that varies from a few nanometers to a few microns. Chemical composition of our nanoparticles was analyzed with the XPS technique. Data obtained served us to make deconvolutions, where we can verify that our results coincide with the reported by the scientific literature. As a conclusion, we present in this work three new formulations to synthesize CoS, CrS and Cr₂S₃ nanoparticles.



[NSN-220] Raman Spectroscopy of Simple Wall Carbon Nanotubes (SWNTCs) with cylindrical and oval symmetry obtained by theoretical calculations Ab Initio.

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We present in this work a theoretical study on two phases referred to the modeling of carbon nanotubes. In both phases, which we call carbon nanotubes with oval or cylindrical geometry, the differences of its geometric and vibrational structure are shown; showing the Raman spectra of these phases. In both structures their ends are capped with hydrogen atoms with which they are functionalized. Since the discovery of the interesting optical and electronic properties of carbon nanotubes, their behavior as a metallic or semiconductor material or both, which depends strongly on the dimensions of the diameter of the carbon nanotube determined by the chirality indices (n, m) With respect to the emitted wavelength (λ). We analyze the Raman spectra of the two phases of carbon nanotubes comparing and studying the influence of oval geometry on the cylindrical in particular the main bands: 1) The Radial Breathing Modes (RBM) which extract information on the diameter and chirality of the same; 2) the tangencial G band, whose spectral profile reveals the semiconductor or metallic character of the nanotubes; and 3) The D (“Disorder-induced”) and G’ (sobretono de D) bands. The computational tool that supports our work is the software SPARTAN and GAUSSIAN in which we model both types of molecular structures, using Ab initio calculations.



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[NSN-241] Characterization and application of Ag, Au and Cu nanostructures substrates for surface enhanced Raman spectroscopy using Methylene blue as a test molecule.

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The influence of the morphology and distribution of nano-structured gold, silver and copper substrates on the localized surface plasmon resonance wavelength and surface enhanced Raman signal (SERS) is investigated. The Ag, Au and Cu nanostructures are synthesized by laser ablation using a Nd: YAG laser emitting in the third harmonic, at a wavelength of 355 nm and a pulse duration of 10 ns. Nanostructures are made by varying the number of pulses typically from 200 to 20000 using about 100 mJ as output laser energy and focused in a spot of 1 mm in diameter. The nanostructures are characterized by UV- Vis spectroscopy and TEM. The surface plasmon wavelength shows a strong dependence on the nanostructures morphology which evolves progressively from nanospheres to more complex shapes. The SERS studies were performed using methylene blue as test molecule. It is found that the SERS signal increases monotonically with the size of the Ag, Au, Cu nanoparticles and the surface plasmon exhibits a red shift, until reaching a maximum in intensity and decreases afterwards.



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[NSN-246] Preparation of copper nanoparticles by laser ablation in distilled water.

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The aim of this work is to report the synthesis of copper nanoparticles by laser ablation of a Cu target immersed in distilled water. The laser used was a Nd:YAG emitting at 355 nm with a pulsed length of 20 ns. The effect of the liquid and the laser energy density (12 J/cm^2) on the size and size distribution of the nanoparticles was investigated. The nanoparticle size was determined from transmission electron microscopy (TEM) micrographs. In general, the range size was from 4 nm to 30 nm. Copper nanoparticles, as synthesized, were highly crystalline in nature. UV-Vis measurements showed typical plasmonic absorption band characteristic of Cu metallic spherical particles of nanometric size. Furthermore different experimental conditions were studied such as height of water above the target spot size and the presence or absence of an ultrasonic field. The main results are presented in this work.



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[NSN-252] Sustaining the one-dimensional order of InAs nanostructures in the growth on high-Index substrates

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In the last decade, the low dimensional systems (LDS) has been widely studied in order to develop new generation optical and electronic devices. For their synthesis, the self-assembling of nanostructures in a variety of systems (i.e. InAs/GaAs, InAs/InP, CdSe) has been extensively employed. For this approach in order to maximize the LDS-based devices performance, research about the control of the nanostructures self-organization is required. The molecular beam epitaxial growth (MBE) on high-index substrates has demonstrated to be an excellent alternative for propitiating self-alignment of nanostructures on corrugated surfaces. However, both the corrugation and the nanostructures formation are promoted by strain, thus raising the complexity of the heteroepitaxial system. In this work, we study growth of InAs to promote the self-organization of nanostructures. The surfaces under study were GaAs(221)- GaAs(631)- and GaAs(775)-. For InAs/GaAs structures, the deposition of fractional monolayers of InAs can be used to switch the surfaces from corrugated to flat surface ^[1,3], finding a new energy minimum, and leading to a stochastic growth. On the contrary, our work demonstrates that under suitable growth conditions the one-dimensional order of nanostructures such as quantum dashes, quantum wires, and quantum dots can be achieved in spite of the strain introduced by InAs. These novel 1D arrangements are discussed in terms of the formation of stable {110} facets and microfaceting that allows for the restoration of the buried buffer layer corrugation, which still can serve as nanotemplate for the alignment of nanostructures.



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[NSN-270] Bio-conjugation Method for ZrO₂:Yb³⁺-Er³⁺ Nanoparticles to Detect Ki-67
Overexpressed Protein in HeLa Cells

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Abstract.

Up-conversion luminescent ZrO₂:Yb³⁺-Er³⁺ (2–1 mol%) nanocrystals were coated with AntiKi-67, through a conjugation method. This biomolecule can be used as a prognostic marker in many types of cancers. The conjugation was successfully confirmed by Fourier transform infrared, zeta potential, and dynamic light scattering. The internalization of the conjugated nanoparticles in human cervical cancer (HeLa) cells was followed by two-photon confocal microscopy. It was studied the luminescence change due to the biomolecules adsorbed. These results demonstrate that ZrO₂:Yb³⁺, Er³⁺ nanocrystals can be successfully functionalized with biomolecules to develop platforms for biolabeling and bioimaging.

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[NSN-280] p-Type Doping of Cubic GaN by Magnesium

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Gallium nitride (GaN) is a semiconductor that possesses unique characteristics that make it a strategic material for applications in optoelectronics and power devices. Most of their potential in these fields are due, respectively, to the unique properties such the wide band-gap, high electron saturation, high breakdown electric field, high thermal conductivity, and high chemistry and mechanically stability.

The interest in cubic nitrides is motivated by the advantages with respect to the stable hexagonal phase, due to higher crystalline symmetry, that results in more isotropic properties and no spontaneous polarization induced-electric fields in the direction parallel to the c-axis.

Several groups has been successfully grown cubic gallium nitride (c-GaN) on different substrates such as GaAs (001), 3C-SiC, Si (100), and nano-patterned silicon (100). However, the development of optoelectronic devices based on c-GaN requires of an efficient p type doping and high quality crystal structure. Just a few reports of c-GaN devices has been found in the literature^{1,2}, this is in part for the no efficient p type doping or the main disadvantage in the synthesis of c-GaN, the lack of a native substrates and a low quality crystalline film due to the hexagonal inclusions.

In this paper was carried out a study of the effects on the structural, optical and electrical properties of Mg doping on c-GaN grown by epitaxy by molecular beams on MgO (100) substrates. The influence of varying the Mg flux (with magnesium effusion cell temperature in a range of 250 to 900°C) in the growth conditions of c-GaN films grown at 720°C.



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[NSN-282] Chemical and structural properties of p-type cubic GaN

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Galium Nitride (GaN) is a semiconductor of high importance for developing a wide variety of devices, such as LED's, laser diodes, transistors and solar cells. This is mainly due to their outstanding optical, structural and electrical properties. However, one of the major challenges to achieve these applications is to obtain p-type GaN, because of the GaN is intrinsically n-type doped and has high acceptor-ionization energy. On the other hand, GaN can be synthesized in two crystalline structures: stable-hexagonal (h-GaN) and metastable-cubic (c-GaN). c-GaN presents remarkable advantages due to of its high degree of crystallographic symmetry. In this work we present a chemical and structural study of p-type GaN doped with Mg. The samples were grown by the Molecular Beam Epitaxy (MBE) technique. The thin films were synthesized at the growth temperature of 720°C, with a Ga beam equivalent pressure (BEP_{Ga}) of 2.28×10^{-7} Torr. and a Nitrogen (N) plasma source operating at 150 W with a N_2 flow of 4.1 sccm. The BEP_{Mg} was varied in the range of 3.3×10^{-9} to 3.24×10^{-8} Torr. The thicknesses of the Mg:GaN samples are 450 nm. We found by SIMS measurements that by increasing the Mg flux, the Mg concentration increases in the GaN samples. Likewise, we obtained that the hole concentration also increases with the Mg incorporation, as it was shown in the hall effect measurements. The highest hole concentration was $7.83 \times 10^{19} \text{ cm}^{-3}$. Finally we obtained the binding energy of the Mg:GaN by XPS measurements.



[NSN-286] Detection of ketorolac in blood plasma by using Surface-Enhanced Raman Spectroscopy

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The detection of drugs in the bloodstream has been for many years one of the top reasons for performing chemical tests on blood samples obtained from patients. An alternative for doing these tests is Surface-Enhanced Raman Spectroscopy (SERS), which consists in the adsorption of the sample on a metallic surface that leads to an enhancement of the Raman signal. In this work the Raman signals of ketorolac, an anti-inflammatory drug of common use, were detected in the spectre obtained from blood plasma. The Raman signals were intensified by using metallic nanoparticle solutions.

The Raman intensity enhancement given by the metallic nanoparticles was tested by taking the Raman spectre of a diluted ketorolac solution, which characteristic Raman signals were found at 1000, 1450 and 1600 cm^{-1} , adsorbed on two different kinds of nanoparticles. Three ketorolac samples at 10^{-4}M were prepared, one diluted with methanol and the other two diluted with silver and gold nanoparticles solutions, respectively. In the spectre of the methanol-diluted sample without nanoparticles, the signals were weak or some did not appear. Whereas the spectre taken from the adsorbed samples on the nanoparticles showed signals with a high intensity despite the low drug concentration. Afterwards, nanoparticle solutions were used to adsorb a sample of blood plasma after the administration of ketorolac to enhance the characteristic Raman signals of the drug. We found a remarkable improvement of the drug's Raman signals by using SERS instead of conventional Raman which allowed us to detect the drug in the blood plasma sample. The comparison between the Raman and SERS spectres proves the potential that SERS possesses as an alternative technique for detecting or monitoring medicines or drugs within the body.



[NSN-299] **Mechanosynthesis of a ternary thermoelectric compound via high-energy milling**

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Solid–solid reactions have been traced during high-energy milling of Pb–Sn–Se powder precursors under controlled composition, pressure and temperature (*C-P-T*) vial conditions in order to synthesize the PbSnSe₂ ternary thermoelectric compound. Systematic analysis of transformation in the resulting phases of milling has been envisaged to characterize microstructures i.e. morphology and particle size as a function of milling time. The as-milled reaction products were analyzed by X-ray powder diffraction and Atomic Force Microscopy.

Chemical arguments are postulated to discern the high-energy milling mechanism to transform Pb–Sn–Se micropowders onto PbSnSe₂-nanoparticles. Then, a set of reactions were evaluated at around room temperature. The results reveal that the microconstituent powders transforms gradually to PbSnSe₂-nanoparticles when active nano-heterogeneities are added during milling.



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[PLV-63] Physical properties of hydrothermally treated ZnO:M (M=Ag,Au,Cu)
nanostructured thin films grown by PLD

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Pulsed laser deposition of ZnO thin films doped with transition metals (Ag, Au, Cu), on silicon substrates at room temperature in an O₂/Ar atmosphere. For the laser ablation process two metallic targets were coaxially arranged (Zn and Ag, Au or Cu). The pressure in the chamber was kept constant at 2×10^{-2} Torr for every deposit. Plasma parameters were used in order to control the concentration of dopants. The mean kinetic energy of the plasma was kept constant and plasma density was varied. Plasma parameters were calculated from “time of flight” curves obtained with a Langmuir planar probe. In order to homogenize the samples, films were hydrothermally treated. Crystalline, electric and optical properties of the ZnO:Ag,Au,Cu deposited thin films were investigated. The XRD patterns of the films reveal the presence of a strong peak corresponding to the (101) of hexagonal wurtzite ZnO. The average grain size was estimated to be 9.5 nm with Scherrer equation. Band gap energy was obtained from optical transmission spectra of the films.

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[PLV-74] AlN thin films deposited by the combination of PLD and Microwave plasmas

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Aluminum nitride thin films were deposited using the plasma obtained from the combination of nitrogen microwave plasma and the plasma formed during the pulsed laser ablation of an aluminum target. In order to characterize the plasma, two types of Langmuir probes were used; a cylindrical one was used to measure the plasma density and the electron temperature of the microwave plasma and a planar probe to measure the plasma density and the mean kinetic energy of the ions of the laser ablation plasma. Optical emission spectroscopy was used to measure the type of excited species present in this combination of plasmas. A Nd:YAG laser emitting in the fundamental (1064 nm) with a pulse duration of 5 ns and a repetition rate of 10 Hz and maximum output energy of 450 mJ per pulse, was used to form the laser ablation plasma. For the ablation a high purity aluminum target was used. The ablation process was carried out in nitrogen microwave plasma, with a density that could be varied from $5 \times 10^{10} \text{ cm}^{-3}$ up to $3 \times 10^{11} \text{ cm}^{-3}$. The mean kinetic energy of the aluminum ions ranged between 100 and 300 eV. This combination of plasmas allowed depositing nanostructured aluminum nitride thin films. The stationary microwave plasma allows reducing the typical splashing formed on the substrates during the laser ablation process, and the oxygen content in the films. The deposited films were characterized by TEM, in order to observe and characterize the AlN nanocrystals.

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**[PLV-138] Plasma spectroscopy as a tool to monitor the growing process of a thin film
produced by a magnetron sputtering system**

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In this work we present a thorough study on the relation between the plasma spectroscopy and the optical properties, composition and deposition rate of thin films grown by reactive magnetron DC sputtering (MS). Silicon and titanium oxides and silicon nitride thin films were grown under diverse deposition parameters and the emission of the plasma was interrogated in real time by means of optical emission spectroscopy (OES) observing at the target and at the substrate positions simultaneously. The film growth was also measured in real time by means of *in situ* spectroscopic-ellipsometry. Both results were compared with the aim to propose plasma spectroscopy as a monitoring tool of the deposition process to assure repeatability of the resulting thin films. That is, to deduce changes in film stoichiometry and/or deposition rate from the evolution of the line ratios from different spectral transitions observed within the plasma column.



[PLV-168] Characterization of pulsed laser deposited silicon copper oxide nanolayers

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The combination of plasmas in pulsed laser deposition of thin films has proven to be a powerful tool for doping, alloying or synthesizing composite materials. In the present work, silicon and copper targets were simultaneously ablated to combine both plasmas using a parallel configuration in an oxygen atmosphere to grow oxide layers. The chamber was evacuated to a base pressure of 2×10^{-6} Torr. A working pressure of 20 mTorr of a mixture of Ar(80%)/O₂(20%) was used. The plasmas were characterized independently and combined using a Langmuir planar probe in order to calculate the mean kinetic energy and density of the silicon and copper ions. Fixed values for plasma parameters of Si were chosen while the Cu plasma density was varied with the aim to modify the Cu content on the films.

Nanolayers with thicknesses ranging from 40 to 60 nm were obtained. Samples were structurally characterized by XRD and Raman spectroscopy. Optical properties of the films were analyzed by UV-Vis spectroscopy. XPS was used for chemical composition measurements and determination of Si and Cu oxidation states.

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[PLV-41] Effect of plasma ion density on the physical properties of Zn_{1-x}Sn_xO_y
nanostructured thin films grown by pulsed laser deposition

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The energy band alignment between the different layers in thin films solar cells strongly affects their performance. A buffer layer is added to avoid cliff behavior alignment. In recent studies Zn_{1-x}Sn_xO_y has shown to be a superior alternative for such layer in CIGS and CZT(S,Se) photovoltaic devices.

It is necessary to control the physical properties of the buffer layer to reach the optimal conduction band off-set to avoid interface recombination. Pulsed laser deposition has shown to be an adequate technique to manipulate thin films physical properties through the control of plasma parameters.

In this work Zn_{1-x}Sn_xO_y thin films were grown by the simultaneous ablation of high purity Zn and Sn targets under an oxygen atmosphere. The plasma parameters were monitored using Time of Flight curves obtained from Langmuir planar probe measurements. The structural, electrical and optical properties have been studied to achieve an adequate thin film for optoelectronic applications. The ion kinetic energy and density were fixed individually in order to alternately variate the ion density in the formed plasma. The samples were characterized by X-ray diffraction, Raman spectroscopy, atomic force microscopy, scanning electron microscopy, X-ray photoelectron spectroscopy, energy-dispersive X-ray spectroscopy, UV-Vis spectroscopy and Hall Effect. The results were analyzed as a function of the variation of the Sn and Zn ion densities in the plasma.

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[PLV-53] Study on the structural, optical and electrical properties of ZnO:Nb thin films

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Thin films of ZnO doped with Nb, were deposited by the technique of reactive co-sputtering at room temperature, under a reactive atmosphere of oxygen and argon. After deposition the films were heat treated for one hour at 300°C in an atmosphere of argon. X-ray diffraction (XRD) characterization revealed a hexagonal structure, for all the deposited samples. Using absorption and emission spectroscopy it was observed that the films have transparencies of the order of 70% in the visible region. A Hall Effect technique in Van Der Pauw configuration was used to measure a resistivity of 10^{-2} Ω·cm. Additional samples were heat treated for one hour at 400°C under similar conditions. An improvement in all physical properties is observed. The crystalline quality increases and the films are highly oriented along the Z axis and perpendicular to the surface of the substrate. The films show transparencies of approximately 90% in the visible region, and a resistivity as low as 5.47×10^{-3} Ω·cm was obtained.



[PLV-80] Background pressure effect on the crystalline phase of pulsed laser deposited nanometric CdTe films

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Due to its optoelectronic properties, cadmium telluride is one of the most promising polycrystalline materials for thin film solar cells. CdTe has a high absorption coefficient in the visible and infrared spectra and has a nearly optimum bandgap value for efficient thin film solar cells according to the Shockley-Queisser limit of solar cell efficiency. In this work CdTe thin films were grown by pulsed laser deposition on glass substrates at room temperature. Pure argon was used as background gas and the deposition was made at different pressures (10^{-5} to 10^{-3} Torr) while the time remained constant at 10 minutes. Plasma parameters (mean kinetic ion energy and density) were measured using a Langmuir probe. Crystalline structures were characterized by X-ray diffraction and Raman spectroscopy, optical characterization was obtained by UV-Vis and PL spectroscopies, morphology was studied by scanning electron microscopy and chemical composition of the films was obtained by energy dispersive X-ray spectroscopy. Some changes in crystalline structure were observed, which are attributable to different background pressures.

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[PLV-111] Pulsed laser deposition of Ag-Cu mixtures as a back contact layer for photovoltaic applications.

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The diffusion capabilities of copper in semiconductors via a variety of mechanisms are well understood, being present in most types of copper based solar cell contacts, and entails the degradation of the films and malfunction of the cell by short-circuiting of both contacts.

In the present work we make use of coaxially arranged Silver and Copper targets, with separate Nd:YAG laser spots, in order to combine the laser produced plasmas. By means of a Langmuir planar probe it is possible to measure the plasma of both materials separately and in a combination with the aim of controlling the composition for the obtention of an alloy or a nano-composite film, which fits the electrical properties for an ohmic contact to CdTe. The plasma energy and density of Cu was maintained constant while varying the Ag energy, using the same ion density used for Cu. Another approach is made by depositing the Silver film before the Copper one, in this case we take the conducting properties of Copper and use the Silver as a diffusion barrier for Copper, simultaneously isolating the Silver from oxidizing in the atmosphere.

Given the requirements for the contact to work properly, samples were characterized by means of UV-Vis spectroscopy, X-ray diffraction, scanning electron microscopy, energy dispersive microanalysis and electrical resistivity measurements; analyzing the relation between morphology and composition with the electrical properties. Results are discussed as a function of the Ag plasma for each experiment, thus making a physical connection of the whole process interactions.

JGQG acknowledges the partial financial support from SEP-Mexico through PRODEP program (under project UDG-PTC-1274).



[PLV-137] Physical and tribological properties of ZrN and ZrN:Ni nanocomposite films

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In this work, the physical and tribological properties of reactively sputtered ZrN and ZrN:Ni nanocomposite films, deposited on aluminum sheets and crystalline (100) silicon wafers as substrates are reported. These films were grown using a fixed power to the Zr target (80 W), but with a variable power to the nickel target. The chemical composition was obtained from EDX measurements. X-ray diffraction revealed that a two-phase nanocomposite material was formed, for the both cases. The nanocomposite consisted of nanocrystals of (Ni, Zr)N, embedded in an amorphous matrix. The optical constants were measured using spectral ellipsometry and were simulated using a Drude-Lorentz model. The hardness and elastic modulus values were measured by nanoindentation and were correlated to the microstructure of the films. Nanoindentation tests showed that the coatings had an average nanohardness of 24 GPa. The surface of coatings revealed smaller grains and smooth surface. Pin-on-disk tests indicated that ZrN:Ni coating exhibited excellent wear resistance.



[PLV-139] Comparison of the deposition rate of titanium dioxide thin films and the plasma optical emission spectroscopy

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TiO₂ thin films grown by reactive magnetron sputtering were used in this work to support low-e multilayer coatings. The required thickness of these films is very specific to accomplish the pursued optical properties, that is, high transmittance and high reflectance at the visible and the infrared region of the electromagnetic spectrum respectively. However, providing a good quality control is challenging, thus the aim of this work is to suggest a real-time monitoring of the process via plasma spectroscopy. During deposition, the thickness of the TiO₂ layer was monitored and controlled via spectroscopic-ellipsometry and the process was stopped once the desired thickness had been reached. Simultaneously, optical emission spectroscopy of the plasma column was performed during the Ti target cleaning and the TiO₂ deposition phases. Intensity ratios of different emission transitions within the plasma (Ti, Ar and O) were obtained to observe the evolution of the deposition process and verify, first of all, if the target was sufficiently clean to perform such film deposition; and, afterwards, to determine those transitions which can give information about the actual deposition rate.



[PLV-163] Characterization of nanostructured Al-Si-N thin films deposited by laser ablation

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Coatings based on Al-Si-N have attracted the attention of many research groups as they can improve the hardness, transparency and oxidation resistance of AlN coatings, depending on the Si content. This type of coatings is usually deposited using plasma assisted techniques. Pulsed laser deposition is a technique that allows the deposition of ternary systems, in which one of the elements must be incorporated in a controlled manner. In this study Al-Si-N thin films were deposited using simultaneous laser ablation of two targets (Al and Si) in a reactive atmosphere of N₂, with a substrate temperature of 200 °C. The plasma parameters (ion mean kinetic energy and plasma density), were used to control the experiment and were studied using a Langmuir planar probe and optical emission spectroscopy (OES). The ion mean kinetic energy and plasma density of the particles from the Al target, were kept constant at values of 200 eV and $9.3 \times 10^{19} \text{ m}^{-3}$, respectively. The ion mean kinetic energy of the particles produced from the ablation of the Si target was approximately 40 eV for all the experiments and the plasma density was varied from $0.7 \times 10^{18} \text{ m}^{-3}$ to $3 \times 10^{18} \text{ m}^{-3}$. XPS measurements showed a clear evidence of a linear dependence of the Si content regarding the plasma density obtained from the ablation of the Si target, which also depends on the working pressure. In accordance with the characterization performed (optical properties examination, band gap evaluation and the hardness behavior) of the Al- Si-N thin films, the band gap could be varied from 4.7 up to 5.5 eV, the formation of an amorphous matrix of Si₃N₄ is suggested and a maximum value of hardness of $30.3 \pm 1.5 \text{ GPa}$ was reached at 4 at.% Si content.



[PLV-175] Elemental Characterization of Mexican Amber by Laser Induced-Breakdown Spectroscopy (LIBS)

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The Mexican amber is located in the south of the country in Chiapas State, this fossil resin was produced millions years ago by coniferous tree from the Hymenaea family. The Amber has great commercial importance because its transparency and diversity of colors is useful for jewelry and handicrafts. This causes that in the informal trade are generating false pieces of amber, due to this, arises the necessity of a reliable, quick identification and that does not damage the stone. Laser Induced-Breakdown Spectroscopy (LIBS) is a technique employs a low-energy pulsed laser and focusing lens to generate a plasma that vaporizes a small amount of a sample. A portion of the plasma light is collected and a spectrometer disperses the light emitted by excited atomic and ionic species in the plasma, a detector records the emission signals, and electronics take over to digitize and display the results. This technique is fast and non-destructive. This work presents an analysis of the Amber stone of Chiapas by LIBS spectroscopy with the aim of characterizing inorganic amber and identify the variations that exist in its composition depending on the varieties of colors and that is non-invasive, easy and fast. For the 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. A pulsed Nd: YAG laser emitted at 1064 nm and a Q: passive Er: YAG switch generating a 6-pulse train with a total energy of 120 mJ was used for the LIBS analysis. In the analyzes, elements such as Na, Al, Fe, Si, Ni, Co, Mg, Mo, K were identified, varying depending on the type of sample.

Acknowledgements

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X International Conference in Surfaces, Materials and Vacuum
September 25th-29th, Cd. Juarez, Chihuahua, México**

[PTP-300] Thermal annealing and chemical composition effects on thermal conductivity of nanostructured PbSnSe₂ material using photoacoustic and photopyroelectric techniques

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We report the effect of thermal annealing and different chemical composition traces on the thermal conductivity (k_T) of PbSnSe₂ nanoparticles measured using photoacoustic (PA) in open cell configuration (OPC) for the diffusivity determination and photopyroelectric (PP) technique in inverse configuration for the effusivity determination. PbSnSe₂ nanoparticles were obtained by the high-energy milling (HEM) technique under controlled composition, pressure and temperature (C-P-T) vial conditions. A difference in k_T was observed after each thermal annealing step and different chemical composition traces. Thermal annealing and chemical composition traces can be a potential method to improve the thermoelectric efficiency of PbSnSe₂ nanoparticles, not only by enhancing the electrical conduction as demonstrated before, but also by suppressing the thermal transport at the same time.



[PTP-304] Photoluminescence in porous silicon single and bilayers

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In this work, it was studied the photoluminescence (PL) spectra of single layers of porous silicon (PS) and bilayers as a function of the temperature.

Four samples were studied; the layers “A” and “B” correspond a single layer of PS etched at 5 mA/cm² and 40 mA/cm² respectively. The other two samples are a combination of the structure “A” and “B”, it means, there are bilayers compounds of AB and BA. The same properties of the heterostructures were guaranteed by in situ photoacoustics that controls the etch reaction.

The PL spectrum was carried out from 11 to 300 K and different laser power. It was found that the excitonic spectrum of the single layer is not sensitive to the temperature, it means that the origin of the exciton is not directly related with the with the of the quantum well and it is necessary to consider the surface chemistry.



[PTP-33] Phase separation technique of photoacoustic spectroscopy in the study of chlorophylls

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When a plant absorbs light, the phenomenon of photosynthesis occurs; it's ever accompanied of thermal emission, fluorescence and photochemistry energy, then it is used by the molecules of chlorophyll to carry out photosynthetic activity in plants. Photoacoustic Spectroscopy (PAS) is used to study thermal emission resulting from non-radiation de-excitation following absorption of radiation [1]. This work, use PAS as a tool to monitor photosynthetic activity in the visible range (400 - 700 nm) where occurs absorption of photosynthetic pigments as a complement to the analysis of the photobaric effect using the photoacoustic technique [2]. The plants under study are of Aquatic Lirium (*Eichhornia crassipes*), which are exposed at acoustic and photosynthetic activity is monitored in days 1, 3, 6, 9 and 12 after acoustic application. Besides, it was used PAS phase separation technique to study the behavior of the reaction centers of chlorophyll "a" (peak at 660 nm) and "b" (Peak at 620 nm) in the range 600 to 700 nm. Results show a significant decrease in the bands of chlorophylls "a" and "b" in the visible range at 12 days after exposing acoustic. And therefore, the utility of the ultrasonic irradiation, as well as, of the photosynthesis monitoring by means of PAS, for the elaboration and establishment of methodologies in the control of this aquatic plant, whose propagation causes many consequences extremely unfavorable for the environment and for the diverse human activities that are developed on the bodies of water in the tropical and sub-tropical regions of the world.

Keyword: Photoacoustic, photosynthesis, ultrasound.

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[PTP-88] Study of the thermal properties of compact silica nanoparticles in function of their size by the photoacoustic technique

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This work reports the synthesis of silica nanoparticles using Stöber method. Particles with different diameters size were obtained by hydrolysis and condensation of tetraethyl orthosilicate (TEOS) in ammonium hydroxide and alcohol solution. We varied ammonium hydroxide that allowed control size, shape and dispersion silica nanoparticles. It observed mainly spherical and monodisperse silica nanoparticles. Employing different amount catalyst (10-2 ml) it got nanoscale SiO₂ particles since 90 to 660 nm. When it employed higher ammonium hydroxide there were bigger silica nanoparticles. The effect of size silica nanoparticle on thermal properties reveal increase thermal diffusivity about the biggest silica nanoparticles. The thermal diffusivity was determined by photoacoustic, using the open photoacoustic cell (OPC) method. Scanning electron microscopy (SEM), transmission electron microscopy (TEM) and electron dispersive scanning (EDS) were used for silica nanoparticles characteristics.



[PTP-105] Photothermal characterization of silver nanoparticles from Neem contained in centrifuged citrus oils

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Thermal lens spectrometry is a very sensitive non-evasive technique and offers a reliable alternative for the measurement of very low thermal diffusivity.

In this work, silver nanoparticles from leaf extract of *Azadirachta Indica* (Neem) and silver nitrate were synthesized using reverse micelle microemulsion.

The thermal lens (TL) technique was used to obtain the thermal diffusivity of nanoemulsions of silver nanoparticles contained in centrifuged oils.

In relation to the silver nanoparticles, the thermal diffusivity was measured as a function of the reaction time and control of particle size. The results showed an increase in the thermal diffusivity of the nanoemulsion with the increase in nanoparticle concentration and size. Also, the nanoemulsion exhibited improved thermal diffusivity in comparison of the base fluid.

Transmission Electron Microscopy (TEM) was used to determine the morphology of the nanoparticles. They were spherical in shape and the average size was 20 nm. UV-Vis spectrometry was used to observe the absorption spectra of nanoparticles plasmon.

This study has a future application in dermatological therapies against allergies, in tissue regeneration and in the cosmetic area, because of its antibacterial properties.



[PTP-106] Neural network model for the determination of the thermal conductivity of higher nanoparticles concentrations in nanobiodiesel

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Thermal conductivity of nanobiodiesel was investigated theoretically and experimentally. It has been demonstrated in the literature that the addition of nanoparticles to conventional diesel can lead to significant increase in thermal properties. The thermal lens technique was used to determine the effect of the presence of Au nanoparticles on the biodiesel thermal diffusivity. The characteristic time constant of the transient thermal lens was estimated by fitting the experimental data to the theoretical expression for transient thermal lens. The results showed that the thermal diffusivity of the bionanofluids, pure biodiesel and biodiesel containing Au nanoparticles, seems to be strongly dependent on the presence of the nanoparticles. The maximum diffusivity was obtained for the bionanofluids when concentration of nanoparticles increases. The thermal conductivity of nanobiodiesel shows an enhancement lineal for nanoparticles of small concentrations. However, at higher nanoparticles concentrations, the thermal conductivities of Au nanobiodiesel are higher than that of the base fluid, and their enhancement is nonlinear. A possible explanation for such thermal phenomena is given. Therefore, a model was developed for the biodiesel, to represent the experimental data, using simple artificial neural networks. On the other hand, the Halmiton-Crosser cannot represent adequately the enhancement in thermal conductivity as a function of nanoparticle concentration. This



study evaluates the thermal properties Jatropha (*Jatropha curcas*) oil as alternative base oil for new generation systems of refrigeration and heating technology.

[PTP-112] photoacoustic phase resolved method of optical absorption spectrum of rat blood with hepatic damage.

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Photoacoustic spectroscopy (PAS) has been applied to the study of blood and some diseases related with these human fluid [1]. In the present research, the optical absorption spectra of Fisher rat blood, with hepatic damage, were obtained by using Photoacoustic technique. Then by applying the photoacoustic (PA) phase resolved method it was separated the Soret band (γ at 412 nm) to the two other characteristic absorption bands of blood (α and β at 562 nm and 540 nm respectively).

The hepatic damage was induced according to the animal model proposed by Semple *et al.*, [2]. In the phase resolved method, the optical absorption spectra of Fisher rat blood with induced hepatic damage, was obtained by PAS, then by applying the photoacoustic phase resolved method it was obtained only the Soret band and finally by the same method, was obtained the other absorption bands from the blood sample.

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[PTP-132] Thermal diffusivity determination in n-type and p-type porous silicon by mean of photoacoustic technique and numerical analysis

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Samples of porous silicon (PS) were prepared by electrochemical anodic etching with several etching times. It was used n-type, phosphorous doped, (100)-oriented crystalline silicon wafer (CS) (thickness: $500 \pm 15 \mu\text{m}$) of 1-5 Ωcm resistivity and p-type, boron doped, (111)-oriented crystalline silicon wafer (CS) (thickness: $430 \pm 10 \mu\text{m}$) of 120-230 Ωcm resistivity. In all cases was used a constant current density of 40 mA/cm^2 and a HF (40%) solution. The porous layers were prepared with etching times of 5, 10, 15, 20 and 30 minutes.

The measurements of the effective thermal diffusivity at room temperature of the samples were performed using the photoacoustic (PA) technique. On the other hand, the thermal diffusivity of the porous layer was determined by means of numerical analysis from the experimental results.

Keywords: porous silicon, electrochemical etching, photoacoustic technique, photothermal infrared radiometry.

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[PTP-165] Photobaric and photothermal analysis of acoustic waves irradiation effect in the photosynthetic activity in aquatic liriium plants.

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The main objective of photosynthesis is the production of energy necessary for the physical development of the plant. The general process consists in the oxidation of water (removal of electrons with release of oxygen as a by-product) and reduction of CO₂ for the formation of organic compounds such as carbohydrates [1]. The modulated laser light absorbed by the plant leaf is first used in the photosynthetic process which gives rise as one of its products the emission of O₂. The Time-resolved Photoacoustic Technique (PA-*t*), allows you to make measurements “*in vivo*” and “*in situ*”, non-invasive and non-destructive on aquatic liriium leaves, in order to monitor the evolution of oxygen through the photothermal and photobaric contributions to the photoacoustic signal of irradiated aquatic liriium samples [2]. This work uses the PA-*t* technique as a tool to monitor the photosynthetic activity as a complement to the analysis of optical absorption response using photoacoustic spectroscopy. Aquatic liriium (*Eichhornia crassipes*) plants were exposed to sonic irradiation, using a frequency of 4 kHz and 5 W of power in order to analyze the effect of different exposure times on the plants. Irradiations were carried out for 1, 3, 5 and 7 hours. The results show a significant decrease in both photobaric and photothermal contributions at the passage of the days after irradiation, in particular at 12 days. The fall of the photobaric step show the decrease in the amount of oxygen emission of the photosynthetic process and the significant decrease in intensity of the photothermal contribution, which is caused by the structural change of the leaf resulting from the cavitation mechanism. These results show the utility of the sonic irradiation, as well as, of the photosynthesis monitoring by means of the photoacoustic technique, for the elaboration and establishment of methodologies in the control of this



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aquatic plant, whose propagation causes many consequences extremely unfavorable for the environment, as well as for the diverse human activities that are developed in the bodies of water in the tropical and sub-tropical regions of the world.

Keyword: Photoacoustic technique, photobaric, photothermal, sound irradiation, aquatic liriium.

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[PTP-287] Study of the optical properties of sugar cane leaves using photoacoustic spectroscopy and multispectral photography

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This work it has focused on the optical characterization of sugar cane leaves. We have used the photoacoustic spectroscopy (PAS) technique in order to obtain the optical properties of these biological samples. The absorption spectrum of the samples has been taken using the phase separation of the photoacoustic signal in order to distinguish between that coming from the waxy layer (cuticle) of the leaves and the other one coming from the upper epidermis. The samples under study have been leaves of sugar cane taken from small plants growth in laboratory. The spectra of leaves of sugar cane have been taken periodically in order to do a follow up of their conditions after became infected with a kind of microscopic fungus (*Curvularia* spp). We have also taken the photoacoustic absorption spectrum of the isolated fungus. We have extended our study about the evolution of the infection of microorganisms on leaves using multispectral photography in order to get a scaling in the fungi detection based on the results of the PAS technique.



[PTP-305] Design of bragg reflectors based in porous silicon assisted by photoacoustic technique

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The Porous Silicon (PS) is a useful material to make heterostructure or multi-layered systems for optoelectronic devices. One of the most common systems based on a multilayer system by PS 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, this route making the PS layers with variables properties because it depends on of multiple parameters during the etching process and the operator (experimentator) skills. In this work, it used an effective medium theory to calculate the refractive index of the layers, and it was simulated the optical response of the heterostructure. This procedure was made for design a specific DBR. The photoacoustic technique is useful for monitoring in situ the PS multilayer formation [1] 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. It was simulated reflectance function, and it was used for simulating the photoacoustic signal profile that the DBR must have. This theoretical design was carried out using a photoacoustic technique for monitoring in situ the PS multilayer formation by the controlled way and to guarantee the quality of the DBR in an attempt to reproduce the simulated photoacoustic profile. The amplitude and shape of the photoacoustic signal recorded during the PS formation contain information about the thickness and porosity [2] of the every single layer. This work represents a methodology to design and perform heterostructures based on PS like Bragg reflectors that allow that there are highly reproducible.

Keywords: Porous Silicon, Bragg Reflectors, Photoacoustic

References:



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RENEWABLE ENERGY: SOLAR CELLS AND MATERIALS (RWE)

Chairmen: Mario Fidel García Sánchez (UPIITA-IPN)



[RWE-32] semitransparent CdTe solar cells deposited by CSVT technique

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The semitransparent solar cells integrated in the architecture of buildings, is considered the technological solution to the problem that entails the use of extensive areas of earth, derived from the exponential development of the photovoltaic installations. In particular ultra-thin solar cell technology and laser scribing, to create light transmission zones in conventional cells, are the two current trends for the use of semitransparent cells in buildings and automobiles. The CdTe is considered as one of the best alternatives for the application in semitransparent solar cells. The techniques of sputtering and close space vapor transport (CSVT) are the best potential in this new application.

In the present work the advances obtained in the processing of semitransparent solar cells in the ESFM-IPN

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[RWE-176] Biodiesel production by direct transesterification using heterogeneous catalysts from ricinus communis seeds

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Nowadays, biodiesel production has emerged as one alternative fuel produced from vegetable oils and/or animal fats. Biodiesel 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 *sodium zirconate* (Na_2ZrO_3) was evaluated in biodiesel production from *ricinus communis seeds* using the direct transesterification method (one-vessel process) the heterogeneous catalyst such as *sodium zirconate* was synthesized via a solid-state method. The catalyst was characterized using X-ray diffraction, scanning electron microscopy and N_2 adsorption. The influence of some parameters was investigated, such as the reactant concentrations (molar ratios), catalyst percentage, reaction time, temperature and re-use of the catalyst. The direct transesterification reaction was performed by extracting directly from seeds with methanol obtaining biodiesel in 4 h of reaction time and yields of ~99%. The biodiesel characterization was carried out using infrared spectroscopy with Fourier transform and proton nuclear magnetic resonance. The direct transesterification method has shown that the reaction *in-situ* can be a good alternative to obtain higher purity biodiesel, facilitates the oil extraction from the seeds and the transesterification reaction without two different processes.



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[RWE-216] “Synthesis and characterization of composites based on bismuth oxides Bi₂O₃-Li₂O mechanically mixed with LiFePO₄ as cathodic material 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 bismuth oxides shows a high theoretical specific capacity between 274-530 mAh/g depends on the phase. The oxides were prepared via ceramic synthesis method. However, poor reversibility of these oxides limits the application of them in lithium ion cells as the active material in the positive electrode. In this work, we propose to use the composite form for lithium bismuth oxides (Li₃BiO₄, Li₅BiO₅ and Li₇BiO₆) in a mechanically mixed with LiFePO₄ (commercial reagent), for increase the reversibility and keep a high specific capacity.

We thank to the Fondo Sectorial CONACyT Secretaría de DEnergía-Sustentabilidad Energética for generous support to this research. I.C. Romero Ibarra acknowledges the SIP-IPN Project 20170488 and the “Red de Almacenamiento de Energía CONACyT”



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[RWE-224] Reactor design for biodiesel production based on physicochemical properties of transesterification reaction.

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Environmental Pollution is a worldwide problem caused for the use of fossil fuels in areas as energy production and transportation. It is necessary find a partial or total substitute to the fossil fuels that present the same or better properties than conventional fuels. One of these substitutes can be biodiesel, which have notorious advantages compared with conventional diesel. Biodiesel is obtained from vegetable oils or animal fats in presence of a catalyst. Biodiesel is a sustainable, renewable, non-toxic, biodegradable diesel fuel substitute that can be employed in current diesel infrastructure without major modification to the engines. In this work, we use waste oil to produce biodiesel. In this way, we boost garbage's revaluation of oil into products with value added and avoid to the pollution caused by the management of this type of waste. The optimal conditions to produce biodiesel by homogeneous transesterification were determined experimentally. Parameters as temperature, catalyst concentration, waste oil-methanol molar ratio, viscosity and density (for both, oil and biodiesel) were evaluated. This information is used to calculated mechanicals parameters for a design of a pilot-level reactor emphasizing the system of agitation and materials selection.

We thank to SECITI/065/2016 project "Manejo integral de residuos urbanos para la obtención de biocombustibles y otros productos de valor agregado en el marco del programa basura cero de la Ciudad de México", and "Laboratorio Nacional de Biocombustibles IPN".



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[RWE-281] Nanocomposite polymer electrolytes with potential applications for Li-ion batteries.

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The research and development of new materials for energy storage applications have become critical to meet the technological and environmental requirements demanded for sustainable power sources. This field is generating many exciting new materials with novel properties. Nanocomposites are very interesting for their electronic and charge transport properties. In this work novel poly(poly(ethylenglycol)methacrylate) (pPEGMA) nanocomposites electrolytes (NE) based on montmorillonite (MMT) with a lithium salt and an ionic liquid are synthesized. During the synthesis the sonication technique is successfully used to introduce the fillers into the polymer matrix to provide uniform dispersion in order to ensure a polymer amorphous structure. The influence of the inorganic particle content (1, 3 and 5wt. %) is discussed in terms of their thermal and morphological properties. SEM and TEM techniques reveal an efficient embedding of the fillers into pPEGMA. These materials present adequate morphological, thermal and mechanical properties and a significant enhancement of Li⁺ ion conductivity for materials to be considered as potential nanocomposite electrolyte for Li-ion batteries.



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[RWE-289] Scaling of photovoltaic solar modules to areas of 25 and 100 cm-square based on thin film technologies of CdS/CdTe

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Currently, there are technologies for the large-scale production of CdS/CdTe thin film photovoltaic modules. These devices, are already produced in commercial modules. In First Solar¹, they have been able to manufacture modules with photovoltaic conversion efficiencies of 16.3%. This company, to the best of our knowledge, uses the vapor transport technique in the near space (CSS) for the CdTe deposit and a chemical bath deposit variant for the CdS films. Activation (chlorination) of the cells or modulus is carried out by means of an aqueous solution of CdCl₂ sprayed onto the CdTe film and subsequently treated in oven at temperatures close to 400 °C.

In recent years, Romeo et al² developed a new method of chlorination by heat treatment in an atmosphere of a gas containing chlorine.

At this conference, we present our results of high efficiency solar cells (greater than 14%) based on thin films of CdS/CdTe. In these solar cells, are used ZnO thin films deposited by sputtering as buffer, CdS (window layer) and Cu/Mo bilayer are used as a back contact. The CdTe absorbent film is deposited by sublimation in near-space (CSS) on a substrate at a low temperature (500 °C) and the process of activation (chlorination) is carried out with Freon gas mixed with another gas at 400 °C. Cells with more than 14% efficiency are obtained with this procedure without special treatment to the CdS film³.

In the Si-based learning curve, it is pointed out that once small area solar cells with more than 14% efficiency can be manufactured, the technology is ripe to manufacture larger area modules. Based on this learning curve, we apply it to the case of CdTe/CdS thin films. As validation, our recent results are presented scaling processes areas for 25 and 100 cm²



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[RWE-307] Study of CdO thin film influence in CdTe solar cells photovoltaic efficiency

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Polycrystalline CdO thin films have been applied successfully on CdS/CdTe photovoltaic devices. CdO thin films was obtained by chemical bath deposition technique (CBD) using CdCl₂ (0.4M) and NH₄OH (5.3 M) as precursor solutions, H₂O₂ at 30% was used as reducing agent, the films growth was carried out to 85±2°C during 30 min or 80 min. CdO thin films were thermally annealed on air atmosphere at 400°C during 60 minutes. FTO substrates used were treated in HCl (0.1 M). CdO films obtained have around 140 nm when using 80 min, and 60 nm when using 30 min deposition time. Electrical, morphological, optical and structural properties were studied before and after thermal treatment. Three devices were obtained, one of them was a CdTe standard solar cell, and others two adding CdO thin film before and after CdS thin film. Final conversion efficiency increasing from 3% to 7% when CdO was added before CdS thin film.

Keywords — CdO, chemical bath deposition, solar cells.

Acknowledgements

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[RWE-308] The effects of ZrO₂ on the electrocatalysis to yield active chlorine species on Sb₂O₅-doped Ti/RuO₂ anodes

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Dimensionally Stable Anodes (Sb₂O₅-doped Ti/RuO₂-ZrO₂) are synthesized at four different Zr/Ru molar ratios using the Pechini method to account for the effects of ZrO₂ content on the active chlorine formation. X-ray diffraction for ternary catalysts reveal co-deposited phases consisting of a tetragonal crystalline structure (*P4₂/mnm*) for RuO₂, and two phases corresponding to monoclinic (*P2/m*) and tetragonal (*P4₂/mnm*) crystalline structures for ZrO₂. SEM micrographs show that ZrO₂ alters grain growth and film morphology as its content is increased. Electrochemical tests performed in 1 mol L⁻¹ H₂SO₄ and 0.1 mol L⁻¹ NaCl demonstrate that the kinetic rate to perform the oxygen evolution reaction (OER) decreases with the simultaneous augment of ZrO₂ and Sb₂O₅ compositions in the ternary anode, while in the ZrO₂ absence, Sb₂O₅ catalyzes the OER (Ti/SbRu) compared to the Ti/Ru and ternary electrodes. Although the chlorine evolution reaction (CER) preferentially occurs by the suppression of OER in chloride media, the CER rate mainly increases due to the rise of the ZrO₂ content. This finding is corroborated with an iodometric method using UV-Vis spectroscopy, which shows that the electro-generation capacity to form active chlorine species is significantly enhanced when ZrO₂ is added, compared to Ti/RuO₂ and Sb₂O₅ doped Ti/RuO₂ materials. Accelerated life tests conducted with all catalysts indicate that all ternary anodes present failure times considerably longer than Ti/Ru, Ti/SbRu and Ti/RuZr electrodes, suggesting a stability enhancement due to the combined presence of Sb and Zr species.

Keywords: DSA, microstructure, oxygen evolution reaction, chlorine evolution reaction



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[RWE-309] GaN Nanostructures based solar cells

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Intensive use of fossil fuels and their undesirable impact on the environment have generated a great interest in the development of safe, reliable and sustainable sources of energy. Effective use of solar radiation by solar cells has been one of the topics of greater interest due to the high irradiance that is intercepted by the earth's surface, solar panels durability and multiple methods of manufacture of these. The third generation of solar cells include multilayers of amorphous and crystalline semiconductors which has allowed to increase the efficiency of carrier generation around 45% the last 5 years. In this work is presented a comparative design of GaN nanostructured-based solar cells. We review the nanostructuring of materials (quantum wells, dots and wires), the carrier dynamics in low dimensional structures and the impact on the internal quantum efficiency. Devices based on GaN/InGaN multiple quantum wells can absorb photons whose energy is in the wavelength range (300-1200 nm) of the solar radiation and the internal electric field separates the photo-generated carriers reducing optical recombination losses. Reflections at the multiple interfaces of these structures increase optical absorption and generate important interference effects, which could increase internal quantum efficiency [1]. On the other hand, quantum dots-based solar cells have an intermediate energy band formed by levels of electrons in the quantum dots which allows multiphotonic absorption by tuning the size and shape of the dots. Finally, the use of vertical nanocolumns improves the radiation absorption due to the dispersion of light, which acts as anti-reflective layer for long wavelengths, one-dimensional carrier conduction also occurs and the polarization of emitted light is influenced by vertical alignment of the nanocolumns.

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[RWE-5] An absorbent material based upon P3HT: PCBM CdS/TiO₂ for photovoltaic solar cells application

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Organic solar cells are placed in the third generation of solar cells solar cells. They are a promising alternative with a higher cost-benefit over silicol cells such as low fabrication cost and eco friendliness with the posibility of use them in industrial aplicacion e.g. roll-to-roll printing. In the present work, we proposed a novel absorbent material based on a conductive polymer and semiconductor nanoparticles (Nps). We proposed to improve the optical and electrical properties of an absorbent material based upon a: donor/acceptor system: regioregular semiconducting polymer (P3HT), and, a fullerene derivative (PCBM). Improving was made by mixing the donor/acceptor system with semiconducting cadmium sulfide and titanium dioxide nanoparticles (CdS/TiO₂ Nps). A methodology for obtaining semiconductor CdS Nps from Chemical Bath Deposition (CBD) and co-precipitation was carried on. Thin films with different mixtures of P3HT:PCBM: CdS Nps were prepared by the spin-coating technique. The optical and electrical properties of these thin films were characterized by X Ray diffraction, UV-Vis spectroscopy and Four Point Probe technique, respectively, and its correlation with the preparation parameters was studied.

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Keywords: P3HT: PCBM, organic solar cell, Cds/TiO₂ Nps



[RWE-29] CdS/PbS thin films deposited by chemical bath deposition on glass and flexible substrates for photovoltaic applications

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The developed of photovoltaic devices based on CdS / PbS semiconductors offer an alternative to silicon, which require to apply high temperatures to synthesize, generating a high cost in the production to apply this material in the electronic. Chalcogenide semiconductors offer the prospect, ease application in large areas semiconductor devices, high stability, low cost, and high drive currents. Using chemical bath, large-scale photovoltaic devices can be produced; it is not necessary high-tech tools neither working to elevated temperatures reducing the production costs. The present work reports the preparation of CdS/PbS thin films deposited by chemical bath deposition (CBD) on glass/ITO and PEN/ITO commercially transparent conductive substrates; chemically deposited n-type CdS (92 to 113nm thickness) and absorbed layer of p-type PbS (36 to 250 nm thickness). The optical properties were analyzed by UV-Vis spectroscopy. The microstructure of the films was studied by scanning electron microscopy and X-Ray diffraction. The roughness for the films was determinate by atomic force microscopy. After films semiconductor depositions 100 nm of aluminum was deposited. The electrical behavior of the photovoltaic device based on chalcogenide semiconductors as deposited and annealed was determinate with measurements determining the open circuit voltage, short-circuit current density and J-V under solar radiation. This is a first development to photovoltaic dispositive where the semiconductors were deposited at low temperature on solid and flexible substrates (43 °C) by solution process.



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[RWE-51] Effect on the deposition parameters of lead sulfide thin films by SILAR method as semiconductor material for solar cells at low temperature

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Lead sulfide (PbS) is a chalcogenide p-type semiconductor material, and it has been an excellent candidate for devices as photovoltaics in the research of solar cells. Lead sulfide thin films have been deposited by the SILAR method using chemical precursors as lead nitrate complexed with triethanolamine as cationic source and thioacetamide as anionic source. Several conditions have been varied as can be the immersion time on the precursors and rinsing time during the deposition cycles as well as the number of deposition cycles and a post cleaning on the formed thin film. Also, a variation in the pH of the cationic precursor was examined. Later, a cubic structure formation has been obtained and studied by XRD along with the determination of the crystallite size. The order of the optical transmittance and the band gap value were calculated from the UV-vis analysis. The morphology distribution was studied from SEM and the stoichiometry by XPS analysis. Measurements of current-voltage have been required to investigate the order of the dark electrical characteristics of the thin films and its potential application as an absorber layer for solar cells technology.

Keywords: Chalcogenides, lead sulfide, semiconductor material, successive ionic layer adsorption and reaction (SILAR) method.



[RWE-86] Chemical bath deposition and characterization OF CdSe thin films for photovoltaic applications

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By means of the chemical bath technique thin films of stoichiometric CdSe nanocrystal were prepared on glass substrates in the range 55 – 70 °C of temperature. The layers grow in the cubic zincblende crystalline phase with no preferred orientation. Firstly, Cd(OH)₂ films were deposited on glass substrates, after, these films were immersed in a growing solution prepared by dissolution of Se in hydroxymethane sulfinic acid to obtain CdSe. The average size of nanoparticles lies in the range 10 – 15 nm and the thickness of the films is in the interval 70 – 100 nm. Raman spectroscopy reveals the LO phonon mode and the first overtone of the CdSe semiconductor. In general, the analysis of the CdSe films indicates that the material have good structural and optical properties to be used in terrestrial solar cells preparation.



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**[RWE-90] ZnO nanoparticles confined within SiO₂ matrix, obtained by reactive Sputtering,
with application on photovoltaic solar cells**

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ZnO nanoparticles have shown rectifying behavior, which is useful in the photon energy conversion to electric energy on solar cell structures. In this work ZnO particles were synthesized and confined within a SiO₂ matrix by the radiofrequency assisted (RF) cathodic erosion method using an oxygen rich working plasma. A sequential deposition of SiO₂/Zn/SiO₂ films were produced at 400 °C. This process has the advantage of been cheaper and straightforward compared with others procedures to obtain ZnO nanoparticles. A SiO₂ buffer layer was deposited on substrates to obtain a rough surface which will serve as a nanometric template for the metallic Zn particles. These particles were oxidized during the deposition of a second layer of SiO₂, which covered them completely allowing the production and confinement of ZnO nanoparticles. The samples were characterized by TEM, SEM, XPS, SIMS, UV-Vis spectroscopy and IvsV measurements.. The results of the chemical, structural and electronic properties indicated the successful production of ZnO nanoparticles with transport properties showing a rectifying behavior which can be applied on solar cell to improve the efficiency of solar cells.



[RWE-101] analysis of the optoelectronic and structural properties of a DSSC with union ZnO / TiO₂ and its effect on conversion efficiency.

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The growing demand for energy and the large amount of waste generated worldwide makes the current energy model unfeasible where non-renewable sources of energy are paramount. There is no doubt that a new paradigm is required where the supply of energy for global development is based on environmentally friendly, renewable, economic and for all sources. Solar energy still presents challenges in the technological and economic aspects that can only be solved as the arduous task of the researcher is bearing fruit.

Nanoparticles of zinc oxide and titanium dioxide were synthesized by precipitation and forced hydrolysis methods, respectively. The influence of the optical, electronic, structural and electrochemical properties of the ZnO / TiO₂ bond on the performance of photovoltaic efficiency was studied. The synthesized samples have been characterized structurally, morphologically, optically and electrochemically using XRD, MEB, UV - Vis spectroscopy and electrochemical impedance and their application in a dye - sensitized solar cell (DSSC) based on the N719.

The average size of the zinc oxide crystal is in the range of 17-24 nm while the average size of the titanium dioxide crystal is between 50-60 nm. The optical band gap of these materials is 3.5% lower than that reported for zinc oxide and 1.5% lower for titanium dioxide. The DSSC based on N719 showed an increase in conversion efficiency (50%) due to the interfacial structural change in ZnO / TiO₂ binding.

Increasing the conversion efficiency of photovoltaic cells translates as a better use of solar energy, as long as the costs of materials and processes involved are cheap and their toxicity is relevant.



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[RWE-104] Organic Selective Coatings for applications in Solar Thermal Energy

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Organic Selective Coatings thin films were prepared by an efficient electrolytic procedure, a simple electrolytic undivided cell was designed using copper and tin plates as electrodes, recycled water and a 6 V battery provided the required energy. The system was characterized as a selective absorber surface and its solar selectivity parameters, solar absorptance (α), and thermal emittance (ϵ) were evaluated. The solar parameters of such a system were mostly affected by the thickness and phase composition of the film. Interestingly, the best solar parameters ($\alpha = 83.9\%$ and $\epsilon = 0.03$) were associated to the thinnest films.



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[RWE-162] Synthesis and characterization of halogenated hybrid perovskites ($\text{CH}_3\text{CN}_3\text{PbX}_3$ with $\text{X}=\text{Br}$ or I) for application in solar cells

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Recent studies have reported perovskite-based solar cells with promising photovoltaic efficiencies, useful for the manufacture of organic and hybrid devices that will be used in daily life. These devices employ a crystalline and well-oriented thin film of organo-lead perovskite as both light absorber and carrier conductor, deposited on e.g. glass slide or ITO substrate through a simple spin-coating process. Our interest in organo-lead perovskite is because they exhibit a direct bandgap and a broad range of light absorption covering the visible to near-infrared spectrum as well as a high extinction coefficient. All-solid-state solar cells with organo-lead perovskite as light absorber, exhibit high power conversion efficiencies (PCEs) of great potential in real applications. Perovskite successfully acts as both light harvester and hole conductor. In particular, dual function (i.e., light absorber and carrier conductor) active layers are widely used in fabricating polymer-, organic-, and inorganic-based solar cells. This work presents a detailed description of $\text{CH}_3\text{CN}_3\text{PbX}_3$ with $\text{X}=\text{Br}$ or I type perovskite synthesis, thin films preparation, XPS chemical analyses, UV optical study, XRD structural and AFM morphological characterization; current work is in progress concerning to the development of perovskite-sensitized with conjugated polymers, which preliminary results will also be presented.



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[RWE-164] Ultra-thin solar cells of CdS/CdTe as processed by the magneto-planar-sputtering (MPS) technique.

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Ultra-thin solar cells of CdS/CdTe are one of the most promising innovations to be used as window generating electricity in sustainable and architectural buildings, and sun-roof for cars, among other applications [1]. On the other hand, the impact of transparent and conductive 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. Usually they consist on wide gap degenerately doped oxides, and thus, they are known as Transparent Conductive Oxides (TCO) [2]. Fluorine-doped SnO₂ (FTO) is the most commonly TCO used in commercial CdTe-solar cells, as it can be deposited during glass manufacturing and it is in general inert to subsequent processing [3]. Usually, a double layer structure is used, which consist on a highly-doped primary layer and a nominally-undoped 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 [4]. By MPS technique it is possible 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 solar cells. These three materials, SnO₂, 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 project is to develop ultra-thin solar cells of CdS/CdTe with a buffer layer of SnO₂ by the MPS technique with different contacts. Our processed heterostructures were characterized by XRD, UV-Vis and electrical measurements. We present the materials characterization results as well as PV-performance of our solar cells.



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[RWE-200] Solar Cells Glass/ITO/CdS/CdTe/Ag Tandem Thin Films by Chemical Bath
Deposition and Serigraphy

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This work is focused in the study of solar cells type: glass/ITO/CdS/CdTe/Silver. The study of more options to fix the multilayer to improve the energetic efficiency and the cost reduction in the cells is a continuous search. Recently, the synthesis methods for the CdTe is by sputtering, evaporation and pulsed laser. Our synthesis for the CdTe is by using a serigraphy method which is a low cost method with a high area of work and easy to apply. One of the applications of the thin layer of the CdTe is like a semiconductor type p which is an absorbent material. The semiconductor type n which is a window material is the CdS. The ITO is the front contact and the silver is the rear contact. Our synthesis for the CdS is by chemical bath deposition. The technique of characterization was: UV-VIS, XRD, I Vs V. The results obtained by UV-VIS was a CdS band gap of 2.42 eV and a CdTe band gap of 1.5 eV. The result of the XRD of the CdTe presents signals which identify with the Miller index 110, 220, 311, 400, 331, 442, 511 where the preferential peak ends to be the 110. This was identified with the PDF 15-0770 of the CdTe. The result of the C vs V we obtain a maximum power of 6.8×10^{-11} W, with an efficiency less than 1 % of the solar cell. In conclusion we obtain a solar cell reproducible starting from the serigraphy synthesis and CBD. It is planned to do a heat treatment to the CdS and to the bilayer of the CdS/CdTe to improve the contact between both semiconductors and the silver contacts to improve the job function between the CdTe and the silver. The porosity of the material CdTe is an important factor to increase the efficiency of the solar cell.

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[SCD-59] Esparcimiento de luz en tejidos biológicos

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Cuando una onda de luz interactúa con la materia en particular tejido biológico una parte se refleja y otra se transmite. La parte que penetra interactúa con moléculas dando lugar a la absorción, esparcimiento y remisión de energía a otra longitud de onda (fluorescencia). El fenómeno de esparcimiento supone un cambio en la dirección y la redistribución de la energía. Este tipo de problemas son muy complicados por lo que se usan dos tipos de teorías: la teoría analítica (ecuaciones de Maxwell) y la teoría del transporte (Ecuación de Transferencia Radiactiva (ETR)).

La ETR es una ecuación íntegro-diferencial para la intensidad específica que describe la propagación de la intensidad de la luz en el tejido biológico y emplea como parámetros las propiedades ópticas del medio (coeficientes de absorción y de esparcimiento, y el factor de anisotropía). Sin embargo esta ecuación no tiene solución analítica en el caso general por lo que se utiliza el método de Monte Carlo, que simula la trayectoria de fotones durante su interacción con los centros de absorción y esparcimiento.



[SCD-95] El sol es una fuente inagotable de energía: ¿cómo usarla? *

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Es aceptado que la vida en la tierra depende completamente de la evolución estelar del sol. La formación de la tierra y sus características han sido determinadas por esta estrella. La evolución estelar del sol permite estimar que sus parámetros físicos actuales perduraran otros 5000 millones de años; pero, ¿la humanidad será capaz de mantener el hábitat terrestre durante este tiempo?. Para que la pregunta anterior tenga una respuesta positiva es necesario un desarrollo tecnológico amigable para toda la humanidad.

La creciente demanda de energía genera graves riesgos que impiden un desarrollo sustentable de la humanidad por lo que es necesario contar con fuentes de energía que generen un impacto mínimo sobre el ecosistema terrestre. La fuente natural de energía de la tierra es el sol y sería deseable aprovechar la gran cantidad de energía que incide diariamente sobre la tierra para generar electricidad [1]. Sin embargo, existen otras alternativas para aprovechar la energía solar. En esta plática presentaremos algunas de las alternativas propuestas haciendo énfasis en los generadores de vapor por calentamiento de capas superficiales de agua.

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*: Trabajo apoyado parcialmente CONACyT.



[SCD-114] Electrónica Moderna con la Tecnología Nacional PolyMEMS INAOE

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"Internet de las cosas" (Internet of Things) representa una fase más de desarrollo dentro de la tecnología y nuestro entorno. 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 con aplicaciones interdisciplinarias a partir de la ya consolidada industria de los circuitos integrados (CI's) 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 las señales eléctricas (Sensores inteligentes). Desde sus inicios, los MEMS presentaron aplicaciones restringidas hacia áreas de electromecánica: pero posteriormente, con el desarrollo de diversos materiales compatibles con los chips, los Microsistemas se han diversificado hacia áreas tales como biología, óptica, fluídica, medicina, magnetismo, entre otras, y en Internet de las cosas.

Hasta la fecha, los prototipos MEMS totalmente integrados con amplio uso industrial son enfocados hacia aplicaciones específicas, algunos ejemplo son los acelerómetros para protección en colisiones, los cartuchos para inyección de tinta en las impresoras y recientemente los circuitos para control de frecuencia en sistemas temporizadores.

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 estudio 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 micro-maquinados



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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, utilizando la Tecnología nacional PolyMEMS INAOE[®], los cuales por sus características de innovación y bajo costo resultan de alto interés público.



[SCD-213] Depósito de TiN, TiTaN y TiTaAlN mediante pulverización catódica

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La modificación superficial por medio del depósito de películas delgadas es un proceso industrial relevante, empleado para proteger el sustrato de la corrosión, el desgaste y la fatiga, entre otros fenómenos relacionados con el daño superficial. Hoy en día, en ingeniería de superficies, los procesos de Deposición Física en fase de Vapor (PVD, por sus siglas en inglés) son ampliamente usados para mejorar las propiedades mecánicas, ópticas y eléctricas, entre otras. Esta técnica proporciona amplia flexibilidad para diseñar películas con composición química y microestructura específicas, y así, al establecer y controlar los diferentes parámetros del proceso, es posible obtener recubrimientos con las propiedades requeridas. Dentro de las técnicas de PVD basadas en la pulverización de un blanco y asistidas por plasma para mejorar la calidad de los recubrimientos, se encuentran diferentes variaciones en cuanto a la aplicación de potencia al sistema: corriente directa (DCMS: Direct Current Magnetron Sputtering), corriente directa pulsada (PDCMS), potencial de elevado impulso (HIPIMS). En el presente estudio se ha logrado depositar nitruros de titanio dopados con tantalio y aluminio empleando estos modos de potencia. En éste, el modo HIPIMS resulta especialmente interesante porque los pulsos de elevada potencia son sincronizados con los pulsos de polarización del sustrato (pieza a recubrir), a la vez que combina con corriente directa mientras, es así como se logra erosionar eficientemente tres (3) elementos al tiempo para obtener recubrimientos de TiTaN y TiTaAlN. Es así como se ha conseguido reducir el contenido de oxígeno en estos recubrimientos y, por ende, incrementar su densidad, mejorando sus propiedades mecánicas y eléctricas, entre otras. Mediante ensayos de polarización potenciodinámica se ha estudiado la resistencia a la corrosión de estos recubrimientos en un ambiente salado de NaCl al 3.5% y temperatura ambiente. La composición química ha sido evaluada mediante



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espectroscopía de rayos X (XPS) empleando modo angular (XPS-Sputter). Los resultados obtenidos han sido correlacionados y comparados en función del modo de potencia empleado.



[SCD-226] El hidrógeno como fuente energética renovable

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El hidrógeno aparece en la actualidad como una de las fuentes de energía renovables, aunque se conoce muy poco sobre ella. 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. Entre estos aspectos 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-265] ¿Cómo incrementar la sinergia de la sociedad desde el punto de vista para la fabricación de materiales cerámicos?

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Las cerámicas son fuertes, rígidas y quebradizas, pero sus propiedades son afectadas dramáticamente no sólo por las características de las materias primas y también por las condiciones de su proceso de fabricación. Del mismo modo, la motivación y el carácter de una persona juega un papel muy importante en el desarrollo de la sociedad, además en la interacción de persona a persona (P2P), la relación es el punto clave para desarrollar la sinergia social. Es obvio que la relación humana en la sociedad es más compleja que la preparación de materiales cerámicos, pero indudablemente los humanos siempre se han aprendido de fenómenos naturales. Por lo tanto, quiero contribuir para aumentar la sinergia humana desde el punto de vista del proceso de materiales cerámicos. En este contexto, propongo una forma de aumentar la competitividad del grupo comparando el comportamiento humano en la sociedad con el comportamiento de partículas y grano en materiales cerámicos. Se discute el rol de las propiedades de las partículas y los granos, las interacciones superficiales y los límites de los granos, en el proceso de los materiales cerámicos comparando con la conducta de una persona, relaciones humanas y sinergia del grupo. La interacción P2P fuerte y rígida es indispensable para aumentar la competitividad de los grupos en una sociedad globalizada. Se discute también el concepto más importante de las relaciones entre fractales y holón como reflexión en la formación de una sociedad estable. En esta presentación, se introduce la importancia de P2P, y se discute la diferencia cultural sobre el concepto de crisis entre las sociedades japonesas y mexicanas con el tema de ¿cómo superar las crisis? También se discute los conceptos sobre los errores ¿cómo enfrentar los errores? Tomando en la consideración de la dificultad en la fabricación de materiales cerámicos, en donde se requiere acomodar y unir los granos con sinergia, se presenta ¿cómo formar la sociedad competitiva con la sinergia enfrentando los dos paradigmas inevitables, el síndrome del estudiante y la ley de Parkinson?



[SCD-283] Como aprovechar la energía solar, que es casi....infinita

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Se ofrecerá, una plática amena y divertida sobre la Energía Solar utilizando jugentes y dispositivos simples. Actualmente, hay dos formas muy populares para cosechar la Energía Solar. Una es la Energía Solar Fotovoltica (ESF) en la cual se utilizan dispositivos llamados celdas solares, que convierten la luz del sol en energía eléctrica. La otra es la Energía Solar Fototermica (ESFT) en la cual se utiliza una parte de la luz solar que no es visible al ojo humano, llamada infra-rojo para convertirla en calor.

Existen muchos otros procesos que son generados por la Energía Solar. Se resalta, el más importante: la existencia de la vida y su sobrevivencia en la Tierra. De este y otros, se darán ejemplos, en una forma sencilla y simple, intentando que se mantenga la parte fundamental del proceso solar en cuestión.



[SCD-291] Calor y temperatura, dos conceptos estrechamente relacionados pero diferentes.

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Como parte del que hacer científico y en la vida cotidiana estamos acostumbrados al uso de los términos calor y temperatura, palabras que hemos hecho nuestras y que con el uso hemos modificado su significado ya que simplemente representan ideas poco claras. No obstante, hasta el primer cuarto del siglo XIX, se imaginaba al calor como un fluido indestructible que pasaba de un cuerpo a otro, aumentando o disminuyendo la temperatura; se le denominaba “calórico”. Para poder escalear esta confusión es necesario identificar y precisar tres conceptos: energía, su transferencia y temperatura.

La energía es “algo” que se conserva y que le da la capacidad a los sistemas para realizar un trabajo. El concepto de calor se puede describir como un flujo de energía que se desplaza desde un objeto de mayor temperatura a otro que está más “frío”. Así, entre ambos objetos se llegaría a un estado de equilibrio térmico.

El "calor" presenta dos aspectos que son esenciales. Primero, es una forma de energía. Segundo, es energía en tránsito debido, exclusivamente, a una diferencia de temperaturas. Por lo que el calor como tal es una forma de transferencia de energía, refiriéndose a la energía total del movimiento molecular en un cuerpo, que depende de la velocidad de las partículas, de su número, de su tamaño y de su tipo. En contraste, la temperatura es la medida de dicha energía que no depende del tamaño, ni del número ni del tipo de partículas. Calor y temperatura, estos dos conceptos se confunden frecuentemente entre sí, utilizándose de manera errónea. Si bien están estrechamente relacionados, no son idénticos. Queda establecido que, mientras el calor es una forma de transferencia de energía, la temperatura es la cualidad que determina la dirección del flujo calórico y que cuantifica la energía presente en un sistema.



[SCD-292] Rayos X, los detectives de la materia

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Desde que Wilhelm Conrad Röntgen en 1895 descubrió que, una radiación desconocida era capaz de mostrarnos el interior del cuerpo humano, las aplicaciones para estos “*rayos X*” no han parado. Este tipo de radiación que se forma cuando un haz de electrones se frena contra un metal, es capaz de interactuar con los materiales y así ayudarnos a descifrar su estructura y composición. Los rayos X son ampliamente utilizados, desde los dentistas que a quienes ayudan a observar el avance de una caries, hasta los científicos en el *Linac Coherent Light Source (LCLS, Stanford)* que pueden fotografiar a 120x por segundo las estructuras biológicas y las propiedades de la materia,

En este trabajo se aborda de una forma breve el origen de la teoría atómica, los descubrimientos que dieron origen al concepto de átomo, el efecto fotoeléctrico descrito por Heinrich Hertz y explicado de forma teórica por Albert Einstein y el papel de los Rayos X en la generación de este conocimiento.

Por último, se muestra un caso práctico del uso de la espectroscopia fotoelectrónica y cómo esta nos ayuda a entender el universo nanométrico de los materiales, los mecanismos de reacción, las especies intermediarias y cómo esta información sirve para diseñar procesos que sean más eficientes y a eliminar aquellos que no son necesarios.



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[SCD-301] El láser: de la microcirugía a la guerra de las galaxias

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Los láseres tienen poco más de cincuenta años. En este periodo de tiempo han pasado de ser “*una solución en busca de un problema*” a ser herramientas fundamentales en muchos ámbitos de nuestra vida, hasta el punto de ser considerados como uno de los grandes inventos de la segunda mitad del Siglo XX. En esta conferencia mostraremos cómo funciona un láser, cuáles son sus propiedades fundamentales y por qué éstas los han convertido en herramientas tan versátiles como para ser utilizados en campos tan diversos como la medicina, la astronomía, las comunicaciones, el procesado industrial de materiales o la energía, entre otros.



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Semiconductors (SEM)

Chairmen: Maximo López López (CINVESTAV-DF)
Salvador Gallardo Hernández (CINVESTAV-DF)

SEM-ORAL SESSION



[SEM-83] Study of the passivation of InP@ZnS quantum dots.

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In recent years, the colloidal core/shell type InP@ZnS quantum dots (QDs) have generated great scientific interest because this type of nanoparticles contains two semiconductor materials in a single structure. The importance of this type of material is that the shell enables optical properties improvements such as quantum efficiency and shelf life, as well as providing a physical barrier between the optically active core and the surrounding medium, thereby generating the QDs are less sensitive to environmental changes, surface chemistry and photo-oxidation. In addition, the shell provides effective passivation of the surface states by increasing the photoluminescence response. This effect is a requirement for the use of quantum dots in applications as biological markers. In this work, we describe the synthesis and characterization of InP@ZnS QDs, using a single-step chemical synthesis method without injection of hot precursors, varying the concentration of indium myristate. Color variation of the InP@ZnS quantum dots from blue to yellow was found, indicating the formation of InP@ZnS core@shell structures. The absorption spectra of the InP@ZnS QDs have a main shoulder around 400nm, by means of this wavelength the band gap of the InP@ZnS QDs was determined. From the photoluminescence spectra we were able to observe the presence of quantum dots due to their emission peaks from 350 nm to 550 nm, as a consequence of the quantum confinement effect. The size and shape of the QDs were investigated using TEM, with sizes ranging between 1.8 nm and 4.2 nm in spherical shapes



[SEM-159] Growth and Characterization of cubic GaN doped with Mg by MBE

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GaN in metastable cubic phase is a promising material because has several advantages over its hexagonal counterpart. The first advantage is that no spontaneous and piezoelectric polarization is expected, and in addition due to its symmetry the mobility of the holes should be greater than those obtained for the hexagonal phase. Finally, because its smaller energy gap, less concentration of Indium is required to achieve the $\text{In}_x\text{Ga}_{1-x}\text{N}$ ternary alloys that emit in the green color.

Due to these advantages, it is important to study nitrides in cubic phase with the aim of developing semiconductor devices such as LEDs and photovoltaic devices. For these applications is essential to have "p" type films with hole concentrations in the range of 10^{17} to 10^{19} cm^{-3} , and moreover to achieving Ohmic contacts with low specific contact resistance a hole concentration of 10^{19} cm^{-3} is required.

Typically the hexagonal phase GaN has been doped with Mg. However, because the high ionization energy (approximately 200meV), low concentrations of holes have been observed. On the other hand, there are very few reports of the cubic phase GaN doped with Mg. To our knowledge, the state of the art is in the range of 5×10^{17} - $8 \times 10^{18} \text{ holes/cm}^3$ [1-4].



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Therefore in this work, we present our investigation on the growth of cubic GaN doped with Mg by molecular beam epitaxy (MBE), and the electrical, chemical and structural characterization by Hall, SIMS and XRD respectively.

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[SEM-249] Strain effects of GaAs/InGaAs heterostructures on the self-assembling of quantum dots by molecular beam epitaxy.

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Quantum dots (QDs) also known as zero-dimensional system have been investigated in the past years due to their unique physical and electronic properties. This kind of semiconductor devices have demonstrated to accomplish new requirements for high performance electronic-optoelectronic devices such as high efficiency LEDs, lasers, detectors, storage devices and/or solar cells of third generation, also they have achieved a decreasing size for these new devices, encouraging even more their interest in low dimensional systems.^[1, 3] However there are still some challenges to be overcome in order to reach the successful implementation of the QDs structures in common devices. Self-assembled quantum dots growth can be approached through the Stranski-Krastanov growth mode which is based on the lattice mismatch of two different materials, like InAs/GaAs, propitiating an increase of strain at the interface.
[2]

In this work the authors investigate the structural and optical properties effects by stress accumulated in the formation of self-assembled QDs by molecular beam epitaxy. The synthesis of InAs self-assembled QDs on GaAs / In_xGa_{1-x}As / GaAs / GaAs(100) heterostructures, varying the thickness in the last layer of GaAs (Σ) from 1.2 to 33 nm, this variation was performed in order to change the stress belonged to the QDs and/or the layer of the InGaAs quantum well (QW). It is observed that the moment of nucleation of QDs determined *in situ* by the changes in the intensity of reflection high energy electron diffraction (RHEED) patterns increases as Σ increases. As a consequence, the size and distribution of



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QDs changes dramatically: the QDs density decreases from $5.0 \times 10^{10} \text{QD}/\text{cm}^2$ to $1.2 \times 10^{10} \text{QD}/\text{cm}^2$, results determined by Atomic Force Microscopy (AFM). Also, there were performed High Resolution X Ray Diffraction (HRXRD), confirming that the InGaAs QW is strained as well, these results showed a shift in the curve assigned to the InGaAs layer, its respective analysis allow us to determine the incorporation in atomic concentration of Indium, letting us to calculate its lattice constant and its energy band gap, demonstrating that the lattice constant was increasing slightly but its band gap decreased as Σ increased. Similarly, we studied the transition energy levels by Photoluminescence (PL) and Photoreflectance (PR), observing a decreasing behavior in the energy gaps as Σ increased, concluding in evidences of stress in the different layers of the heterostructures.

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[SEM-255] Molecular beam epitaxy of Ga1-XXAs for PV devices.

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The development of new materials with improved electrical and optical properties has conducted to obtaining of high performance devices, sometimes with either increasing capacity, profitability, or velocity, depending on the specific application. For example, the ternary alloy GaNAs has been envisaged as a promissory material for photovoltaic applications. GaNAs is a material studied due to the formation of the so-called Interband, which is formed for splitting the conduction band into two sub-bands: a band called E + which is considered as the new conduction band and a band called E- whose position is inside the GaAs gap. The separation between E+ and E-, increases with the N concentration (N%) of the GaNaAs alloy. In this work, the optical and structural properties of GaNAs thin films grown by molecular beam epitaxy are studied as a function of deposition parameters like power of the RF source (P_{RF}), molecular N₂ flow (F_{N_2}) and arsenic beam equivalent pressure (P_{As}). The first set of samples were made at $F_{N_2}=0.1$ sccm and changing P_{RF} from 100W to 200W. Similar N% was estimated by HRXRD patterns. The results suggested that $P_{RF}=100W$ is sufficient to dissociate the entire F_{N_2} to atomic N. For another set of experiments P_{RF} was set at 150W, while F_{N_2} was varied from 0.2 to 0.3 sccm. We observed that N% increases with F_{N_2} from 0.52 to 0.64, indicating that 150W dissociates the entire F_{N_2} to atomic N. The third series was performed by increasing F_{N_2} to 0.9 sccm and reducing P_{As} to propitiate less competition between N and As. The results obtained in RHEED demonstrates the presence of the 3x reconstruction that is expected for this type of material. This reconstruction had not been observed in previous growths. The obtained concentrations are %N= 0.97 and %N= 1.85. We can conclude that by varying the former parameters we can achieve a wide range of N concentrations in GaNAs. PR measurements were also performed in order to observe the interband transition. It was also observed that the increase in the power of the RF source, decreases the energy of E- indicating that %N increase. It is also observed that increasing F_{N_2} without increasing P_{RF}



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does not really provide a significant difference in the N concentration. It was also seen that the reduction of P_{As} results on much higher %N concentrations in the GaNAs films. Raman spectroscopy showed three main resonance modes: LO GaAs-like which demonstrates the presence of GaAs (1 0 0), TO GaAs-like which is possible to observe due to the incorporation of N in GaAs and TO GaAs-like associated with GaNAs. It is observed that for % N less than 1% there is a shift to higher frequency of modes.

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[SEM-263] Photoreflectance of the E- and E+ transitions in highly mismatched MBE grown GaNAs alloys

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The interband solar cell is simply described as an interband material within a p-type and n-type semiconductor junction. In these devices, the interband allows the absorption of photons of energy E_- lower than the band gap, besides of the absorbed photons in the usual BV-CB transition, which energy is denoted as E_+ . A third photon of energy $DE = E_+ - E_-$ is required to be absorbed to realize the E_- -CB transition. Therefore, within a single material such as GaNAs, photons of three different energies are expected to be absorbed and generate photocarriers, increasing the solar cell efficiency [1]. In this direction, an N concentration (%N) close to 2% is required for the GaNAs alloys. Note that if %N=2% then $E_- = 1.3$, $E_+ = 1.9$, and $DE = 0.7$; three energies located within the curve of maximum available energy of the sunlight spectra. The best way to demonstrate the formation of the interband is photoreflectance spectroscopy (PR). In this work, we studied the E_- and E_+ transitions by PR in GaNAs alloys. We employed molecular beam epitaxy (MBE) for the growth and varied the deposition parameters. The results show the presence of the 3 searched transitions. In a first set of samples by varying the power of the RF source %N changes from 0.41 to 0.60 and the E_- and E_+ transitions goes from 1.395 to 1.339 eV and 1.727 to 1.772 eV, respectively. Additionally, it was corroborated that PR is more reliable in determining %N as compared with XRD patterns. This is associated to lattice distortion effects that are introduced even for small %N in the GaNAs matrix, that hinders the actual %N usually obtained through the Vegard's law. By increasing the N_2 flow, E_- changes from 1.341 to 1.314 eV while E_+ varies from 1.666 to 1.754 for %N ranging from 0.52 to 0.9. These results are not consistent with what



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was expected because higher concentrations were obtained in comparison with the previous set. This discrepancy is related to the mechanism of inclusion of N into the GaAs matrix: whereas in the first set of samples the N atoms occupy interstitial sites, in the second set N enter into substitutional ones. In contrast, the concentrations obtained by XRD ranges from 0.52 to 0.64. By changing the As flux %N to 0.97 and 1.85, as measured by PR and XRD, the intermediate band E₋ and the E₊ transitions were located at 1.24 and 1.14 eV, and 1.80 and 1.825 eV, respectively. The results show that the reduction of the As flux has more remarkable effect on %N of the GaNAs alloys, allowing to get the desired 2%. Finally, PR experiments as a function of temperature showed that the E₋ and E₊ transitions have different a and b Varshni parameters, associated to the different nature of these energy bands.

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[SEM-267] $\text{In}_x\text{Ga}_{1-x}\text{N}$ nucleation by In^+ ion implantation into GaN

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$\text{In}_x\text{Ga}_{1-x}\text{N}$ is one of the most important semiconductors after Si and GaAs due to its special properties such as tunable band gap, high absorption coefficient, resistance to high temperatures and radiation. The band gap is well established in the range from 0.7 to 3.4 eV varying the Indium concentration suitable to absorb and emit radiation. $\text{In}_x\text{Ga}_{1-x}\text{N}$ based devices such as LEDs, photodetectors, and solar cells have been proven [1,2]. The critical issue for $\text{In}_x\text{Ga}_{1-x}\text{N}$ structures is the difficulty to achieve high Indium concentrations without phase separation during epitaxial growth: these results in a high surface roughness and a poor crystalline quality of epitaxial $\text{In}_x\text{Ga}_{1-x}\text{N}$ [3].

Therefore, as an alternative to $\text{In}_x\text{Ga}_{1-x}\text{N}$ nucleation, we propose a study of high dose and low energy In^+ ion implantation into GaN. The In^+ ion implantation into GaN has been performed by our group to fabricate low resistance ohmic contacts [4]. However, the effects of implantation on the GaN photoluminescence have not been reported yet. The existing reports of In^+ implantation into GaN are focused on the radiation damages at different energies and doses. In addition, GaN and InN nanocrystals have been observed after implantation and annealing of N^+ ions into GaAs or InAs respectively. Nevertheless, to our knowledge, the $\text{In}_x\text{Ga}_{1-x}\text{N}$ or InN nanocrystals have not been observed into GaN by this method.

In^+ ion implantation was carried out at 25 keV with a dose of 5×10^{15} ions/cm² at room temperature into Mg-doped and n-doped GaN templates, as a result, we demonstrated that the implantation effect is independent of the substrate conductivity. The structural characterization was realized by HXRD, Raman, and STEM. The results revealed the formation of $\text{In}_x\text{Ga}_{1-x}\text{N}$ with a variable concentration of Indium and interplanar spacings of 0.266nm and 0.2675nm were measured by STEM. The crystalline structure for the as-implanted and after thermal annealing confirmed by Raman, HRXRD, and STEM,



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let us suggest that the thermal spike regime with the formation of quenching of melting pools during 25keV In⁺ ion irradiation of GaN should be considered. After implantation and annealing at 500°C, an interesting green emission was observed. The green emission was explained consistently by the nucleation of the In_{0.327}Ga_{0.673}N ternary alloy which, can be used to absorb or emit green radiation in future applications.

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[SEM-15] Zinc sulfide thin films doped with copper by the chemical bath deposition method

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In this work ZnS deposited thin films doped with Cu by chemical bath deposition method at a low temperature (56 ° C) were studied. The thin films were deposited on glass substrates considering the variations of the number of dips during the CBD process and also annealing effect was studied. The doped semiconductor thin films were optical, structural and electrically characterized. XRD characterization showed that the homogeneous films were deposited with amorphous structure. The absorption measurement (UV-Vis) of the deposited ZnS:Cu films was used to estimate the optical band gap. The energy band gap values are in the range from 3.6 to 3 eV depending on annealing effect and number of dip. The electrical conductivity increased two orders of magnitude for the ZnS:Cu thin films compared with the ZnS films. These characteristics in ZnS:Cu films make them suitable candidate for various semiconductor device applications, obtained by a rapid and low- cost technique.



[SEM-17] Synthesis and deposition of CuO as semiconductor thin films by wet chemistry

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Different transition metal oxides have a numerous applications. One of these is cupric oxide (CuO) as an important P-type transition metal semiconductor oxide has been extensively studied. CuO has been established as a number of applications like gas sensors, solar photovoltaic, and lithium ion electrode. There are various established ways of fabricating CuO thin films like spray pyrolysis, spin coating, dip coating, SILAR to name a few. Among all these sol gel process assisted by spin coating technique has stoichiometry in multi-component system and splendid control of chemical uniformity.

CuO films were synthesized by sol-gel method and deposited by spin-coating process at room temperature in order to compare their properties. We have investigated the influence of the variation of the speed deposition number of layers and annealing effect on the deposited thin films in order to improve the optical and electrical properties. The optical properties were analyzed using a spectrophotometer (UV-Vis) in a range of 1100-300 nm. The microstructure for the films was studied by scanning electron microscopy and X-ray diffraction. The electrical behavior of the thin films was studied by four points and by studied of I-V characteristics.

Keywords: CuO, semiconductor, thin films



[SEM-54] Optical, electrical and structural analysis of p-type ZnO:Ag,N thin films

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P-type ZnO:Ag,N thin films were deposited by dual acceptor co-doping with nitrogen and silver by DC reactive magnetron co-sputtering. The films were annealed at 673 K and 723 K for one hour in nitrogen atmosphere. The electrical properties were measured by Hall Effect measurement, and the optical transmission and absorption spectra were obtained by Uv-Vis spectroscopy. The annealed films present p-type conductivity with a low resistivity, and very high hole concentration (10^{19} cm^{-3}). The SEM micrographs of all the films exhibited uniformly distributed spherical grains over the surface of the films. Raman and IR spectroscopy confirmed the incorporation of Ag and N into the ZnO structure and the possible formation of $\text{Ag}_{\text{Zn}}\text{-N}_{\text{O}}$ pairs and/or $\text{N}_{\text{O}}\text{-Ag}_{\text{Zn}}\text{-N}_{\text{O}}$ triangles. The photoluminescence results suggested the suppression of native defect levels due to the incorporation of Ag and N in to the ZnO films.



[SEM-60] Current-Voltage (I-V) characterization of ZnO:B/ZnO:(Al-In) diode structures
fabricated by the Sol-Gel method

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Transparent conducting oxides (TCOs) have been widely applied in various fields, such as front surface electrodes of solar cells and flat panel displays, low emissivity windows, etc. Various techniques have been extensively employed to fabricate high performance, homo- and hetero-junctions based on ZnO, although the results were not satisfactory overall with respect to the rectification ratio and cut-in voltage. Physical techniques can certainly result in high performance diodes, however, the fabrication costs are very high. We have preferred the sol-gel method to fabricate a transparent dispositive. This method provides a convenience in scientific and technological studies because its properties provide a stable structure by avoiding high-temperature reactions, and the ability to use very small amounts of compounds.

We report the fabrication of a transparent semiconductor junction formed with two layers of ZnO doped with Aluminum, Boron and Indium by the sol-gel method, and deposited on ITO substrates by spinning coater.

In previous studies we found that Boron doped films presented the higher resistivity as compared with the aluminum-Indium doped films. Therefore, we selected the ZnO:B films as the insulating film to be deposited on ITO. After thermal treatment at 500⁰ C, the ZnO:Al-In film was deposited over the first film and thermal treatment at 500⁰ was again applied. Several levels of impurity, as well as different thicknesses were studied. In order to obtain the optimum thickness of the films, the coating procedure was repeated for several cycles. Dark I-V curves of the p-ZnO:B/nZnO:Al-In showed the characteristic rectification of diode. Depending on the Impurity/ZnO ratio, as well as the thickness, ideality factors obtained from the relation $h = (q/kT)(dV/d\ln(I))$, between 3 and 4 were found. The divergence from the ideality factor, suggests the presence of interfacial traps between the layers, as well as current conduction mechanisms other than thermionic emission, and presence of barrier inhomogeneities. The



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leakage current under reverse bias is very low, and the forward threshold voltage is about 0.4 V. As resulted from XRD studies on the separate films, no other phase than ZnO was observed. On the other hand, optical measurements resulted in band-gaps very close to those of ZnO. Therefore, we suggest that this dispositive is a transparent (> 85 %) homo-junction.



[SEM-76] Photoluminescence study of fluorine-doped zinc oxide films prepared by sol-gel spin-coating

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Fluorine doped zinc oxide (FZO) has received considerable attention due to its potential applications in ultraviolet light emitting devices and in flat panel displays as a low voltage [1]. The FZO luminescence properties strongly depend on intrinsic defects such as oxygen vacancies, oxygen interstitial and zinc vacancies [2,3]. PL spectroscopy is an attractive technique to study the intrinsic and extrinsic defects of the materials and provides more information about the nature of the impurities and the existence of defect energy states even when they are present in very low concentration [3,4]. In this, work we report PL spectroscopy study of FZO films prepared by sol-gel spin-coating to identify the type of defect that controls their optical properties. The FZO precursor solutions were prepared from zinc acetate, as metal source, isopropanol as solvent and monoethanolamine as stabilizer agent. Ammonium fluoride was employed as the fluorine source. The concentration of fluorine was controlled from 5 to 15 at%. The FZO films were deposited onto monocrystalline Si (100) substrates. Then, FZO films were annealed at 600 °C for 2 h. XRD studies revealed a wurtzite hexagonal structure (JCPDS: 36:1451) exhibiting (002) preferential orientation, which decreased as fluorine concentration increased. The FZO films exhibited optical transmittance above 80 % in the visible region. The optical band gap of the films increased as the fluorine concentration increased. The PL measurements were carried out in the range 10-300 K. These measurements indicated that the oxygen vacancies have a strong influence in optical properties of FZO films.

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[SEM-102] Electrical characteristics of a C-CNTFET and an SB-CNTFET through compact modelling for different chiralities

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In this work we report an analysis of the electrical characteristics (I-V) of two different types of CNTFETs, using a generic compact modelling. In these devices the channel is conformed by a semiconductive SWCNT characterized by (n,0) quirkality index. Another important characteristics in this type of devices is the ballistic charge transport in the channel. Because the CNTFET is a 1D system, it leads to take into count the contribution of various energetic sub-bands that determine the value of electrical current which is modulated by gate and drain bias. By considering different quirkalities ((13,0), (19,0), (38,0)) we obtain the behavior of I_{DS} values, which in a certain point may allow predicting an specific performance in the device. The compact modelling used in this work gives a current equation I_{DS} derived from Landauer formulism in the perfect contact approximation between source and drain with CNT, and it is called generic because it gives the possibility to adapt many different types of CNTFETs.

It is analyzed I_{DS} as a function of V_{DS} and V_{GS} bias considering the first case of ohmic contacts, and the second case which includes the Schottky barrier effect, such contacts are metallic, and in both cases we study the temperature effect on I_{DS} performance.

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[SEM-117] Zinc phthalocyanine films for its possible application on devices

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The optical and electrical properties of thin sandwich type structures (Al/Si-p/ZnPc/Au, Al/Si-n/ZnPc/Au) have been studied in a quantitative fashion. The ZnPC films were studied with following optical techniques: FTIR, Photoluminiscence and Transmittance. Here, the structures are formed of two form the firts is with Al(150-300nm)/Si-p/ZnPc (50-335nm)/Au(170nm) and the second is with Al(150-300nm)/Si-n/ZnPc (50-335nm)/Au (170nm). The devices were assembled by deposition in vacuum and they were studied by mean of measurements current-voltage (I-V). The I-V curves show a behavior of rectification in dark, when they are expose to light white increased the current and have a behavior symmetrical in forward and reverse. The device have a fast photoresponse with visible light and respond efficiently to pulse light. A correlation of resultsoptical and electrical was realized.

Keywords: phthalocyanine, zinc, devices

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[SEM-149] Effect of different irradiation time on transparent and conducting Al-doped ZnO films

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The effect of different irradiation time on the final structure, morphology, optical, electrical and mobility properties of Al-doped ZnO thin films, obtained through microwave assisted method has been investigated. The thin films were growth by using $Zn(NO_3)_2$ 0.1 M and $AlN_3O_9 \cdot 9H_2O$ 0.01 M as precursors. The irradiation times were of 3, 4, 5 and 6 minutes. The temperature and pH for all reactions were of 82.5 °C and 11.5, respectively. The characterization of the samples has been carried out by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), photoluminescence (PL), UV-vis spectra and Hall-effect measurements. XRD patterns revealed that all samples had hexagonal wurtzite structure corresponding to ZnO. SEM results showed that average crystalline size was observed to increase with an augment in the irradiation time. FL spectra showed that Al-doped ZnO samples exhibited a UV emission peak at 395 nm and one defect peak corresponding to blue emission near 580 nm. Hall-effect in the Van der Pauw configuration was used to measure the electrical properties of the films. The data were collected at room temperature. Al-doped ZnO films showed n-type conductivity, with a carrier concentration average of $3 \times 10^{15} \text{ cm}^{-3}$, a Hall mobility value of ($\mu_H = 17 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) and a resistivity value of $80 \Omega \text{ cm}$ on all samples independently of irradiation time.



[SEM-166] Antireflection ZnO-based coatings deposited by spray pyrolysis

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Antireflection ZnO-based coatings were deposited on glass substrates; the deposition process was realized on four stages: in the first one, crystalline-ZnO was deposited using zinc acetate as precursor; in the second stage crystalline-ZnO was deposited using zinc nitrate as precursor, for the third layer, a very thin ZnO film was deposited using zinc acetate as precursor to seal the previous layer of nanocrystalline ZnO and finally, in the last stage a ultrasonic treatment was applied for 10 minutes. The solution concentrations were 0.1 molar for zinc acetate and 0.3 molar for zinc nitrate; the solution decompositions were carried out at 450 °C under different atomization fluxes. The crystalline structure and the surface morphology of the thin layered films were characterized by X-ray diffraction (XRD) and scanning electronic microscopy (SEM). The results showed that the structure for ZnO corresponds to the typical hexagonal wurtzite. The Transmittance behavior was increased from 80% to 85-90% in the visible region, at the same time, the reflection diminished to values around 15% as the direct effect of the change on the surface morphology.



[SEM-174] Oxygen environment effect on the morphology and composition of pulsed laser deposited nanometric CdTe films

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Cadmium telluride is a highly promising semiconductor material for thin film solar cells due to its optoelectric properties; it has a nearly optimum bandgap value for efficient light conversion according to Shockley-Queisser's limit. In this work CdTe thin films were synthesized by pulsed laser deposition (PLD) on glass substrates. Oxygen was incorporated in the process by working in an Argon (80%) and Oxygen (20%) environment. Deposition was made at different pressures going from 2.5×10^{-5} without gas to 10^{-2} by increasing the gas flow; the main objective was to look for oxygen as a dopant while looking for changes in the film crystalline structure in a 10 minute synthesis in which the only variable parameter was the background pressure. Oxygen was used since it can act as an acceptor in CdTe p-type films. Mean kinetic ion energy and density of the plasma were measured by using a planar Langmuir probe. The crystalline structure of the films was characterized by X-ray diffraction, UV-Vis spectroscopy was used for optical characterization; finally morphology and chemical composition were analyzed by scanning electron microscopy and energy dispersive X-ray spectroscopy, respectively.

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[SEM-202] Dynamic build-in voltage by Current Voltage analysis in Co(Mn)-doped ZnO/YMnO₃ n-p heterojunctions.

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Fast advance in communication technologies have let that the very large scale integration (VLSI) fabrication techniques have an accelerate enhancement. Current research are focused in new properties of semiconductor materials as the small devices that obeying the Moore's Law can supply all the today demand in technology. Semiconductor heterojunctions are bilayers with dissimilar semiconductors where the band gap and/or electron affinity changes at the interface¹. Furthermore the electrical properties of a semiconductor diode material can be modified by doping, electrical fields or light. Due to these changes in the properties of semiconductors, they can be used for amplification, switching, and energy conversion.²

The purpose of this work was the study of the dynamic behavior of build-in voltage by C-V curves of n-p Co(Mn)-doped ZnO/YMnO₃ heterojunctions. We systematically change the Co(Mn) concentration, 0.0, 0.1 and 5.0 atom percent. Samples were grown by pulsed laser deposition technique where we varied the frequency of the laser pulses at 1500 and 2500 for the doped ZnO films maintaining constant all the other growth parameters.

We obtained from the experimental data the donor concentration, thickness of the depletion n-layer formed in n-ZnO, n-ZnCoO or n-ZnMnO (W_d) and p-YMnO₃ (W_a) layer for all samples by using the junction the capacitance equation according to Poisson's equation and assuming an abrupt interface.^{3,4} The donor concentration, N_d , build-in voltage, V_d , for all np heterojunction devices, NpHJDs, were calculated assuming the acceptor concentration, $N_a = 10^{20} \text{ cm}^{-3}$. Results indicate a dependence of N_d , V_d and widths of the depletion region with at%Co, at%Mn, and growth parameter frequency of laser.



We found that the W_d was larger than W_a for all samples; when Co or Mn doping concentration increased, whereas the N_d decreased when at%Co or at%Mn increased, except for 5at%Mn doping increased after a minimum in 0.1at%. For our heterojunctions the hysteresis behavior in C-V curves had a decreasing capacitance during the backward sweep due to possible reduction of V_0^+ after applying +V, on contrary which was found in classical semiconductors⁴. Donor concentration behavior was increased and leading a reduction of the depletion width and therefore an increase in the capacitance.

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[SEM-237] Properties of TiO₂ thin films deposited on different metal substrates.

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Titanium Dioxide is a promising photocatalyst for its strong oxidation potential and its moderate potential reduction due to the generation of electron - hole pairs in the valence band (VB) and conduction (BC). The excited electrons in the BC reduce oxygen in super oxide radical, and holes in the BV oxidize water molecules into hydroxide radicals. These radicals are potent intermediates in the decomposition of organic molecules. In addition, the TiO₂ is physically and chemically stable and nontoxic therefore has a variety of applications such as self-cleaning surfaces, antimicrobial and environmental purification.

In this work TiO₂ thin films have been deposited on different metal substrates, using reactive Rf sputtering technique. The structural and chemical bonding characteristics were analyzed by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). UV-Vis reflectance spectroscopy was employed to determine the band gap energy. The electrochemical properties of films on different metal substrates were obtained using the electrochemical impedance spectroscopy, mott schottky and cyclic voltammetry. The results shown a strong dependence of the metal used as substrate with the properties of the films.

This work was supported by SIP-IPN (project 20170201)



[SEM-238] Growth and characterization of TiN_xO_y thin films to be used as glucose biosensor.

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Promoting direct electron transfer (DET) between an electrode and immobilized molecules is of scientific importance in the investigation of the fundamental mechanism of biological redox reactions and of practical significance for the development of advanced bioelectronic devices, such as highly sensitive enzymatic biosensors and highly efficient biofuel cells. Due to its superior photocatalytic capability and excellent electron-transfer behavior, TiO₂ has been extensively investigated for use in a broad range of applications, including dye sensitized solar cells hydrolysis catalysts, electrochromic devices, and lithium-ion batteries. Nanocrystalline TiO₂ films have recently been introduced to improve the catalytic activity of enzymes in the applications of gas sensors and biosensors. TiO₂ shows low electrical conductivity, and TiN have a high electrical conductivity; hence the composite of both materials could be have a interesting properties for the use as biosensor.

In this work is presented the methodology to develop electrochemical biosensors with high sensitivity, fast response times, and stability for the determination of glucose concentrations. The main goal is to evaluate the use of TiN_xO_y thin films obtained by the RF-Sputtering process for the construction of enzymatic and nonenzymatic biosensors. The results includes the optical and electrochemical characterization of the samples, the procedure to fix the enzyme on the films, and analysis of the results obtained during the research.

This work was supported by SIP-IPN (project 20170201)



[SEM-239] Effect of deposition parameters on properties of TiO₂ thin films prepared by RF-magnetron sputtering

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The life expectancy of the human is increasing, so it a necessity to produce biocompatible products enhancing the quality of life. It has been reported that TiO₂ has good biocompatibility properties. In this work we presented the effect of deposition parameters on the properties of TiO₂. Thin films were prepared of TiO₂ on stainless steel (AISI 316L and AISI 304) substrates. The thin films were prepared by reactive RF-magnetron sputtering technique from a Ti target. We varied the thickness, substrate temperature and sputtering power. The thickness was varied from 50 nm to 400 nm; the temperature was varied from room temperature to 500 °C and the sputtering power was varied from 50 W to 250 W. The samples were characterized by scanning electron microscopy (SEM), Reflectance, and electrochemical. Reflectance measurements showed that the absorption edge there is no significant change in terms of variation in the thickness, the temperature and sputtering power. We obtained that the value of the band gap corresponds to the TiO₂, for all samples. Using scanning electron microscopy (SEM), we found tha the films did not show cracks or major defects. Was also carried out the electrochemical characterization (Tafel and impedance) which showed that the TiO₂ thin film increase the corrosion resistance of the stainless steel.

This work was supported by SIP-IPN (project 20170201)



[SEM-248] Design of logic gates through surface states engineering

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Logic gates commercially available are restricted to specific parameters in their logical voltages levels, hindering the design of devices which requires low power consumption in each one of their elements. For example the 1.8V-CMOS family, for an acceptable high logic input state, require at least 1.17 volts while operated nominally with a 1.8-volts power supply. These parameters are increased for families as TTL, 5V- or 2.5V-CMOS. In this work, the authors propose the manipulation of surface states, surfaces charge and depletion zone of a silicon-on-insulator (SOI)-substrate in order to design a device which follows Boolean algebra. In this design, surface states are created by the breaking of symmetry in the crystalline structure when grooves are digged in the SOI, producing nano-channels where the current flux can be controlled by the applied bias, such as in the self-switching diode (SSD) developed by A. M. Song [1]. The performance is studied by numerical simulations. The typical performance of AND and OR logic gates is obtained when an appropriated geometry and distribution of the grooves is employed. The possibility of modifying the logical voltages level that are required to establish either high or low input can be controlled by the geometry of the device. It is demonstrated that high level input voltage can be lowered to 0.5 V. This makes the concept attractive for applications demanding low voltage signals. In addition, the concept has been proved using when the nominal power supply voltage was 1 V. Transient simulations indicates that the propagation delay time exhibited by the gates is short even for 1 GHz square waves.

[1] A. M. Song *et al.* Appl. Phys. Lett. **83**, 1881 (2003).

Acknowledgments:

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[SEM-284] 2DEG formation at the AlGaAs/GaAs heterostructure using Genetic Algorithms

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The formation of the 2DEG is studied using a genetic algorithm for solving the self-consistent Schrodinger and Poisson equations at the Electric Quantum Limit. Starting from the Fang-Howard like function the system allowed to involve employing the rules of the genetic algorithm. Minimization of the total energy is used to found the one-electron wave function and therefore the energy of the confined states of the 2DEG. The results are compared to the standard straightforward minimization of the one parameter Fang-Howard function.



[SEM-314] Optical and structural characterization of GaAs films obtained by CSVT in different gaseous environments

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GaAs films obtained by the Close Space Vapor Technique (CSVV) using the traditional sandwich set up, obtained at different gaseous environments is presented in this work. Hydrogen or nitrogen was introduced at constant flow in a quartz chamber. The CSVV set up consisted of a GaAs (100) wafer used like source, a fused quartz plate used as a substrate and an O-ring quartz 2mm of thick and 10mm of diameter used as separator. The GaAs source was kept at 800°C in all cases. The time of the process was 5 and 13 minutes. It were observed notable changes in the growth rate of the process. The film growth with hydrogen was thicker than the film growth with nitrogen in almost 3 orders of magnitude for the 5 min film. However the film growth with hydrogen shows a cracked surface and an “orange skin” morphology. The thin film growth with nitrogen shows a very smooth surface. The band gap of the films were very close to the 1.5 eV reported for the bulk, except for the thin film growth with nitrogen, this sample, with a thick of 132nm, presents a band gap of 2.5 eV. Chemical reactions are proposed in order to understand the significant difference produced from the gaseous environment. Also is proposed that the increase of the band gap for the nanometric film can be associated with a quantum effect. The slow growth rate with nitrogen gas make possible obtain very thin films with interesting properties for optical devices.

Keywords: GaAs, CSVV, Thin Films



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SURFACES AND INTERFACES (SIF)

Chairmen: Leonardo Morales de la Garza (CNyN-UNAM)



[SIF-91] Electrochemical performance of nanostructured hybrid Zinc-rich epoxy coatings

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Traditional zinc-rich epoxy coatings (ZREP) contain Zn pigment equal or greater to epoxy's critical pigment volume concentration (CPVC) and have formerly been applied over steel infrastructure as anticorrosive technology. CPVC ensures electrical interconnection between zinc and steel and keeps steel cathodically protected by Zn sacrificial effect. Unfortunately, CPVC can also cause performance issues, such as early blistering; therefore, strategies, such as the use of conductive additives, have been explored to decrease Zinc content but ensure electrical interconnection. Accordingly, hybrid ZREP formulations applied over low carbon steel with Zn below, but close to CPVC and varying content of carbon nanotubes (CNT) as conductive additives, were studied to assess their corrosion protection mechanisms and understand electrolyte-electrochemical system interactions when exposed to nutrient broth enriched-chloride (NB-NaCl) solution.

xCNT-ZREP systems were tested during a 4-week period in NB-NaCl, and characterized through Electrochemical Impedance Spectroscopy (EIS), Open Circuit Potential (OCP), Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS). SEM and EDS revealed coating layer's damage evolution consisting of outermost coating deterioration and zinc dissolution from 7 days of exposure, while the OCP and EIS analysis strongly suggested an anticorrosive mechanistic response mainly integrated by: 1) a barrier effect; and 2) a cathodic protection effect; both are characteristic of traditional ZREP systems; however, it was found that CNT content was critical in such effects' duration.



[SIF-109] Influencia de los parámetros de depósito sobre la resistencia al adherencia de recubrimiento de bronce al aluminio (CU+11% AL-FE) producido con la técnica de proyección térmica por llama y tratados térmicamente.

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En este trabajo se estudió la influencia del tratamiento térmico de sintonización sobre propiedades de adherencia de recubrimientos de Bronce al Aluminio (Cu+11% Al-Fe) depositados con técnica de proyección térmica a la llama sobre sustratos de Bronce Naval. Las superficies de los sustratos fueron sinterizados en horno al vacío y con atmosfera inerte de N₂. Los análisis de composición química se realizaron mediante fluorescencia de rayos X (FRX) y el análisis estructural se realizó mediante difracción de rayos X (DRX). Las interface sustrato – Recubrimiento fueron caracterizada mediante microscopia electrónica de barrido (SEM). En general, los resultados muestran que los recubrimientos mejoraron sus propiedades de adherencia del sustrato.



[SIF-143] Natural zeolite surface modification by a cationic surfactant for tartrazine removal from water

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As a result of the problems of water pollution by different organic molecules, in recent years the importance of different adsorbent materials for the removal of these contaminants has been revealed. Adsorption is nowadays considered one of the best technologies available for the removal of organic pollutants present in the water. Some materials widely used are useful in the purification and separation processes at industrial scale and/or water treatment, although their cost may represent a drawback for their application. That is why the search for alternative, abundant and economic materials for the treatment of polluted water is an important topic in the environmental sciences. The objective of the present study was to evaluate the adsorbent capacity of a natural zeolitic rock from the state of Chihuahua for the removal of azo dye Yellow No.5 (Tartrazine) in aqueous media. The natural zeolite was subjected to a quaternary ammonium salt modification process, and sorption tests were subsequently performed to determine changes in Tartrazine concentration with respect to time. The sorption equilibrium on the zeolite was reached at the first 8 hours of contact time. Kinetic experiments were performed at room temperature (25 °C) and they were best described by the pseudo-second order kinetic model, moreover it was found that the previous modification of the zeolitic rock with a cationic surfactant improves the sorption capacity of the zeolite for the removal of Tartrazine being 1.2 and 15.9 mg / g for natural and modified zeolite respectively.



[SIF-154] Surface characterization of GaAs and InGaAs thin films prepared by magnetron sputtering

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Actually, semiconductor research is focused on finding new low-cost growth methods (e.g. magnetron sputtering) compared with epitaxial growth techniques such as molecular beam epitaxy (MBE). Gallium Arsenide (GaAs) and In-doped Gallium Arsenide (InGaAs) are two semiconductors that are relevant due to their applications in solar cells, if they are grown up on transparent substrates (eg glass). In this work, we report the growth and characterization of GaAs and In-GaAs doped thin films on glass and silicon substrates (100) by magnetron sputtering by varying the substrate temperature and Indium power source-sputtering target. The GaAs and InGaAs thin films were analyzed morphologically by atomic force microscopy and scanning electron microscopy in cross section. These results show that the GaAs and InGaAs thin films are homogeneous with columnar growth, and a well-defined interface between the layer and the substrate. A complementary analysis in depth profile performed by secondary ion mass spectroscopy (SIMS) allowed us to corroborate that the GaAs layer is stoichiometric. A decrease in the Ga and As signals and an increase in the Si signal into the interface was observed, due to GaAs diffusion on the substrate during growth. A similar behavior for the InGaAs thin films were observed. To determine the chemical species on the GaAs and InGaAs surfaces, XPS spectra were recorded in the range of In 3d_{5/2}, As 3d and Ga 3d core-level photoemission lines. The presence of GaAs and InGaAs (Figure 1) oxides was evaluated by comparing the In-s 3d, Ga 2p, As 2p and O 1s region of the XPS spectra [1],[2]. These result show that an increase in the In content in GaAs produce a decreases in the GaO oxides. The low level of oxidation of As, is a consequence of the high grow temperature, since AsO oxides are more unstables than GaO oxides. Finally, we concluded that magnetron sputtering is a good technique to growth polycrystalline semiconductors alloys.

[1] <https://srdata.nist.gov/xps/ElmSpectralSrch.aspx?selEnergy=PE>.

[2] Demanet C.M. and Marais M.A. Surf. Interface Anal. Vol 7 (1985). 13–6. doi: 10.1002/sia.740070104.



[SIF-218] Robust design for superhydrophobic aluminum fabrication process using Taguchi method

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Considering the novel method developed by Cansen Liu, Fenghua Su and Jizhao Liang to fabricate superhydrophobic aluminum [1], a robust design was made to decrease the variance and error of uncontrolled factors during the manufacturing process of superhydrophobic aluminum 7075. The fabrication process mainly consists in three steps: perform an anodic oxidation; immerse the aluminum into an ethanolic solution containing C₁₆H₁₉F₁₇O₃Si (AC-FAS); and finally, heat at a specific temperature. Using Taguchi orthogonal array design, noise factors whose affect the manufacturing process of the superhydrophobic treatment were identified and variance contact angle was minimized to obtain a water contact angle of 157°.

1. Cansen Liu, Fenghua Su and Jizhao Liang, Facile fabrication of a robust and corrosion resistant superhydrophobic aluminum alloy surface by a novel method. *RSC Adv.*, 2014, **4**, 55556-55564.



[SIF-266] Preparation of surface nano-particles and application of the substrate for SERS analysis of biological samples.

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In this work, we report about fabrication of Au and AuTi nanoparticle over silicon and DLC/Si substrates. We used these substrates with nanoparticles for Surface Enhancement Raman Spectroscopy (SERS) measurements of different biological objects: cells, viruses and proteins.

Two method of ultra-thin film deposition were used: electron beam evaporation, and ion sputter deposition. A rapid thermal annealing (RTA) at different temperatures and time was used for the nanoparticles preparation. We search the optimal regime and optimal thickness of the deposited films to control the size of the nanoparticles obtained. A (100) silicon substrate was employed and it was cleaned by following the conventional RCA method.

A Solver Next AFM from NT-MDT was employed to verify some geometrical properties of the formed NPs like size, shape and size distribution.

To prove the Raman signal enhancement, we analyzed different peptides and proteins deposited over the substrates with nanoparticles. The Raman spectroscopy analysis was performed by using two different systems: a NTEGRA system from MT-NDT company with green laser, and a Horiba Micro Raman spectrometer with a red laser. A more pronounced SERS effect was observed for the red laser excitation.

Acknowledgments:

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[SIF-272] **Applicability of the Gibbs Adsorption Isotherm to the analysis of experimental surface-tension data for ionic and nonionic surfactants**

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The Gibbs Adsorption Isotherm equation is a two-dimensional analogous of the Gibbs-Duhem equation, and it is one of the cornerstones of interface science. It is also widely used to estimate the surface excess concentration (SEC) for surfactants and other compounds in aqueous solution, from surface tension measurements. However, in recent publications some authors have cast doubt on this method. In the present work, we review some of the best available surface tension experimental data, and compare estimations of the SEC, using the Gibbs isotherm method (GIM), to direct measurements reported in the literature. This is done for both nonionic and ionic surfactants, with and without added salt. Our review leads to the conclusion that the GIM has a very solid agreement with experiments, and that it does estimate accurately the SEC for surfactant concentrations smaller than the critical micellar concentration (CMC).



[SIF-303] Fermi level position at Ga-polar, N-polar and nonpolar (m-plane) GaN surfaces in vacuum and air ambient

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Keywords: Fermi level, GaN, electroreflectance

Band gap alignment in semiconductor heterostructures is mainly determined by E_g values, doping concentration, dislocation densities, bulk and superficial electric fields, and the Fermi level position (E_F). The last one is well related with the superficial density states, dislocations and point defects on the final surface. In this work we evaluate the dependence of the Fermi level position on superficial ambient for Ga-polar, N-polar and non polar (m-plane) GaN surfaces. Samples were grown by MOCVD technique on GaN substrates with above-mentioned polarity. Contactless electroreflectance spectra were measured on Van Hoof structures by placing the samples between the plates of a capacitor in air ambient and medium vacuum environment ($\sim 1 \times 10^{-4}$ torr). This technique is very sensitive to the surface electric field, which changes with the Fermi level position. A clear variation was observed in the period of the Franz-Keldysh oscillations as the air ambient was changed to vacuum pressure. Oxygen molecules bounded at GaN surface are desorbed when the ambient pressure is changed to vacuum level and then a redistribution of superficial charge is produced, reducing the superficial electric field and modifying the position of the Fermi level. The changes in the surface electric fields were different for each GaN polarity due to binding energies between GaN surface and oxygen molecules, which gives different absorption and desorption process adequate for gas sensors [1].

[1] L. Janicki, et. al., Japanese Journal of Applied Physics **55**, 05FA08 (2016)



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TEXAS-MEXICO SYMPOSIUM (TEX-MEX)

**Chairmen: Perla Garcia (UACJ)
Manuel Quevedo (UT-Dallas))**



TEX-MEX 1:

Solution- processed thin film transistors based on organic-inorganic hybrid gate dielectric

*Rafael Ramirez-Bon,
Cinvestav, México*

[Solution processing has been recently considered as an option when trying to reduce the costs associated with deposition under vacuum. In this context, solution-processable organic-inorganic hybrid gate dielectrics are of significant interest because of their low-cost, low temperatures processing and applications to flexible thin film transistors (TFTs). In this work, we explore the sol gel synthesis to prepare different systems of hybrid dielectric films that allows enhancing the high capacitance of a gate dielectric to enable the transistors operating at low voltages. Furthermore, we complete the thin film transistors structure by depositing, also in solution, the semiconductor active layer and analysed the electrical performance of the devices. The organic-inorganic hybrid transparent dielectrics composed by the mixture of high-k dielectric materials and some polymers as PMMA and PVP were deposited by the sol-gel process. After deposition, the wet hybrid films were cured at low annealing temperatures ($\leq 150^{\circ}\text{C}$) and analysed by UV-Vis spectroscopy, AFM, TGA, SEM, C-V and I-V measurements. The hybrid systems with adequate dielectric characteristics, were deposited as single hybrid layers on ITO-coated glass substrates and tested as gate dielectric in thin film transistors, using CdS as semiconductor active channel deposited in solution. We measured the output electrical response and transfer characteristics of these hybrid dielectric gate-based devices and determined their main electrical parameters as a function of the composition of the hybrid dielectric gate layer. The values obtained for the electrical parameters show that hybrid films are quite suitable for dielectric gate applications in complete solution-processable TFTs.



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TEX-MEX 2:

Sensor Development

Bruce Gnade

Lyle School of Engineering, SMU, Dallas, TX, USA.

In this talk I will discuss two areas of sensor development that we are working on at SMU; large area radiation detectors and rotational spectroscopy. Both technologies have been made possible by advances in semiconductor materials and devices. In the area of large area radiation detectors, thin-film electronics offer the possibility of true 3-D integration because active devices can be fabricated at any level within the system. I will present results on our thin-film neutron detectors with integrated active pixel electronics as an example of how 3D electronics can provide system level performance advantages. In the area of rotational spectroscopy recent advances in silicon-based CMOS THz transmitters and receivers make it possible to develop a low cost rotational spectrometer that can be used in a wide range of gas sensor applications. I will discuss the state of development as well as challenges that still need to be addressed for these technologies, with the goal being to develop areas of possible collaborations.

Acknowledgments: This work has been supported in part by the Army Research Labs, DARPA, The Department of Homeland Security, Nanoholdings, UTSWMC, Texas Instruments and NSF.



TEX-MEX 3:

Photovoltaic Technology: research, development and implementation in Mexico

Xavier Mathew

Universidad Nacional Autónoma de México, Mexico

PV is one of the renewable energy technologies which can meet a part of the energy demand, and reduce the effect of greenhouse gases by limiting the use of fossil fuels. Given the geographical location, Mexico has great potential for harvesting the solar energy. The major R&D activities in Mexico are in educational institutions, with capacity to perform basic and applied research on various organic and inorganic PV materials, device technologies and emerging concepts in energy harvesting. In this presentation the current status of the PV research, development and commercial use in Mexico is discussed.



TEX-MEX 4:

High mobility silicon, germanium and III-V semiconductor thin films on low-cost, flexible substrates for high performance, large-area flexible electronics.

*Venkat Selvamanickam,
University of Houston, USA*

The low carrier mobility values ($1 - 10 \text{ cm}^2/\text{Vs}$) of amorphous silicon, organic and oxide semiconductors limit the performance of flexible electronics devices. Key performance metrics such as switching speed of thin film transistors (TFTs) fabricated with amorphous Si, organic and oxide semiconductors are far below that of TFTs made with crystalline silicon whose mobility values are about 100 times higher. At the University of Houston, we have developed a technology to fabricate single-crystalline-like silicon, GaAs and germanium semiconductors on flexible metal and glass substrates by roll-to-roll processing which has enabled us to combine the superior performance of crystalline semiconductors with flexible and inexpensive substrates. Silicon with mobility values over $230 \text{ cm}^2/\text{Vs}$ and carrier concentration levels below 10^{16} cm^{-3} and GaAs with mobility values of $1300 \text{ cm}^2/\text{Vs}$ and carrier concentration levels of $10^{17} - 10^{19} \text{ cm}^{-3}$ have been demonstrated on metal substrates. TFTs fabricated with such silicon and germanium on flexible metal and glass substrates exhibit high field mobility and high on-off ratios. Progress in the development of nanocrystalline Ge, Si and III-V thin films with single-crystalline-like characteristics and performance on low-cost substrates for large-area flexible electronics applications will be presented.



TEX-MEX 5:

Micro and nano crystalline cvd diamond tl/osl radiation detectors and dosimeters

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Recent advances on the controlled synthesis of CVD diamond have demonstrated the possibility of producing high quality micro and nano crystalline CVD with exceptional performance as detectors and dosimeters, appropriate for high-energy photons and energetic particle beams. Modern radiotherapy methods requires the use of high photon radiation doses delivered in a fraction to small volumes of cancer tumors. CVD diamond is a very attractive material for applications in ionizing radiation dosimetry, particularly in the biomedical field since the radiation absorption by a CVD diamond is very close to that of soft tissue. Furthermore, diamond is stable, non-toxic and radiation hard. In the present work, we discuss the CVD diamond properties and dosimeter performance and discuss its relevance and advantages using thermally stimulated luminescence (TL) as well as optically stimulated luminescence (OSL) methods. The modern CVD method of growth allows introducing precisely controlled impurities into diamond to enhance the dose linearity and minimum dose sensitivity. Clinical dosimetry applications requires, high accuracy of dose measurements, low fading, high sensitivity, good reproducibility and linear dose response, characteristics exhibited by CVD diamonds. In some cases, dose linearity and reproducibility in CVD diamond are better than in standard commercial TLD materials like LiF. In the present work, we discuss the state-of-the art developments in dosimetry applications using CVD diamond.

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TEX-MEX 6:

Nanostructured Materials for Enhanced Photoabsorption and Photocatalytic Properties

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Ever since the discovery of unique quantum effects, materials with nanostructure have been under extensive investigation with an aim of understanding underlying physics behind such effects and also developing new class of materials ideal for advanced devices. Of various studies conducted in this area, nanostructured materials made from compound semiconductors and metal oxide compounds are under particular interest because their properties, including photoluminescence, show extreme sensitivity to the physical dimension as well as chemistry of their surface, which can enable various types of advanced devices with extreme efficiency. This has spurred development of various devices that incorporates nanostructure materials, and examples of such devices include solar cells, light emitting diodes and photocatalyst. In order to further the noble properties of these materials, recent studies attempt to modify their surface chemistry even using graphene oxide. Two-dimensionally structured, the graphene oxide offers band-structure that is advantageous in rendering band-structure of nanocrystals by chemically conjugated bond at interface and also extracting charge carriers from nanocrystals without significant loss. Various quasi quantum dots made of metal compound and graphene oxide have been investigated, and such studies reveal that those materials exhibit even more exciting properties than conventional quantum-dot crystals. However, with limited studies conducted on those materials, the exact nature behind exceptionally efficient photoluminescence and photocatalytic properties originated from surface graphene layer is not very well understood. Majority of studies argue that such enhancement is due to creation of new bond structure at surface, while others speculate that it may be related to activation of the intrinsic defects in metal oxide with change in the band structure.

Our team has been investigated several types of nanocrystals in terms of photo-absorption, carrier extraction and photocatalyst behaviors with a hope of shed lights to ongoing ambiguities. These studies includes quantum structure made of II-IV compounds, ZnO nano rods, and ZnO conjugated with graphene oxide. These studies reveal that many of opto-electronic properties reported in existing studies rooted more to defect chemistry of the crystal itself rather than creation of new structure. Highlights of our findings will be discussed in this paper with weighted emphasis on findings made from ZnO/Graphene oxide nanocrystals.



Sociedad Mexicana de Ciencia y Tecnología de Superficies y Materiales A.C.
X International Conference in Surfaces, Materials and Vacuum
September 25th-29th, Cd. Juarez, Chihuahua, México

THEORY AND SIMULATION OF MATERIALS (TSM)

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Raúl Esquivel-Sirvent (IFUAM)**



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[TSM-8] Semiconductor to metal transition in bidimensional CdSe and CdTe

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Abstract: We have performed first principles calculations to explore the electronic and optical properties of 2D CdSe and CdTe for both, monolayer and bilayer systems using the density functional theory as developed in the *Abinit* package. We have obtained the band gap values for all cases. In the bilayer systems, we have performed a study in which the interlayer distance is reduced in order to tune the band gap. We have determined a critical interlayer distance at which a semiconductor to metal transition occurs. This phenomenon is explained via the projected density of states (a qualitatively good approach within the standard DFT) as well as the electronic band structure corrected by the GW approximation. The study is complemented with the calculation of the dielectric function imaginary part within the Bethe-Salpeter approximation in which the excitonic and local field effects are included. The exciton binding energies are also calculated. The excitonic effects are stronger in monolayer than in the bilayer systems.



[TSM-26] **Zig-zag boron nitride nanotubes functionalization with organic molecules: a density functional study**

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First-principles total energy calculations have been employed in order to investigate the organic functionalization of zig-zag boron nitrides nanotubes (BNNTs) with acetylene molecules. Calculations have been done within the periodic density functional theory (DFT) employing the van der Waals density non-local correlation functional (vdW-DF) with the PBE correction functional. The pseudopotential scheme is used to represent the electron-ion interactions. We have considered BNNTs with different diameters in order to investigate the curvature effect in the adsorption energies. Calculations show that for small diameters chemisorption occurs with adsorption energies of the order of 1.2 eV and physisorption is observed when the diameter of the nanotube increases, the adsorption energies are of the order of 0.15 eV. The ideal BNNTs structures present weak interactions with the acetylene molecules, we generate vacancy-type defects. Boron and nitrogen vacancies have been considered to explore the interactions of the molecules with the nanotubes. Chemisorption occurs with adsorption energies of the order of 5 eV. We find that in the case of boron vacancies the nanotube (9, 0) presents the strongest adsorption energies with 5.32 eV and in the case of nitrogen vacancies the nanotube (4, 0) shows the strongest adsorption energy with 4.60 eV. Studies of the density of states (DOS) show that the organic molecule modifies the electronic structure.



[TSM-30] **Ab initio calculations of Ce, Er and Yb doped SrTiO₃ with perovskite structure**

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Total energy Density Functional Theory (DFT) calculations were performed for undoped and doped strontium titanate (SrTiO₃) with perovskite structure. Dopant atoms are rare earths cerium (Ce), erbium (Er) and yttrium (Yt). Structural and electronic properties were studied. The calculations were performed using the PWscf code of the Quantum ESPRESSO Package. The doping was studied using a 2x2x2 supercell. One dopant atom per supercell was considered, which corresponds to 12.5% atomic concentration. The presence first neighbors' equilibrium positions are modified when we doped the SrTiO₃ with Ce and Er, but they don't change with Yb. Electronic properties were studied through DOS, PDOS, band structure, Lowdin charges and charge density maps. Undoped SrTiO₃ band structure exhibit a semiconductor behavior, with an indirect band gap of 2.4 eV and a direct band gap of 2.9 eV. Formation energies suggest a most favorable substitution of Sr than Ti in the studied cases. PDOS results show that Ce, Er and Yb dopants generate a partially filled band where the gap was in the undoped case. These bands come from dopants 4f orbitals. This effect is probably due the high dopant concentration. Ce and Yb doped systems behave as metals while Er doped SrTiO₃ behave as semimetal. Charge density maps reveal a high concentration of charge in oxygen atoms in the undoped and doped cases. Also Er and Yb shows a large charge density around them.



[TSM-47] First principles calculations of MoS₂/Graphene bilayers

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Van der Waals heterostructures supply novel applications due to combinations of materials properties. We present first principles calculations to study electronic and structural properties of MoS₂/Graphene bilayer. We used SIESTA package. The energy cutoff was set to 200 Ry and DZP basis-set were used. The MoS₂/Graphene heterostructure was formed by a 2x2 MoS₂ on 2x2 graphene layer. MoS₂ has a lattice parameter of 3.16 Å whereas graphene has 2.46 Å. The mismatch between the layers is about 28%. In order to avoid this mismatch we performed a rotation by an angle of 19°, turning the graphene layer with respect to MoS₂ layer and we obtained a supercell with 26 atoms. We report in this work the bond length between Mo and S, C-C, the band gap and the density of states of the system. We found that the equilibrium position graphene lies 3.19 Å above the S plane of MoS₂.



[TSM-67] **Three-Dimensional Time-Resolved analysis of CdTe heterostructures modelled using Molecular Dynamics**

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Molecular Dynamics (MD) simulations in conjunction with visualization techniques offer unique 3D time-resolved representation of the growth of CdTe with atomic scale resolution. Studying the CdTe at the atomic scale is crucial for the development of good quality CdTe solar cells. Experimental techniques such as Transmission Electron Microscope (TEM) and Atomic Probe Tomography (APT) have recently been used for the study of CdTe with atomic scale resolution. However, these techniques are expensive and time consuming. On the contrary, MD simulations offer a rapid technique to study the structural characteristics at the atomic scale. In this work, we study the 3D time-resolved structures resulted from the MD simulation of CdTe on monocrystalline and polycrystalline substrates. 3D animation across the samples at different thicknesses reveals the resulted shape after growth of various defects such as grain boundaries within a volume of 6000 nm³. Similarly, 3D animation across the samples at different thicknesses and different deposition times reveal the evolution of defects such as stacking faults in the bulk. Both zincblende and wurtzite structures are observed within both the monocrystalline and polycrystalline samples as found experimentally. Overall, highly similar morphology to that of experimental findings is predicted.



[TSM-113] Mn induced 1×2 reconstruction in the τ -MnAl(001) surface

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Spin-polarized first principles total energy calculations have been applied to describe the structural, electronic and magnetic properties of MnAl(001) surfaces. We have concentrated in structural models having 1×1 and 1×2 periodicities, since recent experiments on the similar MnGa(001) surface have found 1×1 and 1×2 reconstructions. Our calculations show the existence of two stable structures for different ranges of chemical potential. An 1×1 surface is stable for Al-rich conditions, whereas a Mn-induced 1×2 reconstruction appears after increasing the Mn chemical potential up to Mn-rich conditions. The Mn layers in both structures have ferromagnetic arrangements, but they are aligned antiferromagnetically with the almost no magnetic Al atoms. Moreover, the on top Mn atoms, which produce the 1×2 reconstruction, align antiferromagnetically with the second layer Mn atoms. These findings are similar to those obtained experimentally in MnGa(001) thin films.



[TSM-212] Formaldehyde Adsorption on Graphane

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Interest in adsorption of organic molecules on graphene has been greater in recent years [1], and hydrogenation of graphene has been demonstrated experimentally [2]. Fictionalization of hydrogenated graphene with organic molecules is of great interest for different sensing applications. Using first principles calculations, we have studied the adsorption of a formaldehyde molecule on a hydrogenated graphene substrate, by a free radical initiated reaction. This kind of reaction begins at a hydrogen vacancy on the graphane layer, in which, the oxygen atom of the formaldehyde molecule attaches. Then, the nearest hydrogen atom is abstracted by the carbon atom of the formaldehyde, forming a stable molecule, and leaving behind a new dangling bond on the graphane substrate. Our calculations show that the reaction has an energy barrier of the order of 0.56 eV, larger than in the case of silicane [3], indicating that graphane is not a very good substrate for formaldehyde adsorption. Analysis of the electronic structure and spin density distributions help us to understand the proposed reaction.

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[TSM-306] Polymorphism in Ligand-Protected Gold Clusters: The Au₁₄₄ case.

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Ligand protected metal clusters have been thoroughly investigated recently thanks to the prominent place they have in the nanoscale, and to the advancements in experimental methods that allow to get more precise results. Among their features of interest are the properties and morphologies of their core structures, the chemical composition of their ligands themselves, and the way they interact with other structures. Isomers for the allowed core sizes have been mostly characterized, and they rarely change upon ligand adsorption. The Au₁₄₄ cluster protected by ligands has been already studied by several groups and has been characterized as an icosahedron, until a group recently claimed to have found it to be a decahedron. In this work, we use first principle calculations to study the polymorphism of the Au₁₄₄ cluster protected by ligands, by analyzing both the alleged core structures alone, and the influence the ligands induce upon them.



[TSM-7] Magnetic behavior of small CoAu nanoalloys and Co@Au structures

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In this study we report the magnetism of small Co_xAu_y ($x + y \leq 4$) bimetallic clusters and Co@Au structures Co@Au_{12} , $\text{Co}_2\text{@Au}_{17}$ and $\text{Co}_{13}\text{@Au}_4$. Our results show that all the structures considered here show magnetic behavior. For the small CoAu nanoalloys, the global minimum structures prefer planar structures whereas for the core-shell clusters prefer like-icosahedral geometries, except Co@Au_{12} whose minimum global structure is a cubo-octahedron. Our results show the Co atoms are totally covered by Au atoms, these results are in good agreement with other theoretical results and experimental results. The calculations have been performed using the ab-initio total energy and molecular dynamics program VASP (Vienna Ab-initio Simulation Program). VASP solves the Kohn-Sham equations in the augmented plane wave basis set, taking into account the core electrons within the projector augmented wave (PAW) method. For small CoAu nanoalloys, the total magnetization increases with the number of Co atoms in the cluster, whereas for Co@Au clusters, the total magnetization corresponds to the magnetization of Co clusters in the structures.

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[TSM-9] Zinc-blende MnN bilayer formation on the cubic GaN(111)-(2x2) surface: First principles studies

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Atomic layers of manganese nitride (MnN), deposited on the cubic gallium nitride (GaN) (111) surface, are investigated using spin polarized periodic density functional theory calculations, as implemented in the PWscf code of the quantum ESPRESSO package. The adsorption of a manganese atom has been evaluated at different high symmetry sites. Incorporation into the GaN substrate by replacing gallium atoms drives the formation of a site in which the displaced Ga atom forms bonds with Ga and/or Mn atoms at the surface. The energetically favorable configurations show ferromagnetic alignment. Surface formation energy calculations demonstrate that when a full Mn ML is incorporated into the GaN structure, a Ga ML on top of a MnN bilayer may be formed under very Ga-rich conditions. On the other hand, when a full Mn ML is deposited on top of the nitrogen terminated surface, an epitaxial MnN bilayer (with cubic structure) is formed with antiferromagnetic characteristics. Density of states and partial density of states are reported to show the antiferromagnetic alignment in both structures. This behavior is mainly induced by the Mn-d orbitals.



[TSM-10] Numerical evaluation of residual stress on Fe₂B coating

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The present study employ the finite element method for evaluate of thermal residual stress across Fe₂B coatings produced on surface AISI 4140, taking into account the power-pack boriding condition. The thermochemical treatment was carry out at 1173, 1223 and 1273 K, for 8 h time exposition for each temperature. The morphology of the boride layer is saw-toothed, due to the tendency of Fe₂B crystals to grow along a direction of minimum resistance, perpendicular to the external surface and have influenced by the presence of residual stresses [1].

The results of numerical evaluation was carried out in program with code of element finite and the results were compared from the literature data [2]. It was found that the residual stress varied with the temperature and the thickness of the coating, also the distributions of residual stress determined in the Fe₂B coatings are compressive with magnitudes ranging from -1211 to -1349 MPa.



[TSM-13] Magnetism of Fe₁₂, Pt₁₂ and FePt₁₁ clusters

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FePt nanoalloys are candidates for ultrahigh-density magnetic recording media due to their high magnetic anisotropy. Thus, intermixed Fe-Pt nanoparticles exhibit ferromagnetic-like behavior, which can be contrasted to pure Pt and Fe clusters. We report DFT calculations using VASP (Vienna ab-initio Simulation Program) code with the Perdew-Burke-Ernzenhorf 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 (PAW) method. Our results show that all the clusters considered in this work present magnetic behavior where all the local magnetic moments point in the same direction, in all the clusters Fe and Pt atoms tend to mix with each other due to the energetically favorable Fe-Pt bonds.

This work was done with financial support of CONACyT with "Proyecto Aprobado por el Fondo Sectorial de Investigación para la Educación" with reference number 237882



[TSM-28] Optical properties calculations of the phosphorene-CrO₃ system within the G₀W₀ and BSE approximations

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Phosphorene, the two-dimensional counterpart of black phosphorus, is under current intense investigation in order to be applied in gas sensor devices. In regard to the material excited-state properties, these may be sensitive to molecular adsorption. Therefore, in this work we theoretically study the change in the optical properties of phosphorene-CrO₃ systems considering different CrO₃ surface coverage (0.0%, 34.3% and 68.6%). The CrO₃ molecule is a powerful oxidizer and a suspected carcinogen. To determine rigorously the optical properties of CrO₃ adsorbed on a surface is mandatory the use of the G₀W₀ approximation and the solution of the Bethe-Salpeter equation (BSE) with the inclusion of van der Waals forces. As part of the results, this work shows the electrical band gap values obtained by the application of the G₀W₀ approximation, optical band gap values derived from the solution of the BSE and an analysis on the optical in-plane anisotropy of the composed phosphorene-CrO₃ systems. Ultimately, results show that the band gap, the optical absorption spectrum and the optical in-plane anisotropy of phosphorene can be broadly tuned by changing the amount of CrO₃ surface coverage and molecular disposition.



[TSM-35] Strontium germanate doped with europium: ab initio study

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In this work we present an ab initio study of strontium germanate in perovskite form. We used DFT based software, Quantum ESPRESSO, to calculate the structural and electronic properties of the pristine material using two different sets of pseudopotentials. Total energy calculations were performed in order to optimize the cell parameter. In addition, a substitutional atomic doping study was considered, a strontium atom was replaced by a europium atom. The doping was made with two different atomic europium concentrations per super cell size, $x=12.5\%$ and $x=3.7\%$. DOS and bands diagrams have been calculated for SrGeO₃ for the three cases. Charge diagrams has been calculated as well. We show that europium doped strontium germanate improves its electronic properties.



[TSM-50] Studies of first principles of PbS phase

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Lead sulphide, PbS, is a semiconductor material that exhibits variation of the electrical resistance when exposed to infrared radiation, with a prohibited bandwidth by volume of 0.41 eV and with a NaCl crystal structure. This compound is of interest due to its application in the development of optoelectronic devices such as sensors, photovoltaic cells and laser diodes which in turn have wide application in medical technology and in industry. Recent research on PbS shows that it can present different types of stable or meta-stable crystalline structure, which modifies its band structure and gap. First principles calculations have been carried out to determine the structural stability and electronic properties of the PbS compound in the NaCl phase in order to predict possible phase transitions using the DFT, pseudopotential and the local density approximation (LDA). It has been found that the PbS can have different phases applying an external pressure, TII (Cmcm), FeB (Pnma), both are orthorhombic phases, α -GeTe (R3m) cubic phase, analyzing the band structure it is evident that the orthorhombic phases have a semiconductor behavior as opposed to the cubic phase that presents a metallic behavior. The change of phase and therefore in the electronic properties of the PbS will allow to use it in new infrared devices.



[TSM-65] Effect of imperfect contact conditions in piezoelectric composites. application to one-dimensional case

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The development of analytical and numerical models for the knowledge of the physical properties and the couplings phenomena of composite materials have been useful tools for the characterization of multifunctional materials. Through them, it is possible to analyze and understand the design and behavior of heterogeneous material systems.

In this work, the statement of the problem for heterogeneous piezoelectric composite with mechanical and electrical imperfect contact condition is given. Here, a semi-analytical model by mean of asymptotic homogenization method and finite element method is developed to study the behavior of piezoelectric periodic structures. Analytical expressions of the local problems and the elastic, piezoelectric and dielectric permittivity effective properties obtained by asymptotic homogenization method are shown. The local problems solutions are determined by finite element method through the problem's discretization. As an illustrative example, a one-dimensional two-phase periodic piezoelectric composite is considered. Some numerical examples are presented under the presence of both types of imperfection at the interface.



[TSM-66] First principles calculations of BN nanowires

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Studies have been performed on nanowires in the wurtzite crystal structure with the growth axis being along the [0001] direction and having different diameter. The calculations were performed using the PWscf of Quantum ESPRESSO package in the DFT theoretical frame. The GGA approximation was used to treat the exchange correlation energy. Ultrasoft pseudopotentials were used as well. At first, the lattice parameter of BN wurtzite was optimized, it was obtained $a = 2.56 \text{ \AA}$ and $c = 4.23 \text{ \AA}$. Three different diameters were considered for nanowires structures, $d1 = 3.63 \text{ \AA}$, $d2 = 7.26 \text{ \AA}$ and $d3 = 8.01 \text{ \AA}$. Electronic bands structure was calculated for each nanowire and the results indicated a semiconductor behavior in each case. The band gaps calculated are 1.6 eV, 2.3 eV, 3.6 eV respectively. It was observed that as the diameter increases the band gap tends to an insulate behavior.



[TSM-72] First Principles Studies of structural and electronic properties of hydroxyapatite and graphene oxide

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The hydroxyapatite (HAp) [Ca₁₀(PO₄)₆(OH)₂] is the main mineral constituent of bones, 70% by weight of human bone is a modified form of hydroxylapatite. Since HAp provides hardness and rigidity to bones, it would be the ideal biomaterial to replace it, nevertheless, because of its poor mechanical properties, it is only used as filler and support. On the other hand the graphene, an carbon atom sheet, is an exceptional material with very special properties, such as high biocompatibility, superconductivity, hardness and flexibility.

The main purpose of this work is to model the structure and electronic properties of the HAp and graphene oxide (GO). HAp and GO to find ways to improve its characteristics using atomic and molecular simulation employing SIESTA, Quantum Espresso and Materials Studio softwares. HAp and GO structures and properties were studied from first principles approaches based on Density Functional Theory (DFT) to obtain the electron distribution, charge density, electrostatic potential, total energies, forces and stresses. Several pseudopotentials were tested to perform the geometry optimization in order to found the optimal structure parameters such as, atomic positions and lattice parameters in addition to the electronic properties. For both materials our results the optimization (lattice parameters and atoms position) and electronic properties according with theoretical and experimental previously reported results [1-4].

Key words: hydroxyapatite, graphene, properties, DFT simulation.

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[TSM-97] Antiplane effective properties for a piezoelectric composite based on a semi-analytical model

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Calculation of composite materials physical properties applying analytical and numerical methods is a topic of nowadays interest. They support the development of new materials with improved properties. In addition, they provide a better understanding of the heterogeneous material complex behaviors. In the present work, a semi-analytical model is developed to calculate the antiplane effective elastic, dielectric and piezoelectric properties based on a combination of the asymptotic homogenization and finite elements methods. Analytical expressions for the effective properties are reported as a result of applying the asymptotic homogenization. Local problems solutions are needed to obtain the effective properties. These problems are solved by means of the finite element method considering a high order approximation (8 nodes quadrilateral elements). Some numerical results and comparison with literature are reported.



[TSM-99] Numerical evaluation of residual stress on Fe₂B coating

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The present study employ the finite element method for evaluate of thermal residual stress across Fe₂B coatings produced on surface AISI 4140, taking into account the power-pack boriding condition. The thermochemical treatment was carry out at 1173, 1223 and 1273 K, for 8 h time exposition for each temperature. The morphology of the boride layer is saw-toothed, due to the tendency of Fe₂B crystals to grow along a direction of minimum resistance, perpendicular to the external surface and have influenced by the presence of residual stresses [1].

The results of numerical evaluation was carried out in program with code of element finite and the results were compared from the literature data [2]. It was found that the residual stress varied with the temperature and the thickness of the coating, also the distributions of residual stress determined in the Fe₂B coatings are compressive with magnitudes ranging from -1211 to -1349 MPa.



[TSM-144] GaAs on High-Index-Si: A DFT study

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Silicon (Si) is the basic material for semiconductor devices due to the advantages that it presents among them: good mechanical and thermal characteristics and low cost. On the other hand, the III-V compounds, in particular GaAs, offers many advantages over Si such as high carrier mobility and excellent photon emission properties. Therefore, there is a great interest to monolithically integrate the technology of Si with that of GaAs, through the growth of GaAs on Si substrates. This is not an easy task, because there exist a mismatching between their lattice constants and an important difference in their thermal expansion coefficients, which promotes the generation of dislocations and antiphase domains at the interface GaAs-Si. An interesting alternative to face this problem is the use of high-index (HI) Si substrates.

In order to study in depth the physics involved in the interface formation of GaAs/HI-Si, we present the study of the adsorption of GaAs on Si oriented in different crystallographic directions. The pseudopotential density functional theory (DFT) is used for the calculations. Within the DFT approach, we use the ultrasoft pseudopotential approximation for the electron-ion interaction and a plane wave basis set for the wave functions with the use of the PWscf code. For our considered structures, the cutoff energy for the plane wave expansion is taken to be 476 eV. The structure was simulated in two dimensions. The geometry and size in of supercell has been changed according to the studied crystallographic direction and the Γ point for the Brillouin zone integration. In all cases, we have used the Perdew-Burke-Ernzerhof (PBE) pseudopotential with fully unconstrained structural optimizations, using the conjugate gradient method. The convergence in energy was set as 1 meV. We first find stable surfaces for Si in a number of high-index directions. Then, Ga and As atoms are deposited on the silicon optimized surfaces. By means of this simulations we tried to get a criterion for the choice of Si crystallographic directions which could reduce the apparition of interphase defects.



[TSM-184] Structural and electronic properties of III-V nanowires: DFT calculations

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Structural and electronic properties of III-V nanowires have been investigated using first principles total energy calculations within the periodic density functional theory (DFT). Studies have been performed on BN, AlN and InN nanowires in the wurtzite crystal structure with the growth axis being along the [0001] direction and having different diameter. Dangling bonds are present on the relaxed nanowire surface atoms it produces displacement on the nanowire outer atoms. Band structure and density of states (DOS) calculations indicate that the different III-V nanowires behave as semiconductor materials. The partial density of states (PDOS) shows that the valence bands are formed mainly by N-2p orbitals. Formation energy studies were developed. Results reveal that nanowires with larger diameter are more stable than thinner ones.



[TSM-201] DFT study of oxygen adsorption on graphene sheets.

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First principles total energy calculations have been performed to study the structural properties of graphene oxide. Calculations have been performed within the periodic density functional theory as implemented in the PWscf code of the QUANTUM ESPRESSO package. The exchange-correlation energies are treated with the generalized gradient approximation (GGA). Electron-ion interactions are modeled with pseudopotentials. The electron states are expanded in plane waves with an energy cutoff of 30 Ry. 3 x 3 x 1 and 4 x 4 x 1 hexagonal supercell periodicity has been considered. Oxygen atom was placed at different adsorption sites. The results indicate that the most stable configuration corresponds to oxygen atom placed over the C-C bond with adsorption energy of -3.156 eV approximately in both periodicities. The C-C length bond results to be 1.49 Å, while C-O bond is 1.50 Å. Electronic structure calculations indicate a direct band gap near of symmetry k-point with 1.318 eV amplitude. Therefore, we conclude that oxygen adsorption significantly modify the electronic properties of graphene.



[TSM-211] Gallium adsorption on the AlP(111) surface: Density functional theory calculations

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Gallium (Ga) adsorption on the aluminum phosphide (AlP) surface and incorporation into AlP atomic structure are investigated by first principles total energy calculations within the density functional theory as developed in PWscf code of the quantum ESPRESSO package. The electron-ion interactions are described with pseudopotentials and the exchange-correlation energies are treated according to the generalized gradient approximation with the PBE parameterization. Electron states are expanded in plane waves with an energy cut of 30 Ry. To deal with the AlP(111)-(2x2) surface the supercell method is applied. The AlP(111)-(2x2) supercell is composed of a slab containing four Al-P bilayers, each Al (P) monolayer has four Al (P) atoms. The dangling bonds of the bottom surface are saturated with pseudo-hydrogen atoms. To simulate bulk-like environment the lowest Al-P bilayer and the hydrogen atoms are frozen at their ideal positions. An empty space of the order of 15 Å is considered to preclude charge transfer between adjacent slabs. The Ga adsorption and incorporation of $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$ and 1 monolayer are investigated at high symmetry sites: H3, T4, Top and Bridge. Results indicate that the Ga structure formation with different Ga coverage stabilizes at the T4 configuration. However, surface formation energy (SFE) calculations indicate that the most stable structure is the $\frac{1}{4}$ of Ga monolayer adsorption at the T4 site. The total density of states (DOS) and projected DOS are determined to describe electronic properties.



[TSM-219] Variation of volume of unit cell of Mg_xM_{1-x} alloys (M= Al, Ni, Zn; $1.0 \leq x \leq 0.8$)

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In this work we use Density Functional Theory (DFT) and the module CASTEP of the Molecular simulation program Materials Studio, to obtain geometric optimization of three alloys, magnesium-aluminum, magnesium-nickel and magnesium-zinc ($Mg_{1-x}M_x$) for concentrations of magnesium between 0.8 and 1.0, in a crystalline hexagonal closed packed (hcp) unit cell. We optimize the bulk geometry of the alloy and expect that the values of the volume of the unit cell will decrease in the case of the magnesium-aluminum alloy, remain almost constant in the case of the magnesium-nickel alloy and will increase the case of the magnesium-zinc alloy, all this compared to the volume of the unit cell of magnesium.

Keywords: Volume unit cell, geometric optimization, magnesium-aluminum alloy, magnesium-nickel alloy, magnesium-zinc alloy.



[TSM-222] Electronic charge transfer in $Mg_xM_{1-x}H_2$ alloys (M= Al, Ni, Zn; $1.0 \geq x \geq 0.8$)

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In this work we use Density Functional Theory (DFT) and the module CASTEP of the Molecular simulation program Materials Studio, to obtain electronic charge transfer of three hydride metals, magnesium-aluminum, magnesium-nickel and magnesium-zinc ($Mg_{1-x}M_x-H_2$) for concentrations of magnesium between 0.8 and 1.0, in a crystalline hexagonal closed packed (hcp) unit cell. We cleave the bulk alloy in the direction (110) and then interact hydrogen molecule on this surface and optimize the structure of the supercell with hydrogen and without hydrogen. We compare the result of the electronic density of states before and after that the molecule of hydrogen interacts with the surface of the metallic alloy.

Keywords: Electronic charge transfer, magnesium-aluminum alloy, magnesium-nickel alloy, magnesium-zinc alloy.



[TSM-285] Designing a High-Q photonic crystal cavity with Genetic Algorithms

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Cavities in photonic crystals are produced by introducing a defect in otherwise perfect structure. In this work the photonic crystal slab with a triangular lattice of holes is studied, special attention is focused on the L3 defect which consists in removal of three defects along the ΓJ orientation of the lattice. Starting by considering random configurations which consist of shifting the positions and sizes of holes nearby the defect, the configurations are allowed to evolve by using the rules of genetic algorithm searching for high Q-factor cavities, the Q-factor is computed using FDTD. The configurations with the highest Q factors are reported as a function of either the holes position and/or hole radius size.



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THIN FILMS (THF)

Chairmen: Alberto Duarte Moller (CIMAV-Chihuahua)



[THF-14] Study of annealing effects on the physical properties of Bi₂S₃ thin films obtained by chemical bath deposition

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Bi₂S₃ is a metal chalcogenide semiconductor, the optical absorption spectrum of which overlaps reasonably well with the visible and near-infrared part of the solar spectrum. This makes it interesting for electronic applications for example in the development of photovoltaic devices. A large number of methods such as solvothermal, solvent less thermolysis hydrothermal, single source precursor etc. have been employed for the synthesis of Bi₂S₃. In this work Bi₂S₃ thin films grown in monolayers, bilayers and three-layers have been successfully obtained by chemical deposition method. However, most of the optoelectronic applications require of an enhanced electrical and optical behavior. This study focuses on the effect of the annealing process to improve morphological, structural and optical characteristics of the obtained thin films. The annealing process was proposed as a single exposure at 130, 170, and 210 °C in air atmosphere for 5 minutes of thin films. A novel approach was proposed by using microwave radiation as a way of annealing on the same total exposure time at different steps: five times one minute, two times two and a half minutes and one time five minutes. Traditional annealing and microwave annealing were compared. Optical characterization was made to confirm the effect on annealing as well as band gap estimation and four probe measures. SEM micrographics confirm the morphological changes on thin films as a shift to a crystalline conformation supported by DRX analysis. Bi₂S₃ thin films make them a suitable candidate for device applications at low temperature processing.



[THF-37] CuAlO₂ semiconductor films prepared from new precursors by spray pyrolysis method

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The Transparent Conductive Oxides (TCOs), as the CuAlO₂ delafossite phase, are used for creating thin conductive layers for a variety of semiconductor applications such as LEDs and sensors. The CuAlO₂ delafossite phase shows a good p-type conductivity and at the same time an enhanced optical transparency in the visible range of the electromagnetic spectrum respect to other TCOs. This material has been traditionally synthesized by High-Temperature Solid State Methods with large reaction time (24-72 h) and temperatures values as high as 1000- 1200 °C at low oxygen partial pressures (pO₂). Recently, a lot of works has been devoted to preparing CuAlO₂ delafossite materials by thin film methods, but low pO₂ (10⁻⁹-10⁻³ atm) during the films deposition and later a heating process in an inert gas to reach good electronic and optical properties were necessary. The present work presents new precursors to prepare CuAlO₂ delafossite like semiconductor films by the Spray Pyrolysis cheap method using air as carrier gas at low temperatures. The solid precursor optimized in the previous stage (Cu-Al-citrate-ammonium nitrate) was used successfully to prepare both, granular and dense thin films in the 300-450 °C by a combination of spray pyrolysis method and autocombustion reaction. As a second precursor was used a mixture of Aluminum and cupric acetylacetonates. To the later precursor, a study of films properties as a function of the deposition temperature and the effect of adding different amounts of aluminum was carried out. Were used different solvents for the aerosol formation (water, N,N-Dimethylformamide and mixtures of them). Corning glass and (1-1-1) silicon were used as substrates and a flow rate in the 5-10 L/min range of the inert gas was employed. Transmission



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Electron Microscopy and Energy Dispersive Spectroscopy, X-ray Diffraction, Scanning Electron Microscopy, X-ray Photoelectron Spectroscopy, Uv-vis Spectroscopy, Hall Effect, and the Hot Point probe technique resulted extremely useful in characterizing the films as deposited.



[THF-40] Study of thermoelectric properties in thin films of metallic oxides

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The technique of impedance spectroscopy has been selected due to factors such as the simple experimental arrangement and the reduction of the number of equipment used to obtain the ZT figure of merit. By making changes in the structure of the thermoelectric material it is possible to improve its thermoelectric properties in such a way that it can increase the efficiency in the figure of merit. Metallic oxides generate interest in characteristics such as low toxicity, high availability and low cost, as well as good behavior at high temperatures.

In the present investigation are presented results determined by impedance spectroscopy of some thermoelectric properties as well as the equivalent circuit of the system.



[THF-69] Chemical synthesis and characterization of hafnium oxide thin films by SILAR method as dielectric material

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Hafnium oxide (HfO₂) is considered a dielectric that has the property to form electric dipoles in its interior under the action of an electric field and it has been an excellent candidate for electronic devices as it has a higher band gap. Hafnium oxide thin films have been deposited by the SILAR method using chemical precursors as hafnium chloride as a cationic source and as anionic source thioacetamide complexed with triethanolamine. Several conditions have been varied as the concentrations of each precursors, time of thermal treatment and the immersion time on the precursors and rinsing time during the deposition cycles as well as the number of deposition cycles and a post cleaning on the formed thin film. Later, the crystalline structure formation has been studied by XRD. The order of the optical transmittance and the band gap value was calculated from the UV-vis examinations. The roughness and morphology distribution was studied from SEM. This material requires high temperatures to overpass the vitreous phase.

Keywords: hafnium oxide, dielectric material, successive ionic layer adsorption and reaction (SILAR) method.



[THF-70] Synthesis and characterization of bismuth oxide thin films by SILAR method and its evaluation as semiconductor material.

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Bismuth oxides have a relevant importance for modern solid-state technology, owing to their peculiar properties such as energy band gap, refracting index, dielectric permittivity and photoconductivity. These properties have made Bi₂O₃ thin films suitable for large range of applications, such as optical coatings, photovoltaic cells, and microwave integrated circuits. Along with these applications, recently introduced applications of Bi₂O₃ films are in fuel cells, oxygen sensors and oxygen pumps. In this work, bismuth oxide (Bi₂O₃) thin films were prepared, at room temperature, by the SILAR method using chemical precursors as bismuth nitrate complexed with ammonium hydroxide as cationic solution and acid hydrochloric acid as anionic solution. Several conditions have been varied as can be the immersion time on the precursors and rinsing time during the deposition cycles as well as the number of deposition cycles and a post cleaning on the formed thin film. Thin films of Bi₂O₃ has been annealed at different temperature (573, 723 and 823 K). Later, the crystalline structure formation has been studied by XRD along with the determination of the crystallite size. Morphology distribution by SEM. The order of the optical transmittance and the band gap value were calculated from the UV-vis examinations.

Keywords: photovoltaic cells, bismuth oxide, X-ray diffraction, successive ionic layer adsorption and reaction (SILAR) method.



[THF-115] Ti-Zr-Si-N thin film deposited by reactive cosputtering

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Thin films of Ti-Zr-Si-N were grown on stainless steel 316 L substrates using the reactive magnetron cosputtering technique. The films were analyzed through structural, morphological and cyclic oxidation studies. The structure analysis was carried out using X-ray diffraction (XRD), and the morphological analysis was carried out using electron microscopy (SEM) and 3D optical microscopy. The cyclic oxidation studies were done on samples of stainless steel 316 L coated and uncoated with Ti-Zr-Si-N films changing the number of cycle at 600°C, each cycle consisting of 1 hour of heating and 0.5 hour of cooling. The coatings improved stainless steel corrosion resistance at high temperature. Corrosion mechanisms for the coatings are deposited are discussed.



[THF-134] Tribological study of Hydroxyapatite/Silver coating on stainless steel AISI 316L substrates.

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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 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 such as the plasma-spray method, 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 (AgNO₃), and phosphoric acid (H₃PO₄). 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 Vickers was evaluated to normal loads of 50 gf obtained 243.66 HV for 316L Stainless steel and 252.92 HV for the coating of HA/Ag. Wear tests were carried on by a reciprocating tribometer, employing a ball of 10mm diameter Al₂O₃, in dry conditions with a 0.5, 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); and Raman spectroscopy. The HA/Ag coating exhibited volume loss (V) of 3.48x10⁻³ mm³ and a wear rate (k) of 9.66x10⁻³ mm³/Nm against the stainless steel without coating that showed the next values of wear; volume loss



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(V) of $2.84 \times 10^{-1} \text{ mm}^3$ and a wear rate (k) of $7.89 \times 10^{-3} \text{ mm}^3/\text{Nm}$. In summary, an increase in dormancy and in the volume loss and wear rate on the coated substrate was observed with respect to the uncoated substrate, the coated substrate had a low friction coefficient (μ_k) in the tribological tests with respect to the uncoated substrate.

Keywords: Hydroxyapatite; silver; biocompatible coating; biomaterial; electrochemical deposition; stainless steel AISI 316L; tribological tests.



[THF-156] Temperature dependence of Mn₅Ge₃-Mn₁₁Ge₈ phase formation in sputtered thin films.

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Mn₅Ge₃ thin films grown on Ge(001) substrates were obtained by co-deposition of pure Mn and Ge elements using rf-magnetron sputtering at different substrate temperatures, T_s (250 °C ≤ T_s ≤ 550 °C) in order to analyze the influence of the substrate temperature on the structural and magnetic properties of the samples. These films were thoroughly studied by reflection high-energy electron diffraction, transmission electron microscopy, atomic force microscopy, and SQUID magnetometry, evidencing the important role of the substrate temperature on the microstructure of the films. For temperatures higher or equal to 350 °C, a crystalline Mn₁₁Ge₈ phase also appears in addition of the Mn₅Ge₃ one, evidenced by the diffraction and magnetic measurements. Additionally, spin-glass-like magnetic behavior is also observed in all the samples (more evident when the Mn₁₁Ge₈ phase is small), due to the existence of a layer with spin-glass properties at the Ge/Mn₅Ge₃ interface caused by the intermixing of Ge and Mn at that interface.



[THF-158] Electrical and magnetic properties of GaAsMn and GaSbMn thin films growth by magnetron sputtering

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The gallium antimonide (GaSb) gallium arsenide (GaAs) are two of the most important semiconductors with a bandgap of 0.070 eV and 1.42 eV, which falls into the red and infrared spectral region. Recent experiments have demonstrated that if the GaSb and GaAs matrix is doped with Mn, the ternary alloys of GaAsMn and GaSbMn exhibit room temperature and low temperature ferromagnetic properties, important for application in spintronic. Magnetron sputtering (MS) is a low cost non-epitaxial growth techniques, interesting for the deposition of semiconductors thin films, such as GaSbMn and GaAsMn , because that is possible to growth on crystal and amorphous substrates. In this work, we report the electrical and magnetic properties of GaSbMn and GaAsMn thin films prepared by magnetron sputtering on a glass substrate. In order to incorporate low Mn concentrations into GaSb and GaAs host, the thin films were growth at low substrate temperatures. The carrier concentrations of GaAsMn and GaSbMn were determined from Hall Effect experiments at room temperature by using standard four-probe method. Magnetization measurements as a function of magnetic field ($-500 < H < 1500\text{Oe}$) shows a paramagnetic behaviour for the samples of GaSbMn from low to room temperature. However, the GaAsMn thin films show ferromagnetic only at low temperature. These result shows that the magnetic properties are very sensible to the experimental parameters as working pressure and growth temperature.

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[THF-169] Physical properties of CdTe:Cu thin films deposited by combination of laser produced Cu and CdTe plasmas

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Cadmium telluride has shown to be an excellent material for optoelectronic applications because of its remarkable optical absorption properties in the IR-visible region of the spectrum, together with electrical conductivity, and the band gap near to the optimum value for efficient solar energy conversion. CdTe has been synthesized by several physical and chemical techniques. Deposition by laser ablation has proven to produce high quality CdTe films, depending on the laser produced plasma conditions, the crystalline structure can be controlled even at room substrate temperatures. In this work the CdTe plasma was combined with Cu plasmas by the simultaneous ablation of Cu and CdTe targets. The mean kinetic ion energy of Cu plasmas was increased from 74 to 124 eV. Plasma density increased linearly with mean kinetic ion energy. Mean kinetic ion energy and density of CdTe were kept constant at 75 eV and $2 \times 10^{14} \text{ cm}^{-3}$, respectively. Structural characterization of the films revealed that increasing energy of Cu plasma change the orientation of the films. Sample grown using energy of 124 eV is amorphous. Optical properties of the films were obtained by UV-Vis spectroscopy. Scanning electron microscopy was used to study surface morphology. The chemical composition was measured by energy dispersive X-ray spectroscopy.

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[THF-190] Morphological, dielectric and chemical characterization of coatings of nano and micro particles of aluminum hydrated silicate.

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It is well known, that there is the need of an electrostatic discharged environment in an electronics manufacturing floor. This research work has the purpose of to use coatings of nano and micro particles of Aluminum hydrated silicate ($\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2$) also known as pyrophyllite to minimize electrostatic charges. Pyrophyllite has excellent dielectric properties, the resistivity volume can go up to $500\text{M}\Omega/\text{cm}^3$, that means that it achieves the ISO 20345 standards. It is also known that the electrical properties of materials are affected by the levels of humidity. The pyrophyllite absorbs humidity and so may improve the dielectric properties of the coatings made of pyrophyllite particles.

The coatings were prepared in emulsions with a variation on the concentration of nano and micro particles of pyrophyllite of 10%, 20%, 30% wt. The substrates covered with the coatings were characterized in terms of the specific covered surface area, particle size distribution, particle concentration, particle morphology and coatings thickness by means of SEM and chemical composition by means of XPS.

The electrical properties of the coatings were measured by means of a surface voltmeter. The results showed that the dielectric properties of the coatings of micro particles of Pyrophyllite at the lowest concentration improve the performance of the substrate in terms of resistance to electrical charges.



[THF-203] Structural and optical properties of ZnO films fabricated by Screen Printing, for futures solar cells applications.

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Semiconductors in the form of thin films are essential components in the development of solar devices. Uniformity in thickness and composition is then crucial for its application; therefore conditions of deposit are the key for its performance. There exist a variety of techniques and chemical methods by which thin films can be obtained. The screen printing technique is a simple and low cost synthesis method for deposited semiconductor and composites materials. The Zinc Oxide (ZnO) is an important group II-VI metal oxide semiconductor (MOS) used for widely applications like electronic sensors and opto-electronic devices. It exhibits n-type semiconducting properties for the which has many potential applications in fields such as solar cell, light emitting diode, sensors and anti-bacterial.

For this properties the ZnO films are good candidate for used in solar cells, in this work we used this material as n-type semiconductor in a quantum dots PbS solar cell. ZnO films have been prepared by screen-printing technique followed by an adequate heat treatment, we added zinc chloride (ZnCl₂) powder as adhesive and propylene glycol as a binder. The paste thus prepared was screen printed on to a glass substrate and then dried at 200°C for 60 min. The obtained films were characterized structural, optical and electrical.



[THF-215] Resistive switching on Au/La_{0.3}Ca_{0.7}MnO₃/YBa₂Cu₃O_{7-δ}/SrTiO₃ growth on sputtering DC

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It was studied the resistive switching on heterostructures composites with YBa₂Cu₃O_{7-δ} (YBCO) as a bottom electrode and La_{0.3}Ca_{0.7}MnO₃ (LCMO) complex oxide as an insulator layer using a top electrode of Au; the layers were growth in SrTiO₃ (STO) and Sr_xNd_{1-x}TiO₃ (SNTO) substrates and deposited by sputtering DC at high pressure of oxygen (2mbar) and the temperature of 830°C. All the measurement were made a room temperature, where the YBCO have like a metal behavior, also it has a perovskite structure like the LCMO and its deposition temperature. It was carried up an electric characterization with I(V), ρ(T) curves and x ray diffraction to the Au/LCMO/SNTO and the heterostructures Au/LCMO/YBCO/STO with the purpose of analyzing the conduction mechanisms and compare both types of structures, electrical and the resistive switching behaviors. Atomic force microscopy were carried up to analyze the surface of the layers of Au/LCMO/SNTO and the change with the insertion of the YBCO like a bottom electrode. The implications of the stacking an oxide superconducting as an electrode (YBCO) below to a manganite insulator layer (LCMO) with the phenomena of resistive switching and the movement of the oxygen vacancies, conducting mechanisms like space charge limited conduction (SCLC) and a structure deformations were taken in count for the study.



[THF-240] Mechanisms behind the tribological performance of the catalytically active nanocomposite coating

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Lubricants and coatings are playing an important role in the improvement of the durability of components in a diverse number of mechanical applications, as well as reducing the energy consumption through reducing friction under sliding and rolling conditions. The catalytically active coating that we are presenting in this work is made of a metal nitride and a catalyst metal, and is able to reduce friction by at least 20% and decrease the wear of the sliding surfaces to very marginal levels [1]. Here we present the mechanisms that enable a catalytically active coating to extract protective lubricious carbon-based tribofilms directly from the hydrocarbon molecules of the lubricating oil. During the systematic investigation, we found that the metal catalysts are able to reduce the energy that is necessary to crack the hydrocarbon molecules. In this work the use of different tribometers (i.e., Pin-on-Disc and High Frequency Reciprocating Rig) and advanced characterization techniques (such as Raman Microscopy, TOF-SIMS and HR-TEM) allow us to visualize and confirm the presence of the amorphous carbon-based tribofilms. Furthermore, the use of MD and ab-initio molecular dynamics help to confirm the very specific stages that lead to the formation of this solid lubricious film extracted from a liquid lubricant. We will also discuss the effects of having less catalyst in the coating on the formation of the carbon-based tribofilms.

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[THF-23] Synthesis of Oligoparaphenylene with CN functional group deposited on a PVA matrix by Sol-Gel

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In flexible electronic area the use of plastic substrates obtained by solution processable synthesis are preferred because they are easily formed using low-temperature processing, large area applications, compatibility with light weight, and mechanically flexible. In the same way the optimization in the electronic device construction to fewer steps is still a challenge to overcome. The present work is divided into two sections, on the first one, oligoparaphenylene was synthesized by the boration of precursor and Suzuki-Miyaura cross coupling reaction catalyzed by palladium. The molecule was chemical and optical characterized in order to evaluate its properties. The second part, membranes and substrates of PVA with oligoparaphenylene were synthesized by sol gel process. The membranes and substrates were chemical, optical and morphologically characterized in order to evaluate its potential applications in electronic area. The membranes and substrates exhibit remarkable improvement in the chemical and optical properties like a displacement in the band gap with the inclusion of the molecule on the structure. The properties obtained for the new materials offer a very promising in the fabrication of electronic flexible devices.



[THF-31] Pentacene thin films by spin coating technique at room temperature: Effect of solvent dispersion

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Pentacene is an important alternative of amorphous silicon semiconductor in the inorganic electronics field. In this work, we report thin films deposited by spin coating technique of pentacene solutions using different solvents. Pentacene was studied by Fourier Transform Infrared Spectroscopy (FTIR) and ¹H-Nuclear Magnetic Resonance Spectroscopy (¹H-NMR) for chemical characterization. In order to evaluate the behavior of pentacene in solution, pentacene was dispersed in 1,2- dichlorobenzene and chloroform as well. Then thin films were obtained from two different solutions by spin coating technique at room temperature and annealed process was applied. Finally, the films were optical and microstructurally characterized by UV-Vis, RAMAN and AFM techniques respectively. Thin films depositions presented here provides an affordable pentacene films, which can be further applied for research and development of organic electronic applications.



[THF-48] Fresnel coefficients for a multilayer conducting system

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We study the long—range surface-plasma waves found by Sarid using the Sarid configuration, based on total attenuated reflection (ATR). The influence of the incident beam wave on the coupling with surfaces plasmons is analyzed and compared with those obtained using the classical Kretschmann arrangement. We show that these surface waves are more sensitive to the characteristics of the incident beam than the surface plasma waves excited by the Kretschmann configuration.



[THF-73] Growth of SmFeOx thin films as precursors of iron-arsenic based superconducting systems

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Based on the new class of high temperature superconductors (HTs) called "pnictides" containing arsenic, iron and lanthanide, we present here preliminary studies on the growth of SmFeOx precursor thin films. The films have been grown by Metalorganic Chemical Vapour Deposition (MOCVD). The results of the composition evaluated by an energy dispersive X-ray analysis probe (EDX), and results of crystallographic evolution obtained by X-ray diffraction, for different conditions of growth are presented. These indicate that precursor films contain Fe-Sm oxides. The studies will be used with the purpose of optimizing the morphology and chemical composition of precursor films, fundamentally relevant properties in the subsequent processes aimed at the obtaining and optimization of iron-arsenic based superconducting systems in form of thin film.



[THF-92] Detailed study of the magnetic behavior at low scale in $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$

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$\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ (LSMO) is the most interesting compound of the manganite perovskite family due to its Curie temperature above room temperature that makes its remarkable physical properties desirable for practical applications as magnetic sensors. However, it is well known that the ferromagnetic properties of a material weaken in the presence of reduced dimensions. In this research, we have grown $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ thin films by sputtering DC in pure oxygen atmosphere on SrTiO_3 (001) substrates at temperature of 830 °C. From x-ray diffraction (XRD) analysis, we found the Bragg peaks for LSMO thin films only (002) peaks are observed indicating a textured growth. We have characterized morphologically samples by atomic force microscopy (AFM). Additionally, LSMO thin film was patterned by lithography, the sample fabrication consist of creating a well defined channel with current and voltage leads enabling four point resistance measurements. Dependence of resistivity with temperature shows a behavior typical of this ferromagnetic system with metal-insulator transition above 300 K. The devices electrical properties will be contrasted with thin film. We carried out isothermal resistance and magnetization versus applied magnetic field loops to characterize the samples. We study the dependence of magnetic transport properties with film thickness of 25 nm and wire channel size (width and length) for potential applications like magnetic sensors.



[THF-152] Influence of oxygen for crystalline phases formation in Zr thin films, produced under heat treatment in different environments.

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Zirconium oxide is one of the most studied materials, because of the broad range of uses that characterize it. It is known that under heat treatment, Zr undergoes unpredictable and abrupt phase changes. In the present work it is made a study in which effects in Zr thin films are analyzed, when they are submitted to heat treatment in two different environments: in the presence of oxygen and in vacuum (1.0×10^{-5} mBar). Zirconium thin films were deposited at room temperature, by sputtering on silicon substrates and glass, and 500nm of thickness. Later they were submitted to temperatures above room temperature, near 600°C. The morphologic characterization was made by atomic force microscopy (AFM). Structure characterization was made by the use of the Raman spectroscopy. Results show the oxygen presence importance for the different crystallization phases and the sequence of appearance of each of them as the oxygen and temperature changes.



[THF-171] Synthesis of PbS Thin Films by Chemical Bath Deposition

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Commonly, lead sulfide (PbS) semiconductor is a film used for detection devices due to its band gap of 0.37 eV. Solar cells, infrared detectors, as well as thin-film transistors are some of the applications where PbS have been used. Different synthesis methods for this semiconductor have been previously reported, such as electro-deposition, spin-coating, pulsed laser deposition, spray-pyrolysis, chemical bath deposition (CBD), among others. However, these techniques shown a slow growth where thick films are required for light-detection. In this work, we present a traditional CBD synthesis of PbS films by using three different formulations with different complex agents. Commonly, for PbS synthesis triethanolamine (TEA, C₆H₁₅NO₃) is used as complex agent, while sodium hydroxide (NaOH), sulfide ions (thiourea, CH₄N₂S) and lead acetate (Pb(CH₃COO)₂) are used as precursors. Here, we present a comparison of this formulation with two different complex agents. One of them is a combination of PEI with ammonium nitride (NH₄(NO)₃), while the other uses polyethylenimine (PEI, (C₂H₅N)_n) instead of TEA. Chemical and structural analysis was analyzed by XPS, EDAX, SEM, XRD and TEM. The PbS films shown an increase for the deposition rate by changing from TEA to PEI-NH₄(NO)₃ as well as PEI-NH₄(NO)₃ to just PEI as complex agents. However, chemical characterization also presents material incorporation besides the Pb and S elements. Crystallographic results present a cubic galene structure for all films. On the other hand, the superficial morphology shown different granular shapes going from round and soft towards sharpened for the films based on TEA, PEI and PEI:NH, respectively. This study can lead to increase the efficiency of semiconductor devices where thick PbS films are required.



[THF-173] Surface morphological behavior of Ti:Fe thin films heat treated

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In a titanium target highly pure of 2,026.8 mm² surface, pellets were superficially incorporated of approximately 13.5 mm², until reaching exposed surface of 1,916.4 mm² of Titanium and 110.4 mm² of Iron, this in order to generate thin films of Ti_{1-x}Fe_x Through a system of Cathodic Erosion or Sputtering, Using a magnetron sputtering cathodes of 2 inches in diameter. In this way, Nine samples were obtained in the form of thin films, grown on glass substrates with thicknesses of approximately 230 nm, Metallic gray color characteristic of Titanium, with no apparent difference between each of them, this is at first sight. Later, were each divided into dimensions of 10x10 mm for its heat treatment at a temperature of 550°C in an uncontrolled atmosphere (oxidant), for a time of six hours, obtaining totally different samples in physical aspect, ranging from the transparent sample TiO₂ up to brown shades, due to the presence of different iron oxides. Studies done on each of the samples using EDX, they reported the presence of oxygen with a small variation, while a clear decrease of Titanium against a gradual increase of Iron in the different synthesized samples.

Studies on all samples using physical, chemical, microstructural and morphological characterization techniques, show the presence of phases of the different elements present, In the form of oxides or as alloys between them, and the most important of this work: The surface morphological change By the



gradual presence of iron, which favors the agglomeration and crystallization of each sample to a greater or lesser degree depending on the content of this element in the different samples.

[THF-197] Effect of Ni Substitution on properties of Bismuth Ferrite (BiFeO₃) films

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The design of solar cells based on perovskite-type semiconductor materials has showed high efficiencies for the conversion of solar energy to electrical energy. Perovskites based on organometallic halides or with methylammonium lead iodide (CH₃NH₃PbI₃ or MAPbI₃) have been found to have the potential to compete with traditional solar cells. BiFeO₃ is an intrinsic semiconductor widely studied as multiferroic material. However, due to its structural and optical (E_g = 2.3-2.8 eV) properties, this perovskite is attractive for the design of solar cells, and photocatalysis. In this work, it is present a study of the cationic substitution of Bi/Fe atoms by Ni atoms in BiFeO₃ films. The synthesis of BiFeO₃ was made by the sol-gel method. The deposit of the BiFeO₃ films was done by the spin-coating technique. Different calcination temperatures and Ni concentrations were assessed. The optical, morphological, chemical and structural properties of BiFe_{1-x}Ni_xO₃ films were studied by the UV-Vis spectroscopy, SEM, XPS, and XRD characterizations techniques, respectively.

Acknowledgments

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[THF-217] Magnetic and Transport Properties Study of LaCaMnO₃/Pr_{0.8}Ca_{0.2}MnO₃
Bilayers

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Manganese oxide with perovskite structure R_{1-x}A_xMnO₃ (where R and A are rare or alkaline earths metallic elements) has two basal states possible: ferromagnetic metal and antiferromagnetic insulator, accompanied by orbital and / or load systems. This material is known as manganite, where Pr_{0.8}Ca_{0.2}MnO₃ phase is an ferromagnetic(FM) insulator with Curie temperature <150°C. Other manganite that has been extensively studied is a Ca doped lanthanum manganite, for this work we selected La_{0.3}Ca_{0.7}MnO₃, this manganite offer antiferromagnetic (AFM) behavior with Neél temperature < 280°C. The bilayers films were grown in substrates SrTiO₃ (100) by DC sputtering technique fixing the thickness of the array in 80 nm in three different configurations for AFM/FM system: 60/20, 40/40 and 20/60. The bilayers grown were chemically, structurally, magnetically and electrically characterized by EDS, XRD, hysteresis isotherms, R-T curves applying magnetic field and I-V curves, respectively. We find correlation with the thickness of the antiferromagnetic layer and the magnetic response in bilayers and a change in transport behavior particularly in measurements of the resistive switching.



[THF-228] Oxidation mechanism of metallic chromium

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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 thickness¹. In this work, we report the characterization by angle resolved XPS (ARXPS) of different chromium oxidations to quantitative study the oxidation state and the oxidation mechanisms of metallic chromium films.

Metallic chromium 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 growing rate (MASTEK TM-350) was 0.1 \AA/s and the total thickness was 30 nm. The film was characterized with an XPS instrument with a monochromatic X-ray aluminum source (XR5, from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha10, from ThermoFisher).

Metallic chromium films 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. Metallic chromium has a complex multiplet structure making the peak fitting a challenge procedure². Through the active background approach it was possible to obtain an accurate fit of the Cr 2p spectrum³⁻⁴. The block-approach was used to analyze the angular dependence of the metal and its oxide. From the photoemission of the Cr 2p spectrum, we observed contributions from metallic Cr at 909.75 eV and from Cr³⁺ at 912.6 eV. We found that the metal and the oxide coexist along the whole surface layer visible to XPS. Metallic chromium does not oxidize in a layer-fashion as previously assumed².

¹ Biesinger, M. C., Brown, C., Mycroft, J. R., Davidson, R. D. and McIntyre, N. S. (2004), X-ray photoelectron spectroscopy studies of chromium compounds. Surf. Interface Anal., 36: 1550, 1983.



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³ A. Herrera-Gomez. "The peak-Shirley background." Internal Report. CINVESTAV-Unidad Queretaro (2011).

⁴ A. Herrera-Gomez, M. Bravo-Sanchez, O. Ceballos-Sanchez, and M.O. Vazquez-Lepe. *Surf. Interface Anal*, 46, 897, 2014.



[THF-243] Comparative Study of Thin Films Fluorine Doped Tin Oxide deposited by Spray Pyrolysis

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Highly conductive and transparent fluorine doped tin oxide F:SnO₂ (FTO) have been prepared using tetra chloride (SnCl₄·5H₂O) as precursor and ammonium chloride NH₄F as sources of doping impurities and ethanol as a solvent. The films have been prepared by Pneumatic Spray Pyrolysis (PSP) and Ultrasonic Spray Pyrolysis (USP). The films were grown below similar conditions like: temperature, ratio F/Sn, thickness and substrates. The films were deposited at temperatures ranging between 450°C and 460°C with thickness of 300nm and 500nm approximately, and the F/Sn ratios: 0.35, 0.5, 0.65. The samples were characterized using X-Ray diffraction (XRD), Atomic Force Microscopy (MFA), UV-Visible spectrophotometric (UV-VIS) and the conductivity with points four. X-ray diffraction pattern shows the presence of the rutile structure in films FTO with a preferential growth along the (200) direction and besides the films thickness are in the range of 380-400nm. The optimal FTO films on glass present about 2 x10⁻⁵ Ohm.cm of resistivity, high transmission of about 80 % and optical band gap about 4.7 eV.



[THF-253] Photoluminescence and morphology of Gd₂O₃: Eu + 3 films use of surfactants.

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In the present work, the effect of morphology on the luminescence of nanoparticles obtained by sol-gel of Gd₂O₃: Eu³⁺ at 5 mol% deposited on quartz substrates using the dip-coating technique and the use of surfactants (S = Pluronic F-127, DDA, PVP 10,000) using a ratio of Gd₂O₃: Eu³⁺: S = 1: 2, and heat treated from 300 ° C to 800 ° C. The results by X-ray diffraction confirmed the characteristic cubic structure of Gd₂O₃. By scanning electron microscopy (SEM), different morphologies were revealed that were compared with the Gd₂O₃: Eu³⁺. The morphologies observed at 800 ° C using the surfactants, Pluronic F-127, DDA, PVP and Gd₂O₃: Eu³⁺ were: the formation of agglomerated particle strands with sizes ~0.8-1µm. Using ADI; Uniformly distributed oval particles with ~0.5µm sizes were found. Finally, the films of Gd₂O₃: Eu³⁺, are characterized by a homogeneous layer with isolated areas of networks, forming radial chains with sizes of µ1µm. The chemical evaluation of the bonds was determined by Fourier transform infrared spectroscopy (FTIR), whose representative band at 543cm⁻¹ is assigned to the Gd-O network vibration. Photoluminescence studies showed that the highest luminescence intensity corresponds to Pluronic F-127 at 800 ° C, standing at 618 nm corresponding to the 5D₀→7F₂ level of Eu³⁺.



[THF-254] Airy pattern on narrow photoluminescence spectrum of band to band recombination in CdTe:Te thin films

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Semiconductor CdTe:Te films were deposited by means of rf sputtering on glass substrates. The excess of Te gave place to a high number of Cd-vacancies (VCd) producing p-type CdTe films. The density of carriers produced a high strength surface electric field which allowed obtain the bandgap value employing modulated transmittance spectroscopy. The obtained bandgap value of 1.40 ± 0.01 eV was confirmed by absorption spectroscopy measures. The density of holes is so high that bandgap renormalization is observed. Photoluminescence (PL) measurements were carried out with the down-converted 883.2 nm (1.403 eV) line of the 441.6 nm wavelength of a HeCd laser. This energy allows to produce a resonant excitation of the CdTe:Te films, in such a way that electrons from the conduction band (CB) can be just excited to the valence band (VB). The resonant excitation produced a PL spectrum of band to band electronhole recombination showing discrete energy emissions that follow the pattern of oscillations corresponding to the Airy model for a quantum triangular potential well. The average width of signals of the higher energy oscillations is 12 ± 3 μ eV and separation between energy levels is of the order of 12 ± 3 μ eV.



[THF-313]Cu₂O thin films obtained from CuO films treated under argon/dry-air microwave plasma

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Pure Cu₂O thin films can be obtained from CuO films using an argon/dry-air plasma treatment. CuO is reduced to a form of metastable metallic copper that readily oxidizes to Cu₂O. Depending on different process conditions, the crystallite size of Cu₂O can be increased and controlled. CuO thin films were produced by dip-coating on glass substrates from a homogeneous copper acetate solution. Every film consists of 5 coatings deposited at a rate of 8 cm/min and dried at a temperature of 260 °C for five minutes. Different groups of samples were annealed at different temperatures (TA), from 350 °C to 550 °C in increments of 50 °C, for an hour in open atmosphere.

To obtain Cu₂O, CuO thin films were treated for 15, 20, 25 or 30 s, under an argon/dry-air plasma. The treatment took place at low pressure (15 mbar) inside a quartz chamber in a home-made equipment consisting of a 1500 W microwave oven modified for this purpose. The samples were placed on a ceramic plate, with a cut-off window, that allowed both substrate sides to receive the same plasma treatment. Fluxes of argon (60 sccm) and dry air (60 sccm) were controlled by mass controllers and injected continuously before, during and, after the plasma treatment. Depending on the CuO films annealing temperature and time of plasma treatment, Cu₂O, Cu or a mixture of the two were obtained. Interestingly, pure Cu₂O was produced only from a metastable form of metallic copper and only after the plasma treatment, which can take from a couple of minutes to some hours. This partial oxidation of metallic copper was driven by the oxygen availability right after the plasma treatment, when the sample was still hot. To our knowledge, this phenomenon has not been reported before.



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CuO annealing temperatures showed that Cu₂O crystallite sizes tended to be bigger when lower TA's were used. However, there also seemed to be an optimal annealing temperature around 400 °C for which crystallite size can be maximized. Wide variations in crystallite size were observed. Specifically speaking, pure Cu₂O films of about 100 nm in thickness, with bandgaps around 2.17 eV, and crystallite size of 25 nm were obtained by a plasma treatment of 30 s. Four-point resistivity measurements of pure Cu₂O samples reported resistivity values around 2.70×10^2 Ohm-cm. Besides the Cu₂O crystallite size enhancement and control, other advantages of this plasma processing lie in the simplicity, short time of treatment and, low cost of the home-made equipment.



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Ortega Figueroa Carlos Alberto *THF-203*
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Ortiz Francisco *ALD-232*
Ortiz-Saavedra J. *PLV-137, SEM-166, PLV-53*
Ostos C. *RWE-308*
Otero Hernández J. A. *TSM-65, TSM-97*
Oviedo Mendoza M. *RWE-5*
Padilla Islas Miguel Adrian *NSN-147, NSN-150*
Padilla-Islas Miguel Adrian
Palacios-Cabrera Cristian B. *NSN-116*
Palma-Goyes R. E. *RWE-308*
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Paniagua Mercado Ana María *AMC-233*
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Pérez García Claudia Elena *THF-203*
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Peña Bueno Gabriela Alejandra *CHM-230*
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Pelayo Jesús *NSN-82, TSM-306*
Peralta Arriola Miriam *CHM-180*
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Petrov Ivan *SCD-213*
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Portillo Sampedro Mercedes *NSN-141, NSN-126*
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Ramirez Giovanni *THF-240*
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Restrepo Johan *CHM-127*
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Reyes López Simón Yobanny *AMC-199, AMC-231, AMC-271, BIO-129, CHM-230, NSN-142, BIO-258, AMC-128, AMC-125, AMC-131, AMC-121, BIO-140, SIF-143, NSN-145*
Reyes Valderrama Ma. Isabel *TSM-72*
Reyes-Rojas Armando *LPM-36*
Reynoso-Soto E.A. *CHM-61*
Rickards Jorge *NSN-44, NSN-45*
Righini Giancarlo C. *LPM-100*
Rimmaudo Ivan *RWE-289*
Rios Lorena *AMC-259*
Rivas J. M. *PLV-53*
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Rivera L. P. *SEM-174, NSN-179, PLV-168, . PLV-163*
Rivera Laura *PLV-74*
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Robles Aguila Josefina *SCD-291*
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Rocha Alonzo Fernando *NSN-116*
Rodríguez Angel-Gabriel *ALD-290*
Rodríguez Castillo M.E. *PTP-300, NSN-299*
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Rodríguez Rosales Karen *RWE-86*
Rodríguez Victoria Angel Pedro Rodríguez Victoria *NSN-220*
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Rojas-Salinas W.B. *RWE-5*
Roldán Cruz César Alberto *BIO-178*
Román López Jesús *LPM-288*
Romero J. *PLV-111*
Romero de la Cruz María Teresa *TSM-47, TSM-201, TSM-35, TSM-66, TSM-30, TSM-184*
Romero Ibarra Issis Claudette *RWE-216, RWE-176, RWE-281, RWE-224*
Romo Jose *ALD-232*
Romo Herrera José Manuel *ALD-196*
Romo-Herrera J.M. *CHM-61*
Roque-Ruiz José Hafid *AMC-125, AMC-131*
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Rubio-Pereda Pamela *TSM-28*
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Ruiz-Torres Rodolfo *NSN-278*
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Sabino Gutiérrez Marcos Antonio *BIO-42*
Salas González Jesús Antonio *AMC-103*
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Salcedo Prieto Yael Alejandro *TSM-35*
Salgado Zamora Héctor *RWE-104*
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Salinas-Beltrán Susana *RWE-51*
Sanabria Díaz Carlos Alberto *MEM-260*
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Sanginés Roberto *CHM-38, PLV-139, PLV-138, CHM-242, CHM-180*
Sankaranarayanan Subramanian *THF-240*
Santana Medina Luis Carlos *SEM-15*
Santana-Aranda M.A. *PLV-111, PLV-168, THF-169, NSN-68, PLV-63, NSN-179, SEM-174, PLV-80, PLV-41*
Santiago-Cuevas Alan J. *NSN-116*
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Santos-Morales A. A. *SEM-54*
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Sastré Hernández Jorge *RWE-164*
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Sosa Hernández Elisa Marina *TSM-13*
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Soto G. *CHM-61, ALD-196, ALD-123, ALD-232*
Soto Cruz Blanca Susana *NSN-155, THF-243*
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Téllez-Villalobos J. G. *THF-40*
Telles Padilla José Guadalupe *BIO-18*
Tellez Cruz Miriam Marisol *NSN-147, NSN-150*
Tengstrand Olof *SCD-213*
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Torres Barahona Edgar Absalon *THF-115*
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Torres Espinosa Néstor David *NSN-220*
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Torres San Miguel Chistopher René *TSM-10*
Torres-Ochoa Jorge Alejandro *THF-228, CHM-279, SCD-292, ALD-98, CHM-195*
Torres-Palma R. A. *RWE-308*
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Tran Lam T.N. *LPM-100*
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Velarde-Escobar Oscar J. *SEM-284, TSM-285*
Velasco Santos Carlos *NSN-151*
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