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Book of Abstracts

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ATOMIC LAYER DEPOSITION / 47

SATURATION DEGREE IN DOPANT MONOLAYERS AS MODULATOR OF AL-DOPING OF ZNO BY ALD SUPERCYCLE APPROACH

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Transparent conductive oxides (TCOs) have garnered significant attention in scientific and technological circles due to their unique optoelectronic characteristics: high electrical conductivity coupled with optical transparency. The quest for eco-friendly materials in TCO development remains ongoing, with zinc oxide (ZnO) standing out as a promising candidate. Through supervalent doping with elements such as Ga, Al, and In, ZnO optoelectronic properties have been notably enhanced. Among these, Al-doped ZnO (AZO) has emerged as a top contender to replace the environmentally hazardous In-doped SnO2. However, a debate persists regarding the mechanism through which Al-doping influences ZnO optoelectronic properties—whether through substitutional doping or by facilitating active structural defects—. This study delves into the Al-doping of ZnO using atomic layer deposition (ALD) with a supercycle approach. It reveals that reducing the Zn precursor dose during dopant cycles leads to a decrease in the saturation degree of Zn-species monolayers, resulting in morphological and microstructural alterations detrimental to the optoelectronic properties of AZO films. These changes point towards an increasingly defective wurtzite structure while the Al content remains relatively constant. The study underscores the pivotal role of unsaturated surfaces generated by reducing the Zn precursor dose in facilitating Al incorporation reactions. To maximize doping effects, it suggests that complete oxide substitution reactions, rather than conventional ALD, should govern growth while preserving crystallinity. These findings hold implications for optimizing the optoelectronic properties of AZO films deposited by ALD. They steer the debate towards the hypothesis that electrical properties are influenced by Al substitutional doping alongside active defects formed in the film's crystalline structure due to such a doping.

Keywords:

Dopant-layer saturation degree, Al-doped ZnO films, ALD supercycle approach

Reference:

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ATOMIC LAYER DEPOSITION / 138

EFFECT OF ANNEALING ATMOSPHERE ON ELECTRICAL AND OPTICAL PROPERTIES OF MULTILAYER AL2O3/ZNO NANOLAMINATE STRUCTURES DEPOSITED BY ATOMIC LAYER DEPOSITION

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Multilayer nanolaminates of alternate Al2O3 and ZnO were deposited by atomic layer deposition using trimethylaluminum, diethylzinc and water as co-reactants, on a p-type silicon substrate at 200 ℃ in a Beneq TFS 200 system. A set of four nanolaminates with a total thickness of approximately 100 nm were fabricated containing multiple Al2O3/ZnO bilayers with thicknesses of 2 nm. After deposition, the nanolaminates were thermally annealed at 400℃ for 1 hour in N2, O2 and ambient atmosphere to improve the electrical and optical properties of the structures. Optical constants and thicknesses were obtained by ellipsometry measurements. The Al/nanolaminates/p-Si/Al structures were electrically characterized by current-voltage (I-V) and capacitance-Voltage measurements. The obtained results indicate that these nanolaminates have potential for applications in electronic devices.

Keywords:

ALD, electrical properties, optical properties, nanolaminates, thermal annealing

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ATOMIC LAYER DEPOSITION / 150

EFFECT OF ANNEALING TEMPERATURE ON ELECTRICAL AND OPTICAL PROPERTIES OF NANOLAMINATE STRUCTURES DEPOSITED BY ATOMIC LAYER DEPOSITION

Authors: Francisco David Mateos Anzaldo[1]; Jesus Roman Martinez Castelo[2]

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A multilayer nanolaminate of Al2O3 and ZnO was deposited by atomic layer deposition using trimethylaluminum, diethylzinc, and water as co-reactants on a p-type silicon substrate at 200 ℃. A set of four nanolaminates with a total thickness of approximately 100 nanometers were fabricated, each containing multiple Al2O3/ZnO bilayers with thicknesses of 20 nanometers. After deposition, the nanolaminates were thermally annealed at 400, 600, 800, and 1000 ℃ for one hour in an N2 atmosphere to improve the electrical and optical properties of the structures. Ellipsometry measurements revealed the optical constants and thicknesses. Current and capacitance voltage measurements were taken to electrically characterize the Al/nanolaminates/p-Si/Al structures. The obtained results indicate that these nanolaminates have potential for applications in electronic devices.

Keywords:

ALD, electrical properties, optical properties, nanolaminates, thermal annealing

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ATOMIC LAYER DEPOSITION / 187

Investigating Cubic and Hexagonal GaN Crystal Phases on Diverse Substrates at Low Temperature via Atomic Layer Deposition (ALD)

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Gallium Nitride (GaN) is a widely studied semiconductor owing to its outstanding optoelectronic properties, which are enhanced by the presence of a specific crystal phase. The cubic and hexagonal phases of GaN are particularly interesting. The cubic phase exhibits high electron mobility, low acceptor activation energy, and high hole mobility, which are typically achievable only through epitaxial techniques. In contrast, the hexagonal phase offers high conductivity and a reduced lattice mismatch, making it more readily obtainable, often through nitrogen plasma-based methods. This work explores the deposition of GaN on three distinct substrates (silicon, magnesium oxide, and gallium arsenide) at a low temperature of 325℃ and a pressure of 1.9x10^-1 torr using NH4OH and Ga(CH3)3, as precursors. Atomic Layer Deposition (ALD) facilitated the simultaneous growth of all three substrates, enabling a direct comparison under identical conditions. X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and photoluminescence (PL) measurements were performed

for a comprehensive sample analysis and characterization. The initial XRD analysis confirmed the deposition of amorphous GaN on all substrates. Subsequent annealing at 700℃ and 900℃ investigated the influence of elevated post-growth temperatures on the formation of crystalline GaN phases. Interestingly, the deposition on MgO exhibited a portion of GaN in the cubic phase, whereas depositions on GaAs and Si primarily displayed the hexagonal phase. ALD offers exceptional control over the film thickness, uniformity, and large-scale reproducibility for GaN growth. This approach presents a cost-effective alternative to traditional methods while maintaining the desired crystalline properties crucial for GaN-based semiconductor applications.

Keywords:

GaN, Cubic Phase, Hexagonal Phase, ALD, Substrates, Crystallization, Optoelectronic Materials

Reference:

Turrubiartes MMMC, Moran UZ, Gallardo JAL, Borbolla MAV, Luna EL. HIDRÓXIDO DE AMONIO COMO PRECURSOR DE NITRÓGENO PARA EL CRECIMIENTO DE NITRURO DE GALIO POR EL MÉTODO DE CRECIMIENTO POR CAPAS ATÓMICAS. Journal Of Engineering Research. 2023;3(12):2-11. doi:10.22533/at.ed.3173122324042

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ATOMIC LAYER DEPOSITION / 188

Development of a GaN/InGaN/GaN Quantum Well for RGB Light Emission using Atomic Partial Layer Deposition (APLD)

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This work presents the optimization of a GaN/InGaN/GaN quantum well structure for red, green, and blue (RGB) light emission using Atomic Partial Layer Deposition (APLD). InGaN was selected because of its high carrier mobility, compatibility with GaN, and readily controllable bandgap, enabling coverage of the entire visible spectrum. The InGaN quantum well was grown using APLD, whereas GaN layers were deposited via Atomic Layer Deposition (ALD) at optimized at a low temperature of 325℃ and a pressure of 1.9x10^-1 torr with NH4OH, Ga(CH3)3, and C2H4InO2 as precursors. Notably, the deposition was performed simultaneously on Si, MgO, and GaAs substrates. The In concentration in InGaN was precisely controlled by varying the exposure time to the C2H4InO2 precursor. This approach leverages the unique capabilities of APLD, a variant of ALD that uses short precursor exposure times to prevent a complete layer reaction. This allows the subsequent precursors to partially fill the incomplete layer, enabling precise control over the material composition. Post-deposition annealing was employed to promote the formation of crystalline GaN and InGaN phases on all the substrates. This research paves the way for the implementation of GaN/InGaN/GaN quantum wells in optoelectronic devices capable of emitting pure RGB light. The combination of ALD, which offers exceptional control over thickness, uniformity, and large-scale reproducibility, with APLD, providing enhanced versatility and material property control, signifies a significant advancement in this field

Keywords:

InGaN, Quantum Well, RGB LED, Atomic Partial Layer Deposition (APLD)

Reference:

Hernández-Arriaga H, López-Luna E, Martínez-Guerra E, Turrubiartes MM, Rodríguez AG, Vidal MA. Growth of HfO2/TiO2 nanolaminates by atomic layer deposition and HfO2-TiO2 by atomic partial layer deposition. Journal Of Applied Physics. 2017;121(6). doi:10.1063/1.4975676

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ATOMIC LAYER DEPOSITION / 214

TiOx analysis on the ALD obtention process by titanium (IV) n-butoxide: comparison with conventional TDMA.

Authors: Pierre Giovanni Mani González[1]; Jesús Alfredo Hernández Márquez[1]; Matthew Snelgrove[2]; Rob O´Connor[2]

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The motivation of this work is developed semiconductor device patterning technology based on metallic liquid precursor materials. The methods involved the vacuum vaporization by reaction on silicon substrate of vapor phase. This can be directed to the substrate's active sites for controlled growth and manipulating the chamber's vacuum level from low vacuum. Then, dose the precursor into chamber as to allow the deposition, for comparation this TiOx films which had been previously deposited by conventional atomic layer deposition (ALD) onto silicon substrates using Tetrakis dimethyl amido titanium (TDMA). Versatility of ALD processes allow for the phase change due to vacuum by a vaporization process. Films were analyzed with X-ray Photoelectron Spectroscopy (XPS). This photoemission-based technique gives information about O 1s, Ti 2p and C 1s core levels. Energy Dispersive Spectroscopy (EDS) suggests Ti atoms comparable with conventional TiOx ALD process. XPS measurements enabled details of the chemical composition of the thin film to be characterized and offered a robust analysis of both interfaces and discrete layers present in the films. These measurements displayed evidence of bonding interactions between the metals in the silicon substrate which assists in developing an understanding of the preferential vaporization process which needs to be optimized for device fabrication applications.

Keywords:

ALD, metallic precursor, vacuum, XPS, TDMA.

Reference:

Mani-Gonzalez, Pierre Giovanni, Caitlin McFeely, Matthew Snelgrove, Kyle Shiel, Jesus Alfredo Hernandez Marquez, and Robert O'Connor. "Titanium infiltration into ultrathin PMMA brushes." Journal of Vacuum Science & Technology A 39, no. 4 (2021).

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ATOMIC LAYER DEPOSITION / 63

Optical Properties of TiO2 Grown by Atomic Layer Deposition Using Various Oxidizing Agents: The Ellipsometry Analysis of Absorption Properties

Authors: Jorge Luis Vazquez Arce[1]; Tibor Suta[2]; Balint Fodor[2]; Laszlo Makaii[2]; Amin Bahrami[1]; Kornelius Nielsch[1]; Hugo Tiznado[3]

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This study provides an in-depth analysis of the optical properties of TiO2 films grown via atomic layer deposition (ALD) using various oxidizing agents, including H2O, H2O2, O3, and O2 plasma. Our research describes the distinctive absorption band in TiO2 films grown with H2O, named "black TiO2", a phenomenon not observed in films grown with other oxidizing agents. This finding is linked to Ti3+ species within the TiO2 matrix. Additionally, we observe a correlation between increased nitrogen content, presumably from the TDMAT precursor, and the presence of Ti3+ states in H2O-grown films, suggesting nitrogen contamination's role in forming or stabilizing these states. Contrasting this, films grown with H2O2, O3, and O2-plasma, despite having similar nitrogen levels, do not exhibit the absorption band, highlighting the complex interaction between growth conditions, nitrogen incorporation, and the TiO2 matrix. Furthermore, our study notes a decrease in Growth Per Cycle with increasing ALD cycles, aligning with the 'surface memory' effect observed in ALD processes. This research contributes to a deeper understanding of the growth dynamics and optical properties of ALD-grown TiO2 films, offering insights for future photo-technological applications.

Keywords:

TiO2 films, Black TiO2, ALD Films

Reference:

H. Ali-Löytty et al., "Diversity of TiO 2 : Controlling the Molecular and Electronic Structure of Atomic-Layer-Deposited Black TiO 2", ACS Appl. Mater. Interfaces, vol. 11, núm. 3, pp. 2758–2762, ene. 2019, doi: https://doi.org/10.1021/acsami.8b20608.

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ATOMIC LAYER DEPOSITION / 74

Effect of the co-reactant on the electronic structure bands of nickel oxide films synthesized by ALD

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Co-authors: Emilio J. Juárez Pérez [2]; Francisco Servando Aguirre Tostado [1]; Maria Isabel Mendivil Palma [1]

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In this study, we investigate the impact of co-reactants on the atomic layer deposition (ALD) synthesis of nickel oxide films and their influence on the chemical characteristics and electronic structure of the resulting films. The ALD process involves the utilization of nickel acetylacetonate as the organometallic precursor, which undergoes oxidation by Ozone, water, and Oxygen in both thermal (TALD) and direct plasma mode (DPALD), respectively. We found that the growth per cycle of the nickel oxide films range from 0.01 nm to 0.09 nm. X-ray photoelectron spectroscopy (XPS) analysis confirms that the nickel oxide films exhibit a non-stoichiometric nature on the surface, characterized by a high density of Ni^{3+} (13 at. %). This defect significantly influences the electronic band structure of the nickel oxide films, as demonstrated by ultraviolet photoelectron spectroscopy (UPS) analysis, which reveals that the presence of Ni^{3+} leads to modulations in the work function and valence band maximum. Thes modulation can result in variation up to 1 eV between the TALD and DPALD synthesis. Additionally, reflected electron energy loss spectroscopy (REELS) analysis shows insignificant changes in the band gap (E_g) between all synthesis methods. Our findings suggest that nickel oxide films hold promise as hole transport lates (HTL) in perovskite solar cells.

Keywords:

Nickel oxide, ALD, HTL, electronic bands structure

Reference:

Attri, R., Panda, D. P., Ghatak, J., & Rao, C. N. R. (2023). High crystalline epitaxial thin films of NiO by plasma-enhanced ALD and their properties. APL Materials, 11(9).

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ATOMIC LAYER DEPOSITION / 198

HfO2/TiO2 NANOLAMINATES SYNTHETIZED BY ALD FOR MIM CAPACITORS APPLICATIONS

Authors: Jaime Estrada Sánchez[1]; Miguel Martinez Gil[2]; Dainet Berman Mendoza[None]; Rafael García Guitérrez[None]; Rafael Verdugo Miranda[2]; Jesus Javier Alcantar Peña[3]; Frank Romo García[2]

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This work consists in the synthesis of nanolaminates of hafnium oxide (HfO2) and titanium oxide (TiO2), for MIM (metal-insulator-metal) capacitors applications, by the atomic layer deposition (ALD) technique using an Anric AT-410 equipment, devices were manufactured on a p-type Si (silicon) wafe, the architecture consists of Ti (titanium) bottom contact deposited by electron beam evaporation technique, a dielectric layer with different configurations: 1.- 70 nm single layer of TiO2, 2.- 60 nm TiO2 layer between two layers of 5 nm HfO2, 3.-50 nm TiO2 layer between two layers of 10 nm HfO2 and 4.- 30 nm TiO2 layer between two layers of 20 nm HfO2 and Al (aluminum) deposited by sputtering as upper contact. The precursors tetrakis dimethylamido hafnium (TDMAH) and tetrakis dimethylamido titanium (TDMAT) were used for the synthesis of materials, programming different numbers of cycles for each one to obtain the desired thickness, molecular nitrogen (N2) was used as a purge gas and deionized water as reactant (DI H2O). The effect of the HfO2 layers at the interface with the electrodes to reduce the leakage current compared to the TiO2-only capacitor was evaluated by testing current-voltage characteristic (I-V) and capacitance-voltage characteristic (C-V) curves. The results obtained from the I-V curves at 1V for the capacitors without HfO2 and with the layers of 5,10 and 20 nm were 379.96 x10-9, 11.96x10-9, 242.75. 9 x10-9 and 47.55 x10-12 A respectively, where the 20 nm HfO2 layers capacitor presents a greater reduction in the leakage current. A reduction in the capacitance of the devices can be noticed; the average capacitance values obtained at 1 V for the capacitors without HfO2 and with layers of 5,10 and 20 nm were 628.29x10-15, 541.31x10-15, 360.41 x10-15 and 353.42 x10-15 F respectively, which can be attributed to the difference in dielectric constants between the materials.

Keywords:

ALD , MIM CAPACITORS

Reference:

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ATOMIC LAYER DEPOSITION / 210

Synthesis of NiOx thin films by PEALD as active material for supercapacitor electrodes

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Co-authors: Alejandra García García [2]; Angel Osuna [3]; Claudia Rodriguez [1]; Eduardo Martínez Guerra [3]; Hortensia Reyes [1]; Isabel Mendívil-Palma [3]; Luis Silva [3]; Mario Hidrogo [4]; Oscar Edgardo Vega Becerra [5]

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The study of active materials for supercapacitors involves the development of optimal synthesis methods to achieve high surface area and achieve electrode/electrolyte interactions. A plasma-enhanced atomic layer deposition (PEALD) methodology using (Ni(acac)2) as organometallic was proposed. To evaluate the electrochemical properties of the films, approximately 44 nm of NiOx was deposited on an Au/Cr/Glass substrate to assemble a working electrode. The samples were compared without and with heat treatment by varying the electrolyte concentration from 0.1 to 1.0 M KOH in a three-electrode half-cell. Cyclic voltammetry (CV) was performed, and redox pairs were identified less than 70 mV apart, with maximum capacitance obtained at lower sweep rates. The reactions involve the insertion of OH- ions. The maximum capacitance values are 102 F/g, 10 times below the values reported in the literature. The heat-treated films present an average increase of 4.5% of the surface area and decreased lattice parameter AS suggested by MFA and XRD results. The stoichiometry of the films before and after heat treatment indicates an increase of oxygen vacancies from x=0.86 to x=0.75. Electrochemical impedance spectroscopy (EIE) corroborated the existence of a double layer and ion diffusion. The limitations of the film geometry inhibit electrode/electrolyte interactions; however, the reversibility of the process is promising for supercapacitor applications

Keywords:

thin film, growth per cycle, supercapacitor, pseudocapacitance, heat treatment

Reference:

Y. Koshtyal et al., "Atomic layer deposition of nio to produce active material for thin-film lithium-ion batteries", Coatings, vol. 9, núm. 5, may 2019, doi: 10.3390/coatings9050301

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ATOMIC LAYER DEPOSITION / 108

ANTIREFLECTIVE COATINGS BASED ON ZNO/AL2O3 NANOLAMINATES GROWN BY ALD

Authors: Frank Romo Garcia[1]; Jesus Valente Corral Palomares[1]; Miguel Martinez Gil[1]; Rafael Verdugo Miranda[1]; Rafael García Guitérrez[2]

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This work consists in the manufacture of Antireflective coatings (ARC) based on nanolaminates of zinc oxide (ZnO) and aluminum oxide (Al2O3), which were deposited on silicon wafers, glass, and polycrystalline silicon solar cells in a home-made Atomic Layer Deposition (ALD). The number of alumina cycles in the nanolaminate was varied with the objective that the thicknesses were 1%, 3% and 5% with respect to the thickness of the ZnO. The optical properties of the ZnO/Al2O3 nanolaminates on glass and silicon substrates were analyzed using a UV-Vis spectrophotometer for measurements

of transmittance and reflectance percentages. Because the nanolaminates are made up mostly of ZnO layers, they produce a decrease in transmittance at wavelengths shorter than 380 nm because of the exciton energy of the ZnO. Decreasing the wavelength in the UV range is important to improve the efficiency of the silicon solar cell. The nanolaminate which has a thickness of 1% alumina is the one that reflects the least in the range of 1000 nm to 600 nm wavelength and is the one that presents the best reflectance in the range of 550 nm to 300 nm. Silicon solar cells were characterized by IV characteristic curve with the aim of study the efficiency of the photovoltaic device before and after the deposition of the ARC. It was determined that there is an increase in efficiency in the solar cell that was coated with the ZnO/Al2O3 nanolaminates with 1% alumina and the efficiency was increased by 3.1%.

Keywords:

ALD, ARC, Nanolaminates, solar cell

Reference:

F Romo-Garcia, HJ Higuera-Valenzuela, D Cabrera-German, D Berman-Mendoza, A Ramos-Carrazco, H Tiznado, GA Hirata, OE Contreras, R Garcia-Gutierrez. Optoelectronic attenuation behavior of Al2O3/ZnO nanolaminates grown by Atomic Layer Deposition. Thin solid films, doi: https://doi.org/10.1016/j.tsf.2018.11.026

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ATOMIC LAYER DEPOSITION / 304

YSZ THIN-FILM SOLID-STATE ELECTROLYTE WITH BATTERY AND MEMRISTOR CAPABILITY

Authors: Jorge Luis Vazquez Arce[1]; Óscar Romo[2]; Carolina Bohórquez[3]; Bonifacio Can[3]; Oscar Edel Contreras López[4]; Gerardo Soto[None]; Joel Molina[5]; Eduardo Blanco[None]; Manuel Domínguez[None]; Kornelius Nielsch[1]; Amin Bahrami[1]; Hugo Tiznado[3]

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This work presents a novel thin-film solid-state battery design with a wider operating temperature range (up to 200℃) compared to conventional designs. The battery utilizes a 100 nm thick yttria-stabilized zirconia (YSZ) layer deposited by atomic layer deposition (ALD) as the solid-state electrolyte and ruthenium/gold electrodes, achieving an energy density of 200 mWh/cm³. Furthermore, the YSZ electrolyte exhibits resistive switching behavior, enabling the device to function as a memristor. This dual functionality makes the design attractive for high-temperature on-chip energy storage and neuromorphic computing applications in integrated circuits. The study explores the influence of temperature and oxygen vacancies on the battery's performance and the memristor's switching

behavior. The findings suggest that controlling oxygen vacancy concentration can enhance energy storage and memristor characteristics.

Keywords:

Energy storage, solid electrolyte

Reference:

https://doi.org/10.1016/j.jpowsour.2022.231555
https://doi.org/10.1111/jace.19392
https://doi.org/10.1016/j.est.2023.108966
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ATOMIC LAYER DEPOSITION / 259

SYNTHESIS AND CHARACTERIZATION BY PHOTOLUMINESCENCE OF THE ZNO: NI SEMICONDUCTOR OBTAINED BY THE ALD TECHNIQUE

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Zno: Ni thin films were produced on a silicon substrate and doped with varying concentrations of Ni (1 wt%, 3 wt%, 4 wt%, and 5 wt%) using the ALD process. Using Photoluminescence Spectroscopy (PL), the effects of Ni concentration on the structural optical characteristics of the produced samples were examined. ALD is a vital technique that makes continuous advancements in the design of microelectronic devices possible. ZnO doped Ni showed high crystalline quality, according to XRD measurements. The adaptability of ZnO crystal synthesis is what makes it so beautiful. It is possible to produce crystals that range in size from tens of nanometers to a few millimeters by using a variety of procedures. A wide range of optical properties are produced by the crystals' interaction with light as a direct result of this extraordinary control over size. The spectrum of photoluminescence in the Zinc oxide's (ZnO) photoluminescence spectrum exhibits band edge and exciton luminescence in the ultraviolet spectrum. Both pure and nickel-doped ZnO thin films were subjected to surface and chemical composition analyses using X-ray photoelectron spectroscopy (XPS). SEM micrographs further confirm an increase in the average grain size of ZnO thin films doped with nickel, which is consistent with results from X-ray diffraction (XRD) investigations. The hexagonal wurtzite crystal structure is possessed by both pure and doped ZnO, as confirmed by X-ray diffraction (XRD).Measurements using energy-dispersive x-ray spectroscopy (EDX) demonstrated the presence of the Ni contribution.

ZnO thin-film optical characteristics are strongly impacted by nickel doping. A discernible shift in the optical constants between the Ni-doped and undoped versions demonstrates this. A higher surface density was found to be correlated with an increase in the concentration of Ni dopant. Two distinguishing characteristics of the photoluminescence spectrum of nanostructured ZnO are a maximum within the ultraviolet (UV) spectrum actually .

Keywords:

ZNO:Ni;ALD method; Optical properties; PL spectra; XPS

Reference:

Manickam Anandan a,b, Selvakumaran Dinesh c, Benedict Christopher,Multifaceted investigations of co-precipitated Ni-doped ZnO nanoparticles:
Systematic study on structural integrity, optical interplay and
photocatalytic performances, https://doi.org/10.1016/j.physb.2023.415597

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ATOMIC LAYER DEPOSITION / 301

SELF-ASSEMBLED MONOLAYER FOR AREA-SELECTIVE ALD

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Stearic acid self-assembled monolayers (SA SAMs) are a promising candidate for area-selective atomic layer deposition (AS-ALD) due to their soft removal properties.
We evaluated SA SAM formation kinetics and thermal stability on copper. The resulting SAMs were densely packed and highly hydrophobic, exhibiting water contact angles exceeding 110°. The adsorption process followed the well-established Langmuir kinetics for surfactant adsorption on planar surfaces.
Next, we investigated SA/copper as a non-growth surface for ZnO ALD using X-ray photoelectron spectroscopy (XPS). The optimal ALD parameters were identified at 70 ℃ with 25 ms pulses of diethyl zinc and water precursors, separated by 10 s purges. These conditions yielded sustained growth attenuation for at least 40 ALD cycles.
Finally, we explored the removal of the SA monolayer with water, acetone, and ethanol at room temperature. Based on infrared spectroscopy and water contact angle measurements, ethanol proved to be the most effective solvent, achieving complete removal within 30 minutes without requiring sonication or agitation. This demonstrates the soft removal nature of SA SAMs.
In conclusion, SA SAMs offer an efficient and removable passivating solution for copper in AS-ALD, eliminating the need for harsh etching or acid treatments.

Keywords:

selective ALD, Self-assembled monolayer

Reference:

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ATOMIC LAYER DEPOSITION / 363

Atomic Layer Deposition: Tailoring Nanomaterial Properties for Advanced Applications

Author: Hugo Tiznado[1]

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Nanostructured materials hold immense potential due to their unique properties heavily influenced by size, shape, and composition. Precise control over these factors is crucial for engineering the desired functionalities in next-generation nanotechnologies. This report highlights Atomic Layer Deposition (ALD) as a powerful technique for surface engineering, enabling the controlled modification of various physicochemical properties like refractive index, bandgap, and electrical properties. ALD's exquisite control over deposition thickness allows for the creation of diverse nanostructures with precise dimensions, including nanotubes, core-shell materials and nanolaminates. This precise control over surface properties paves the way for the design and fabrication of advanced nanodevices with tailored functionalities, like energy and memory storage, as well as optical devices.

Keywords:

Atomic Layer Deposition, Surface Engineering

Reference:

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https://doi.org/10.1016/j.optmat.2020.110370
https://doi.org/10.1002/aelm.202300608

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ATOMIC LAYER DEPOSITION / 58

STUDY OF THE OPTICAL AND STRUCTURAL PROPERTIES OF Zn AND AZO FILMS GROWN BY ATOMIC LAYER DEPOSITION

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Co-authors: Alonso Concha Balderrama [2]; Cristo Manuel Yee Rendón [1]; Eduardo Martínez Guerra [2]; Isabel Mendívil-Palma [2]; Nayeli Pineda Aguilar [2]

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In recent years, the need to Emerging technology requires the develop of new materials for opto-electronic devices. and nanostructured systems from TCO For many application a Ttransparent conductive oxides (TCO) are required and has has become e a high priority as it is vital for the development of the for the electronics industry. and research.
Transparent conductive oxides (TCO), whichTCO have high flexibility, transparency and transmittance. This group of oxides includes zinc oxide (ZnO) and aluminum-doped zinc oxide (AZO) and zinc oxide (ZnO). These materials gain importance thanks to due to its have a high optical transmittance (band gap > 3.34 eV), low resistivity, low cost and is also non-toxic. However Zinc oxide (ZnO) alone has low conductivity; this problem can be corrected by doping this material with different percentages of aluminum (Al), which is why the study of AZO becomes relevant.
In this work, these materials will be studied, which wereZnO and AZO grown over silicon were synthesized using the atomic layer deposition (ALD) technique with different growth conditions, which allows us optimal control of growth thanks to the fact that it is based on cycles where there are self-limiting reactions on the surface. Another important aspect is to know the optical and structural characteristics of the thin films, for which .The effect of the growth condition of the thin films on the optical and structural properties were analyzed by several techniques.Finally, a correlation will be sought between the synthesis conditions and their effects on the optical and structural properties of these films.

Keywords:

ZnO, AZO, Transparent conductive oxides, Atomic Layer Deposition, Photoluminisence, Photorreflectance.

Reference:

Enabling high-quality transparent conductive oxide on 3D printed ZrO2 architectures through atomic layer deposition.Joel Arriaga Dávila, Jędrzej P. Winczewski, Manuel Herrera-Zaldívar, EduardoMartínez-Guerra.

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ATOMIC LAYER DEPOSITION / 76

Effect of Oxidant Agent on Electrical and Optical Properties of Nickel Oxide Thin Films synthesized by ALD

Authors: Diego Giraldo Guzmán[1]; Eduardo Martínez Guerra[2]; Francisco Aguirre Tostado[3]; Francisco das Chagas Marques[1]; Maria Isabel Mendivil Palma[4]; Mario Hidrogo[4]

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NiO films can be deposited by atomic layer deposition (ALD) employing nickel acetylacetonate as organometallic precursor and make variation of the co-reactant employed, such as ozone (P-Oz, T-Oz), water (P-W, T-W) and oxygen (P-Ox) in thermal and plasma-enhanced mode. The best samples in this study were produced with oxygen plasma-assisted ALD. This deposition technique features high GPC (0.09 nm/cycle), short per-cycle time (12 sec/cycle), reduced carbon concentration at the sample surface (8 at.%). The use of oxygen plasma leads to formation of water molecules, producing many $OH-_{(s)}$ groups that interchange with chemisorbed $Ni(acac)+_{(s)}$, making a chemical synergy with the adsorbed $O-_{(s)}$. This mechanism is not possible when H_2O or O_3 are used as oxidizing agents. The higher transmittance was obtained for the T-Oz and P-Ox films, with the maximum transmittance values reaching 92% and 81%, respectively. In both cases, the transmittance of 80% is maintained for almost the entire visible range. This result is extremely important for photovoltaic applications, where NiO can be used as a hole transport layer. P-W sample features the lowest transmittance value <30% in the spectral range analyzed (300–800 nm) due to its metallic character. The optical band gap shows values of 4.105, 3.858, 2.188, 3.747, and 3.725 eV for T-W, T-Oz, P-W, P-Oz, and P-Ox samples, respectively. These values agree well with the literature data for NiO films deposited with CVD and ALD methods [1, 2]. These results emphasize a pronounced dependence of optical band-gap on the oxidizing agent used, and can be employed for efficient band-gap tuning. The resulting film is slightly non-stoichiometric (Ni:O ratio 0.94); it features p-type conductivity, high optical transparency (85%), high carrier concentration (10^{18} cm^{-3}) and high mobility (7.79 $cm^2/V \cdot s$). These remarkable optoelectronic properties make P-Ox NiO promising for manufacturing hole transport layer in Perovskite Solar Cell.

Keywords:

ALD, Nickel Oxide, HTL, p-type, Semiconductors

Reference:

Antony Premkumar, P., Toeller, M., Adelmann, C., Meersschaut, J., Franquet, A., Richard, O., ... & Van Elshocht, S. (2012). NiO thin films synthesized by atomic layer deposition using Ni (dmamb) 2 and ozone as precursors. Chemical Vapor Deposition, 18(1-3), 61-69.

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ATOMIC LAYER DEPOSITION / 107

OPTICAL CHARACTERIZATION OF AZO/SIO2 THIN FILMS GROWTH BY ALD

Author: Juan Jazziel Favela Lopez[None]

Co-authors: Antonio Ramos Carrazco ; Cristo Manuel Yee Rendon ; Jose Ricardo Rangel Segura ; Rafael Garcia Gutierrez

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The present work reports the study of thin films of AZO (zinc oxide doped with aluminum oxide) growth by the atomic layer deposition (ALD) technique for a future application as a coating in commercial photovoltaic cells. The main objective is to develop a material that filters UV radiation, through the luminescent downshifting (LDS) effect, increasing the efficiency of the solar cell using photons in the visible region. The results of AZO films with different concentrations of aluminum oxide from 0% to 15% are presented. The absorption edge of the films was studied using UV-Vis spectroscopy, and band gap energy values of 3.24 eV to 3.74 eV were estimated with the Tauc graphic method [1]. Using the Photoluminescence technique, the main characteristic emissions of the AZO samples were found with emissions in the UV (3.37 eV) and in the visible region caused by aluminum oxide defects, with these results it was found that AZO films absorb ultraviolet light and transmit in the visible range, which demonstrates their luminescent downshifting properties, thus being a candidate for use as a coating in solar cells.

Keywords:

AZO , ALD , Coatings , semiconductor , thin films

Reference:

Hou, Q., Meng, F. & Sun, J. Electrical and optical properties of Al-doped ZnO and ZnAl2O4 films prepared by atomic layer deposition. Nanoscale Res Lett 8, 144 (2013). https://doi.org/10.1186/1556-276X-8-144

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ATOMIC LAYER DEPOSITION / 120

CHARACTERIZATION OF A LAB-MADE ATOMIC LAYER DEPOSITION SYSTEM USING ALUMINUM OXIDE FILMS

Author: Jackeline Navarro Rodríguez[1]

Co-authors: Jesus Roman Martinez Castelo [2]; Francisco David Mateos Anzaldo [1]; Armando Pérez Sánchez [3]; Juan Antonio Ruiz Ochoa [3]; Rogelio Arturo Ramos Irigoyen [1]; Eduardo Martínez Guerra [4]; Hugo Jesús Tiznado Vázquez [5]; Nicola Nedev [1]

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Atomic layer deposition (ALD) has emerged as a highly promising technique with diverse applications in microelectronics manufacturing because of its ability to control layer growth at the atomic scale. However, the sustainability of ALD technology remains a critical consideration, necessitating quantitative investigation to improve its economic viability and environmental performance. In this study, we present the characterization of a cost-effective laboratory-made (lab-made) atomic layer deposition (ALD) system using aluminum oxide (Al2O3) films through trimethylaluminum and water binary reactions. On a Si wafer (100) and corning glass, an aluminum oxide film can be deposited at temperatures between 100 and 200 ℃ at different doses of precursors and purge times to create uniform films with a growth per cycle (GPC) that nearly matches the GPC reported by other commercial ALD systems. Our results indicate that a lab-made ALD system may perform comparably with a commercial system and can be used for teaching and research purposes. With optimized operational process settings, GPC remains constant even though the number of ALD reaction cycles is changed. This can be used as a metric to verify that material is deposited by a self-limiting surface reaction.

Keywords:

ALD, Lab-Made, Characterization, Deposition System

Reference:

N/A

This work was supported by:

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ATOMIC LAYER DEPOSITION / 207

PLASMA ENHANCED ATOMIC LAYER DEPOSITION OF TIO2 THIN FILMS FOR PHOTOCATALYTIC APPLICATIONS AT VIRUS INHIBITION.

Author: Jesús Alfredo Hernández Márquez[1]

Co-authors: Darragh O'Neil [2]; Naun Lobo [3]; Alejandro Martinez [3]; Matthew Snelgrove [2]; Robert O'Connor [2]; Pierre Giovanni Mani González [1]

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The TiO2 photocatalytic activity is efficient at the wavelength range of UV-Light (~254nm). Devices utilizing TiO2 photocatalysis would see advantages from a layered structure containing both rutile and anatase phases. The heterojunction formed at the interface between rutile and anatase phase promotes spatial charge separation which leads to a rise in photocatalytic activity. In addition, the fact that the thin film increases its photocatalytic activity when it is doped with another metal such as Ni and nonmetals like N well as, is also an important case of study. This doping technique enhances the wavelength threshold for initiating photocatalytic activity, rendering the photocatalytic thin films effective at approximately 380nm. By employing atomic layer deposition (ALD) processes to modify

and introduce dopants into the controllable TiO2 interface, biological issues such as the degradation of the SARS-CoV-2 molecule are addressed. This investigation capitalizes on the surface's potential to degrade micro viral agents through the generation of electrons at the heterojunction interface within its crystalline structures. The primary goal is to offer solutions for inhibiting and halting the propagation of SARS-CoV-2 by crafting rutile/anatase TiO2 thin film stacks and rutile/anatase TiO2 thin film stacks doped with Ni via an optimized ALD process. TiO2 thin films were deposited through PE-ALD with approximate thickness of ~5nm with TDMAT and O2 plasma as precursors. Thin films were characterized using GAXRD (grazing angle x ray diffraction) to assess the crystalline structure of the films, Ellipsometry spectroscopy for thickness and refractive index obtention and XPS (X-Ray Photoelectron spectroscopy) to study chemical composition.

Keywords:

XPS, GAXRD, Photocatalytic, Thin Film, virus

Reference:

P. Yan et al., "Photovoltaic device based on TiO2 rutile/anatase phase junctions fabricated in coaxial nanorod arrays,"Nano Energy, vol. 15, pp. 406–412, 2015, doi: 10.1016/j.nanoen.2015.05.005.

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ATOMIC LAYER DEPOSITION / 391

EROSION–CORROSION WEAR OF (TiAlZrTaNb)Nx HIGH ENTROPY NITRIDE THIN FILMS GROWN ON AISI 4343 STEEL

Author: Julian David Vargas Buenaventura[1]

Co-authors: Ingrid Johana Gonzales Avila [1]; Jhon Jairo Olaya Florez [1]; Juan Pablo Gonzalez Lozano [2]; Oscar Edwin Piamba Tulcán [1]

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The erosion-corrosion behavior of high entropy nitride (TiAlZrTaNb)Nx produced by HiPIMS (High-Power Magnetron Suputtering) on AISI-4340 and was studied. The behavior of the coating against erosion-corrosion synergism is performed using the procedure indicated in ASTM G119-09, by means of a test cell including a Jet type nozzle to achieve different impact angles (30° and 90°) ang changing the velocities. Corrosive deterioration is achieved with an electrolytic solution of 3.5% NaCl whereas erosive wear is achieved by the action of a water jet with SiO2 particles. the synergistic erosion-corrosion effect was studied by combining the above processes. Analysis of the microstructure and morphology of the coatings produced were performed using X-ray diffraction, scanning electron microscopy (SEM) and 3D optical microscopy techniques. The results indicated that the total wear rate could be reduced significantly with respect to steel when this kind of coating is used. For all conditions, erosion was the most important wear mechanism.

Keywords:

HiPMIS, entropy nitride, The erosion-corrosion behavior

Reference:

ASTM International. (2021). ASTM G119-09: Título completo de la norma. Recuperado de [ASTM International (ansi.org)]

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BIOMATERIALS AND POLYMERS / 372

SELECTIVITY OF NANOCOMPOSITE MEMBRANES OF KRAFT AND ORGANOSOLV LIGNINS IN CELLULOSE TRIACETATE (TAC) APPLIED TO WATER POLLUTION

Authors: Carina Oliva Torres Cortés[1]; Julio Cesar Reyes De Leon[1]; María Leticia Pérez Arrieta[1]

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In order to combat water pollution caused by heavy metals and reduce associated diseases, membrane technology is employed due to its high efficiency, low energy consumption, minimal operational costs, and high selectivity. Key parameters for membranes include the manufacturing material, selectivity, and mechanical and hydraulic resistance. Composite materials represent an advanced and efficient alternative for creating effective membranes. The combination of different materials aims to modify their properties in order to meet specific expectations.

This research investigated the conditions required to obtain composite membranes from TAC and modified lignin nanoparticles using the precipitation and dry evaporation method to enhance their mechanical and hydrodynamic properties. The resulting material was then compared with membranes synthesised through wet evaporation. Nanocomposite membranes of Cellulose Triacetate with 3% and 5% Kraft and Organosolv lignin, both commercial and propylated, were synthesised. Morphological characterisation was conducted using scanning electron microscopy (SEM), and tensile properties were measured using dynamic mechanical analysis (DMA). The results indicate that synthesis at low relative humidity and temperature (10% and 45℃) results in a reduction in the material's mechanical properties due to low lignin incorporation and reduced TAC crystallinity. Conduction is the predominant heat transfer mechanism, with convection evident in vapor-induced phase separation (VIPS) processes. The primary membranes obtained were those for microfiltration, with only one ultrafiltration membrane, MLOP5, being suitable for metal removal. The particle size significantly affects the mechanical properties. Hydrophilic lignins contribute to improved permeability properties, but increased surface roughness can negatively impact flow rates. Increasing the lignin load was found to enhance the mechanical properties of the membranes.

The results demonstrate the potential of composite materials incorporating modified lignins in developing advanced filtration membranes. These materials have the potential to lead to more efficient and cost-effective solutions for addressing water pollution and protecting public health.

Keywords:

Nano composite membranes, Cellulose triacetate, Water pollution

Reference:

Kiziltas et al. (2010) studied thermal properties of microcrystalline cellulose-filled PET–PTT blend composites.
Calvo et al. (2010) applied membrane technology to treat highly hazardous liquid wastes.

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BIOMATERIALS AND POLYMERS / 291

Impact of the formulation method of poloxamer-based micellar systems on the incorporation of lipophilic drugs

Author: Daniela Fernanda Rodriguez Chavez[1]

Co-authors: Alejandra Estefania Herrera Alonso [2]; Celia Nohemí Sánchez Domínguez [3]; Margarita Sánchez Domínguez [4]

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While anticancer agents have revolutionized cancer treatment for many patients, most currently used drugs suffer from limitations. These limitations include low biocompatibility, which can hinder their therapeutic efficacy due to poor solubility in water-based solutions Therefore, it is crucial to develop new delivery systems for active pharmaceutical ingredients (APIs) using nanotechnology, specifically employing poloxamer micelles as controlled release systems for multiple fat-soluble active ingredients. These micelles encapsulate drugs within their hydrophobic chains, thereby enhancing the solubility and bioavailability.
This study evaluated the encapsulation capacity of curcumin and fenofibrate in poloxamer micelles prepared using two different formulation methods: solvent evaporation (SE) and film hydration (FH). The main difference between the two methods lies in the solvent evaporation process, which influences the rheology of the systems due to water loss and the consequent increase in concentration and viscosity. The study revealed that micelle size was not significantly affected within the concentration ranges studied.
Regarding the incorporation of the active ingredients, encapsulation percentages of 72% and 90% were obtained for the SE route and 77% and 93% for the FH route, respectively. These results indicate that the FH route presents higher encapsulation efficiency and lower viscosity, making it a more favorable alternative for the development of intravenous drug delivery systems.

Keywords:

Poloxamer, Training routes, incorporation

Reference:

M. Almeida, M. Magalhães, F. Veiga, and A. Figueiras, "Poloxamers, poloxamines and polymeric micelles: Definition, structure and therapeutic applications in cancer,"J. Polym. Res., vol. 25, no. 1, 2018

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BIOMATERIALS AND POLYMERS / 156

Molecular interaction between the protein E serotype II of DEN-V and reuse drug using surface plasmon resonance

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Given the current lack of specific treatment options against dengue virus, a major health issue in tropical and subtropical regions, the study's findings on drug reuse could offer a promising alternative. Our group previously found by molecular dynamics that five FDA-approved drugs show a selective molecular coupling to the E protein of the dengue virus, the main antigen expressed during the disease. This work evaluated experimentally the molecular interactions between the protein E serotype II of dengue virus and three of the reuse pharms selected by molecular dynamics studies: Paritaprevir, Digoxin, and Trypan blue, using surface plasmon resonance to determine the adsorption, desorption, and equilibrium constants of the protein-reuse drugs interactions. Our findings show that Paritaprevir is the proper drug to continue investigating for a possible treatment against dengue virus replication.

Keywords:

Dengue, protein E, reuse drugs, surface plasmon resonance, molecular interactions.

Reference:

N/A

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BIOMATERIALS AND POLYMERS / 204

Study of physiochemical changes of equine hydroxyapatite as a function of the age obtained by calcination

Author: Brandon Alexis Correa Piña[1]

Co-authors: Angelica Marcela Castillo Paz [2]; Mario Enrique Rodriguez Garcia [3]

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Biogenic hydroxyapatite (HAp) is highly valued in medical science for its biocompatibility, bioactivity, osteoconductivity, and non-toxicity. Sourced from bovine, porcine, and human bones, it contains vital ions such as Na, Mg, Zn, K, and CO3, crucial for guided bone regeneration (GBR) and varying with age. This study examines the physicochemical properties of HAp from horse humerus bones at different ages (1, 3, 6, and 8 years), subjected to low-temperature calcination (600 ℃). Thermal analysis showed significant mass loss due to water, collagen, organic compounds, carbonates, and age-related magnesium diffusion. Older bones, with higher fat content, experienced greater mass loss. Phosphorus levels were constant across ages, while calcium and sodium fluctuated with age. Magnesium levels declined with age, highlighting its role in early bone development. The Ca/P ratio deviated from stoichiometric values due to additional biogenic ions. Infrared spectroscopy identified functional groups in carbonated HAp, with noticeable changes before and after calcination. The decrease in the full width at half maximum of the 961 cm-1 band with age indicated improved crystalline quality. Molar absorption coefficients revealed molecular concentration changes and emphasized age-related differences. X-ray analysis confirmed nanocrystalline HAp in all samples, with crystallite size increasing with age. Rietveld analysis showed lattice parameters were influenced by organic material, but lattice constants remained stable, confirming high crystallinity regardless of age. TEM analysis supported nanocrystalline structures, with larger crystallite sizes in older bones. SEM images displayed the characteristic porosity of calcined HAp, with particle size positively correlating with age. Calcination at 600 ℃ preserved the nanoscale properties and microcrystal formation. The results confirm that age significantly impacts the physicochemical properties of HAp extracted from bones, making it a crucial factor in its extraction and use.

Keywords:

Hydroxyapatite, Horse bones, Age-dependent variations, characterization

Reference:

A. Castillo-Paz, B. Correa-Piña, O. Gomez-Vazquez, D. Cañon-Davila, M. Rodriguez-Garcia. Influence of the changes in the bone mineral density on the guided bone regeneration using bioinspired grafts: a systematic review and meta-analysis. Biomed. Mater. Devices. 2022; 1-17. https://doi.org/10.1007/s44174-022-00026-z

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BIOMATERIALS AND POLYMERS / 142

DETERMINATION OF THE CURING TIME OF DIFFERENT BIOCOMPATIBLE DYE RESINS USING THE PHOTOACOUSTIC TECHNIQUE

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The application of photothermal techniques has allowed the study of optical and thermal properties of different photocurable, biocompatible and biodegradable resins. In this work, the study of composite resins based on PCL and PCLMA was carried out using photoinitiators to produce photocurable dye resins. The UV-visible absorption spectrum was analyzed to determine the wavelength for curing the resins. Curing times were compared using the open cell photoacoustic technique, using a 405 nm laser modulated with a lock-in amplifier. Critical times were obtained as a function of the resin curing time and adjustments were made with respect to an exponentially increasing synodal equation. From the results, it was observed that the resins with green and red pigments had longer curing times τ=752.5 s and τ=572.87 s, respectively compared to the curing time of the transparent resin (τ=465.4 s). Due to its versatility and non-invasive nature, this technique can be used in various areas such as biology, medicine, physics, and chemistry. This study has applications for microscaffolds produced by microstereolithography for tissue engineering, among others.

Keywords:

microstereolithography, UV cured, polycaprolactone, methacrylate

Reference:

No references

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BIOMATERIALS AND POLYMERS / 89

Antimicrobial Cotton Gauze Dressings Derived from Poly(N-vinyl caprolactam-co-maleic anhydride) Grafting

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Cotton gauze was grafted with poly(N-vinylcaprolactam-co-maleic anhydride) to create novel wound dressings with varying polymer attachment levels (23%, 40%, 100%). These modified gauzes displayed efficient loading and release of vancomycin, an antibiotic, and inhibited the growth of *S. aureus*. Furthermore, the materials exhibited good biocompatibility with cell lines tested. These findings suggest promise for these grafted gauzes as next-generation wound dressings with combined antimicrobial and drug delivery functionalities.

Keywords:

Poly(N-vinylcaprolactam-co-maleic anhydride), Antimicrobial, Drug delivery, Biocompatibility, Grafted gauze

Reference:

Betancourt-Galindo, R., Carrillo-Rodríguez, J.C., Meléndez-Ortiz, H.I. et al. Poly(N-vinyl caprolactam-co-maleic anhydride)-Grafted Cotton Gauze with Antimicrobial Properties for Their Potential Use as Wound Dressings, Fibers Polym. 25 (2024) 933–943 https://doi.org/10.1007/s12221-024-00490-y

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BIOMATERIALS AND POLYMERS / 288

ANALYSIS OF MECHANICAL, THERMAL AND MICROSTRUCTURAL PROPERTIES OF POLYPROPYLENE/RESIDUAL CERAMICS

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Co-authors: CRISTAL PALOMA GONZALEZ HERNANDEZ [3]; VANESSA ANDRÉS MENDEZ [3]

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Abstract The polyolefin elastomer grafted compatibilising agent (POE-g-MAH) is studied. The composites were fabricated by extrusion and injection moulding processes, and their morphology and microstructure, as well as fracture surface, mechanical and thermal properties were analysed. Characterisation by polarised optical microscopy showed that the ceramic residue particles were well dispersed in the iPP matrix without the presence of agglomerates. However, POE-g-MAH did not show good compatibility when added to the iPP/CW composite. Rockwell R hardness, tensile and flexural measurements showed that the hardness, Young's modulus and flexural modulus increased with the addition of CW and without POE-g-MAH. The ductility of the composites decreased with the addition of CW. POE-g-MAH affected the hardness, ductility, tensile strength, Young's modulus, flexural modulus and interfacial interaction in the iPP/CW composite. X-ray diffraction analysis showed that CW also acted as a nucleating agent, increasing the degree of crystallisation and forming the β-phase. Fourier transformed infrared analysis showed transmittance bands of iPP, CW,

POE-g-MAH and composites. The bands were similar and there were no major changes in the characteristic bands of the composites, but CW and POE-g-MAH produced changes in the shape and intensity of the peaks of the iPP matrix bands. The addition of CW to the iPP matrix modified the thermal properties of pure iPP, such as the degree of crystallisation and the melting temperature in the iPP/CW composites. The addition of POE-g-MAH decreased the crystallisation temperature and the degree of crystallinity in the iPP/CW composite.

Keywords:

ceramic waste; isotactic polypropylene; mechanical properties; thermal properties; POE-g-MAH.

Reference:

H. C. Gonzalez, V. Andres, R. R. Lopez, V. A. Flores, S. V. Castrejon, J. L. Tellez, R. H. Dorantes y V. O. Soriano, «ANALYSIS OF MECHANICAL, THERMAL AND MICROSTRUCTURAL PROPERTIES OF POLYPROPYLENE/RESIDUAL CERAMICS,» MATERIALS SCIENCE pp. 1320-1392, 2023.

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BIOMATERIALS AND POLYMERS / 72

PHYSICOCHEMICAL CHARACTERIZATION, MECHANICAL PROPERTIES, AND ANTIFUNGAL ACTIVITY OF NANOSTRUCTURED CHITOSAN-POLYVINYL ALCOHOL BIODEGRADABLE FILMS

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Nowadays, pollution due to single-use plastics used for food packaging applications has caused serious environmental problems. Therefore, an environmentally friendly solution must be sought. The aim of this work was to compare the effect on the physicochemical and mechanical properties, and on the antifungal activity due the incorporation of nanoparticles (NPs) to biodegradable polymer films. For that, nanostructured films based on chitosan (CS), chitosan nanoparticles (CSNPs), and polyvinyl alcohol (PVA) were elaborated by casting. Three formulations without NPs and four with NPs were prepared varying the CS:PVA ratio. For the nanostructured films, 33% of CSNPs were added. Scanning electron micrographs revealed the cross-section morphology of the films. Fourier-transform infrared spectroscopy (FTIR) showed no difference between samples. With the incorporation of CSNPs, the degree of swelling was higher compared to the films without CSNPs, being between 1.30-1.69% and 0.20-077%, respectively. From the mechanical properties, the highest value of Young's modulus was for the formulation 33%CSNPs:67%PVA (51.4±8.4 MPa) and the highest value of elongation at break was for the 33%CSNPs:50%PVA:17%CS (80.7±0.3%). The in vitro antifungal activity was measured against Botrytis cinerea. Higher inhibition was observed for films with NPs compared to those without NPs. Total inhibition (100%) was observed for the 33%CSNPs:67%PVA film. From films'characterization it was concluded that NPs improved the mechanical properties for

food packaging applications as well as antifungal activity. CS-PVA based nanocoatings could be a technological alternative to conventional plastics for biodegradable films.

Keywords:

nanoparticles, morphology, swelling, tensile testing, in vitro

Reference:

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BIOMATERIALS AND POLYMERS / 65

Influence of purification methods on the extraction of nanocrystals from bio-hydroxyapatite under consideration of the coalescence phenomenon

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Co-authors: Angélica Marcela Castillo Paz [1]; Brandon Correa Piña [2]; Mario Enrique Rodríguez Garcia [2]; Rafael Ramírez Bon [1]; Sandra Milena Londoño Restrepo [2]

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The coalescence of nanocrystals that occurs during low-temperature cleaning thermal treatments of hydroxyapatite from pigs have yet to be investigated. Traditional methods like calcination at high temperatures cause more significant energy expenditure than low temperatures, while chemical cleaning processes using solvents like ketones and ethers can pose health and environmental risks. To minimize waste and energy consumption, the study uses Soxhlet extraction, known for its efficiency in organic material extraction while reducing environmental impact.
To preserve the features of bio-hydroxyapatite, two methods with less environmental impact than traditional routes were investigated: Route 1 (autoclave and Soxhlet) and Route 2 (calcination at low temperatures at different times). The focus is observing the effectiveness of removing fats and proteins while maintaining crystallite size and morphology. DSC showed that the coalescence of crystallites occurred at 422, 518, and 672 ℃. P-Raw has a higher IR FWHM (phosphate band) due to the organic material; P-R1 had a lower FWHM (partial removal of lipids and proteins). Increasing the calcination temperature decreases the FWHM, indicating a shift in vibrational states from surface to bulk, resulting in an increase in apparent crystallite size due to coalescence. No significant changes occur in the IR spectrum for 20-80 hours at quasi-stable temperatures of 400 and 500 ℃. ICP showed that samples P-R1 and P-R2-400℃-20h still contain organic material, while the content of Ca and P is low due to the concentration effect. The mineral contents of the other samples show no change. X-ray diffraction indicates the removal of organic material during calcination, as the peaks become more defined with increasing temperature. The crystallite size is not affected and remains in similar ranges. Purification with hydroxide shows increased lattice parameters and fluctuations due to the ionic substitutions occurring naturally in HAp of biogenic origin.

Keywords:

Biomaterials, hydroxyapatite, cleaning, coalescence, calcination

Reference:

Cañon-Davila, D. F., Castillo-Paz, A. M., Londoño-Restrepo, S. M., Pfeiffer, H., Ramirez-Bon, R., & Rodriguez-Garcia, M. E. (2023). Study of the coalescence phenomena in biogenic nano-hydroxyapatite produced by controlled calcination processes at low temperature. Ceramics International. 49(11).

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BIOMATERIALS AND POLYMERS / 85

Rheological, morphological, thermal and permeability studies of bilayer chitosan-polyethylene oxide-Cerium fibers fabricated via the electrospinning technique

Authors: Claudia Mendoza-Barrera[1]; Josue Perzabal-Dominguez[2]

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The electrospinning technique has received broad approval because of its capacity to fabricate functional biomaterials in the micro and nano scale with the aid of various materials such as metals, ceramics and/or biopolymers for a wide range of applications such as biomedicine, bioremediation, energy storage, tissue engineering and many others. In particular, biopolymer-based micro and nanofiber membranes have diverse advantages: low cost, wide range of applications, exposed functional groups, low or null cytotoxicity, among others. The selection of the physical, chemical, and environmental variables in the fabrication process allows us to control the deposition time, morphology, porosity, and arrangement. In the same manner, the employed configuration allows us to generate simple, coaxial, or triaxial fibers. This work reports the fabrication of coaxial nanofibers of chitosan-polyethylene oxide (80:20) crosslinked (genipin 0.4% v/v) and doped with cerium (1, 2, 3, 4, 5 % w/v) for the shell layer and polyethylene oxide (5% w/v) for the core. It was determined that the increase in the dopant, for constant concentrations of chitosan, induces a decrease in viscosity. For its part, it was observed by AFM that increasing the concentration of cerium up to 4% m/v in the shell layer promotes the reduction of imperfections and the alignment of the fibers. The thermal analysis done by thermogravimetry and differential scanning calorimetry tells us that increasing cerium concentrations results in a decrease in the heat capacity of the membrane, although the membrane's working temperature is enhanced in general. For its part, the permeability study of the membranes in aqueous solutions via contact angle determined a hydrophilic behavior, on an average time of 30 seconds. Moreover, their contact angles grow as the cerium concentration grows in the shell layer.

Keywords:

electrospinning, coaxial fibers, biomaterials, properties.

Reference:

L. A. Hoyos-Lima, et al., Effect of Ce3+ on the morphology, composition, and thermal properties of single and core-shell polyethylene oxide electrospun fibers, Revista Mexicana de Física,69 (2023)021003 1–10. https://doi.org/10.31349/RevMexFis.69.021003.

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BIOMATERIALS AND POLYMERS / 101

Synthesis and characterization of chitosan films reinforced with silver dendrites.

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Skin injuries is a common health problem, and its consequences increase when these skin injuries are produced by high energy processes, such as fire and/or high voltage process, or when the person has chronic diseases such as diabetes, cancer, or other health problems. For that, different projects are dedicated to improving the skin's health. This project shows the initial results of chitosan films reinforced with Silver dendrites (Ch-Ag-d). The Ag-d was synthesized using an electrochemical process with an Ag wire in Acetic acid (Ac) solutions. The Ag-d were morphological and structural characterized using SEM and XRD diffraction, while the Ch-Ag-d were structure, morphology, and chemical characterized using XRD, optical microscopy, and FTIR. The Ag-d presents the combination of Ag and AgO structure at low Ac% and just Ag structure at a high Ac concentration. Including the Ag-d in the Ch film did not present a change in the chemical composition, being the Ch film just the transport of the Ag-d.

Keywords:

Film, Chitosan, Silver dendrites, electrochemistry, Skin injuries

Reference:

Skin Wound Healing: An Update on the Current Knowledge and Concepts
Human Skin Wounds: A Major and Snowballing Threat to Public
Skin Wound Healing Process and New Emerging Technologies for Skin Wound Care and Regeneration

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BIOMATERIALS AND POLYMERS / 109

CANNABIDIOL ENCAPSULATION IN LIPOSOMES

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Essential oils are unstable and susceptible to degradation when exposed to oxygen, light, and temperature changes. In particular, cannabidiol (CBD), recognized for its excellent topical bioavailability and known for its anti-inflammatory, analgesic, and antioxidant properties. Because of this, methods to preserve its properties have been explored, with encapsulation being one of the most promising methodologies. One potential method involves liposomal encapsulation, which acts as a protective barrier, ensuring the integrity and efficacy of the essential oils. To increase its bioavailability and effectiveness in medicine, pharmacy, and cosmetics, CBD nanoliposomes (CBD-NL) were developed. Encapsulation of CBD in liposomes can be a solution by having a nanometric size, avoiding oxidation, and achieving uniform size, improving their use.

The main objective of this research was to obtain stable CBD liposomes of uniform size. To achieve this, the synthesis of CBD-NL consisted of preparing different concentrations of CBD (2 to 4%) / Tween 80 (20, 36, 60, 76%) to evaluate their effect on the stability and size of the liposomes. The system aims to manipulate at the nanoscale, and our methodology is divided into two phases: middle agitation and ultrasonic homogenizer, to obtain nanoliposomes.

Through Dynamic light scattering and Transmission electron microscopy, we determined the hydrodynamic ratio, distribution, and morphology of the nanoliposomes, in addition to identifying and quantifying the components by UV-Vis spectroscopy that affect their changes and stability. Additionally, antioxidant tests showed that the stability of the emulsion is not affected by the encapsulation process, as well as the kinetic parameters to optimize the formulation and ensure a controlled and effective release of CBD.

In conclusion, using the dispersion method (middle agitation and ultrasound), it is possible to form Tween 80 liposomes with CBD. This study provides a solid foundation for future research on improving the bioavailability of CBD through nanotechnology.

Keywords:

Cannabidiol, encapsulation, liposomes, bioavailability, degradation

Reference:

Fraguas-Sánchez, A. I., Fernández-Carballido, A., Martin-Sabroso, C., & Torres-Suárez, A. I. (2020). Stability characteristics of cannabidiol for the design of pharmacological, biochemical and pharmaceutical studies. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 1150. https://doi.org/10.1016/j.jchromb.2020.122188

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BIOMATERIALS AND POLYMERS / 110

SYNTHESIS AND CHARACTERIZATION OF A MOLECULAR IMPRINTED POLYMER

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Molecular Imprinted Polymers (MIPs) are synthetic materials with tailored recognition sites that exhibit high affinity and selectivity for specific target molecules. This work presents the synthesis of a MIP for the selective recognition of a biomolecule, specifically cortisol. The binding properties of the MIP were evaluated using UV-Vis Spectroscopy. Additionally, the reaction kinetics during MIP polymerization were studied. Key parameters influencing the polymerization rate, such as initiator concentration, temperature, and reaction time, were investigated. The kinetic data obtained allowed for the optimization of the synthesis conditions to achieve a MIP with optimal affinity and selectivity towards the target analyte. The results of this kinetic study were integrated with the characterization findings to better understand the recognition and binding properties of the MIP. The results demonstrated that the MIP exhibited high affinity and selectivity for cortisol, with significantly higher binding capacity and selectivity compared to Non-Imprinted Polymers (NIPs). The MIP also showed good stability and reusability. These findings suggest that the synthesized MIP has promising potential as a bioreceptor for the selective recognition and detection of the target analyte in various applications, such as biosensors, separation science, and drug delivery.

Keywords:

Molecular Imprinted Polymers, cortisol, recognition sites, reaction kinetics, binding properties

Reference:

Septia-Yulianti, Elli, Siti Fauziyah-Rahman, y Yudan Whulanza. «Molecularly Imprinted Polymer-Based Sensor for Electrochemical Detection of Cortisol», Biosensors, 12, n.o 12 (2022): 1090. https://doi.org/10.3390/bios1212109

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BIOMATERIALS AND POLYMERS / 132

MICROENCAPSULATION OF CALENDULA ESSENTIAL OIL FOR ANTI-AGING SKIN APPLICATIONS.

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Calendula, is a plant that possesses medicinal properties due to its bioactive molecules, called carotenoids and flavonoids. These molecules have antioxidant activity, which leads to the neutralization of free radicals, preventing cellular damage, and promoting healthier aging. In this study, the essential oil extraction of the marigold flower was carried out through maceration in almond and jojoba oils with the aim of obtaining its bioactive components. The essential oils were monitored daily to ensure the quality of the essential oil. The microencapsulation of the essential oil was performed using the ultrasound method at a power of 250W, with sodium alginate as a stabilizing agent and Tween 20 as an amphiphilic emulsifier with an HLB of 14.9. The characterization of the essential oil and the microemulsion was carried out using optical microscopy and FTIR techniques. The presence of antioxidant molecules in the oil macerate was confirmed. Nanoparticles of each sample were observed through optical microscopy. The functional groups that make up the microemulsion were confirmed using FTIR.

Keywords:

calendula, essential oil , microencapsulation.

Reference:

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Dra. Edith Bravo González.
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BIOMATERIALS AND POLYMERS / 133

Chemical composition and mechanical properties of test of sea urchin Echinometra vanbrunti: materials with potential for biomimetic applications.

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Co-authors: Amir Maldonado Arce [2]; Lerma H. Chan Chan [1]

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The endoskeleton of the sea urchin (Echinodermata: Echinoidea) is formed by three structural components: test, dental apparatus and accessory appendages. Although all parts of the echinoid skeleton consist of the same basic material, its microstructure shows great potential to satisfy various mechanical needs according to a direct and clear structure-function relationship. This characteristic has allowed the sea urchin skeleton to adapt to different activities such as structural support, defense, feeding, cleaning and reproduction. Therefore, these structures can be used as role models for bioinspired solutions in various industrial sectors, such as building construction, robotics, biomedical and materials engineering. The organisms (*E. vanbrunti*) were already collected in Bahía de Kino, Sonora, Mexico. The tests were washed with distilled water and dried and subsequently stored at -20℃ until analysis. The elemental composition will be determined by means of EDS, total ash content, morphological analysis by SEM. Mechanical properties such as robustness tests will also be analyzed, according to the method of Byrne et al. (2014). Based on the main morphological characteristics and mechanical properties of the *E. vanbrunti* tests, we hope to provide scientific knowledge that could determine to a certain extent the biomimetic potential of these materials.

Keywords:

biomimetic materials, sea urchin, test, Echinometra vanbrunti, structure-function

Reference:

M. Byrne. A. M. Smith, S. West, M. Collard, P. Dubois, A. Graba-Landry, S. A. Dworjanyn Warming influences Mg2+ content, while warming and acidification influence calcification and test strength of a sea urchin. Environ Science & Technol. 21 (2014) 12620–12627.

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BIOMATERIALS AND POLYMERS / 146

IMPACT OF THERMAL AND PH VARIATIONS ON THE FUNCTIONAL PROPERTIES AND CONFORMATIONAL STABILITY OF THE VINORAMA (ACACIA CONSTRICTA) LECTIN

Authors: Rocío León Irra[1]; Irlanda Lagarda Díaz[1]; Rosina Cabrera Ruiz[2]; Luz Vázquez Moreno[2]; Amir Darío Maldonado Arce[1]

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Lectins are carbohydrate-binding proteins of non-immune origin that can recognize and bind simple or complex carbohydrates in a reversible and highly specific manner. Lectins are widely distributed in plants, animals, and other organisms. These biomaterials have found practical applications due to their antitumor, immunomodulatory, antifungal, and/or anti-insect activities. Lectin legumes have been studied since some time ago. Their carbohydrate and structure specificities vary widely which greatly influences the recognition of specific targets. Protein functionality relies on their three-dimensional structure, maintained by interactions such as Van der Waals forces, hydrogen

bonds, and disulfide bonds, which can be disrupted by changes in pH and temperature. This study examines the effects of temperature and pH on the conformational stability and functional activity of a lectin obtained from the legume seeds: Vinorama (Acacia constricta). The protein (VL) was studied with several techniques: fluorescence intensity (FI), Circular Dichroism (CD), Hemagglutinating Activity (HA) assays and Dynamic Light Scattering (DLS). Our results indicate an increase in VL's hydrodynamic diameter with rising temperatures, suggesting aggregation, yet VL retained biological activity, indicating thermal resistance. FI analysis showed structural changes at acidic and basic pH, with native VL (pH 7, room temperature) having buried aromatic amino acids. Extreme conditions caused protein unfolding. Thermal analysis showed stable FI up to 55℃, a significant peak at 75℃ due to tryptophan exposure from unfolding, and a 50% decrease at higher temperatures, indicating aggregation. CD spectra revealed a β-sheet structure for VL and a transition temperature (Tm) above 75℃, indicating unfolding at high temperatures. Despite structural changes, VL maintained biological activity across pH ranges but lost activity above 75℃.

Author will attend:

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Keywords:

Vinorama Lectin, Fluorescence Intensity, Circular Dichroism, Hemagglutinating Activity

Reference:

Purification and characterization of complex carbohydrate specific isolectins from wild legume seeds: Acacia constricta is (vinorama) highly homologous to Phaseolus vulgaris lectins
Biochimie, Volume 86, Issues 4–5, April–May 2004, Pages 335-342
A.M Guzmán-Partida, M.R Robles-Burgueño, M Ortega-Nieblas, I Vázquez-Moreno

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BIOMATERIALS AND POLYMERS / 149

ADSORPTION STUDY OF DEXAMETHASONE ON MAGNETIC NANOPARTICLES STABILIZED WITH GLYCINE

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The functionalization of the surface of magnetic nanoparticles (MNP) reduces toxicity, increases the surface area, and provides a certain surface charge that improves their stability. The glycine is an amino acid that in solution it is found as a dipolar ion that allows its interaction with the MNP and, due to its biological nature, improves the biocompatibility. In this work we present the results of the synthesis and characterization of Fe nanoparticles (NPs-Fe), Fe3O4 nanoparticles (NPs- Fe3O4) and glycine functionalized at different concentrations. These samples were used as adsorbents for dexamethasone (DEX) which is a drug used in the treatment of COVID-19.
The NPs-Fe and the NPs- Fe3O4 were synthesized by chemical reduction and co-precipitation, respectively. The results of the characterization performed by Scanning Electron Microscopy (SEM), Potential Z (PZ), X-Ray Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR) of NPs-Fe and NPs-Fe3O4 unstabilized and stabilized with glycine at concentrations of 0.16, 0.32 and 0.48 M are reported.

All samples of the NPs-Fe and Fe3O4 presented quasi-spherical morphology and with average diameters between 121 nm to 85.6 nm and between 20 and 30 nm, respectively. The results showed that glycine improves the stability of NPs-Fe and NPs- Fe3O4.The stabilized and unstabilized NPs-Fe exhibit a BCC crystal structure and inverse spinel crystal structure for the NPs- Fe3O4. The crystallite size decreased from 9.55 nm to 5.54 and from 11.8 to 11.5 nm, for NPs-Fe and NPs- Fe3O4, respectively.
Furthermore, the adsorption kinetics are studied by varying the mass of the adsorbent (NPs-Fe and NPs- Fe3O4) and keeping the concentration of the adsorbate (DEX) constant. According to the results obtained by UV-Vis spectroscopy, it is observed that the use of glycine improves the adsorption of the DEX on the surface of NPs-Fe and NPs- Fe3O4.

Keywords:

Iron, magnetite, nanoparticles, adsorption kinetics, dexamethasone

Reference:

Eljamal, R., Eljamal, O., Khalil, A. M., Saha, B. B., & Matsunaga, N. (2018). Improvement of the chemical synthesis efficiency of nano-scale zero-valent iron particles. Journal of environmental chemical engineering, 6 (4), 4727-4735. https://doi.org/10.1016/j.jece.2018.06.069

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BIOMATERIALS AND POLYMERS / 320

Vegetal material alternatives for industrial chlorophyll production

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The green leaf blade of plants is a cellular biomaterial specialized in photosynthesis (conversion of light to chemical energy with absorption of CO2 and release of O2). This process is possible due to the abundance of cellular chloroplasts that contain chlorophyll. The main recognized uses are dyes (textile and food), vitamins, therapeutic properties and antioxidants. Therefore, in this work, non-traditional alternatives for plant materials are proposed for the industrial extraction of chlorophylls and thereby also promote the agricultural crops from which it comes. Herbaceous species with different uses: coriander, spearmint, chard, spinach and forage crop (lucerne), were treated according to the chlorophyll extractive methodology by Callejas et al. (2013), a minimally invasive (ethanol as extractant) and rapid technique (2 stages) which involves maceration with 96° ethanol and centrifugation, subsequently the absorbance reading is monitored at 665, 649 and 470 nm. With evaporation of ethanol in the extracts generates chlorophylls in a solid state pulverized to be used as inputs in various industrial applications. In the ethanolic extracts, the suspended matter (°Bx) was determined by refractometer and the antioxidant capacity according to Canadanovic, et al.

(2014). The yield was obtained for chlorophyll type a, b and carotenoids (Lichtenthaler, 1987) with respect to fresh leaf. The yields for obtaining the most abundant chlorophyll pigment "a"expressed as µg/cm2 and mg/100g were: spearmint 175.9; 1,639.5 > coriander 48.4; 345.9 > chard 32.5; 194.59 > lucerne 25.92; 165.5 > spinach (traditional species) 45.5; 101.9. The °Bx were similar in all extracts, (19.5-20.5) °Bx. Finally, the antioxidant capacity in % DPPH radical inhibition was highlighted for spearmint: spearmint (39.80%) > lucerne (24.50%)> chard (9.16%) > coriander (5.33%). It is concluded that spearmint showed potential for the industrial extraction of chlorophyll as a raw material for use as antioxidants, even in the field of photographic development.

Keywords:

Chlorophyll, leaf plant material, chlorophyll extraction, antioxidants, DPPH radical

Reference:

Lichtenthaler, 1987

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BIOMATERIALS AND POLYMERS / 153

BIOHYDROGELS WITH HYDROXYAPATITE-WOLLASTONITE FOR POSSIBLE APPLICATIONS IN TISSUE ENGINEERING

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The sodium alginate hydrogels in tissue engineering area, for example, in bone tissues, are limited because of their weak mechanical properties, in addition to the lack of cell interaction and its uncontrollable degradation. In this context, is proposed the preparation of alginate-based hydrogels with Hydroxyapatite-Wollastonite. This bioceramic compound is synthesized by the Sol-Gel method in different component proportions. The wollastonite with high purity and extracted by the NYCO miner and the alginate was obtained of sargassum from Sonora.
The hydrogels characterization by FTIR, SEM, TGA, the mechanic properties through the compression and thermal analysis with DMA, will be shown.
The wollastonite use is based on the contributions that this mineral gives to the hydroxyapatite, because is reported an improvement the mechanical proprieties, in virtue of the acicular crystalline habit that it possesses, which allows the creation of an interwoven reinforcing mesh, that takes advantage by the hydroxyapatite. Also, the mineral enhances the bioactive and biocompatible qualities of the hydroxyapatite.

Keywords:

Sodium alginate, Hydrogels, Hydroxyapatite, Wollastonite, Bone tissues

Reference:

- M. A. Encinas-Romero, J. Peralta-Haley, J. L. Valenzuela-García, Felipe F. Castillón-Barraza; Synthesis and Structural Characterization of Hydroxyapatite-Wollastonite Biocomposites, Produced by an Alternative Sol-Gel Route; J. of Biomaterials and Nanobiotechnology 4 (2013) 327.

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BIOMATERIALS AND POLYMERS / 170

MOF-LDH COMPOSITES FOR SULPHUR DIOXIDE ADSORPTION IN AIR: A STUDY

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Sulfur dioxide (SO2) is an extremely toxic gas, primarily generated by the combustion of fossil fuels and various industrial processes. Its presence in the air can cause respiratory problems and contribute to acid rain, affecting both human health and the environment. Consequently, the development and use of highly efficient methods to eliminate this gas is of great importance. In this study, a nanocomposite material with micro-mesoporous architecture structured by a MgAlFe layered double hydroxide (MgAlFe-LDH) and a metal-organic framework (UIO-66-NH2) was developed through in situ chemical growth of UIO-66-NH2 on the surface of MgAlFe-LDH treated with (3-chloropropyl)trimethoxysilane. Structural characterization of this nanocomposite using XRD, FTIR, SEM, and BET surface area confirmed the successful development of this material. The adsorption behavior of SO2 was evaluated using a vapor and gas sorption analyzer under vacuum conditions (DVS Vacuum), and the influence of important parameters, including the amount of adsorbent, the initial concentration of SO2, and contact time, was investigated. A better efficiency of these parameters was observed compared to other similar SO2 adsorbents such as ZnAl-LDH, CO3MgAl-LDH, OHMgAl-LDH, UIO-66-ox, 18-UIO-66-cyanoacetic, and UIO-66-NH2/PAN6. These findings highlight the potential of composite materials in mitigating atmospheric pollution by enhancing the efficiency of adsorbing harmful gases such as SO2.

Keywords:

Adsorption, Metal-organic frameworks, Layered double hydroxides, Surface functionalization

Reference:

1- N. Kumar Gupta, C. Leyva, H. Viltres, R. P. Dhavale, K. Soo Kim, A. Romero-Galarza, H. Ho Park, Chemosphere, 338, (2023), 139503

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BIOMATERIALS AND POLYMERS / 186

Molecular Dynamic Study of Behavior of Surfactants Under Water Confinement.

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This research used molecular dynamics simulations to investigate the behavior of surfactant molecules when confined in a thin layer of water, simulating a thin liquid film. The anionic sodium dodecyl sulfate (SDS) was chosen as the surfactant model for the study. Our simulation employed the OPLS-AA force field, with various input parameters relating to the initial amounts of water, SDS, and a gas phase. The forces interaction from the water was modeled by the SPC/ε (extended simple point-charge water model), while the gas phase was modeled via long-range Lennard-Jones potential. Isotropic and semi-isotropic NPT ensembles were implemented with the Nose-Hoover thermostat and Parrinello-Rahman barostat. We have conducted several simulations, changing the pressure each time with the object of observing the effect of the pressure on the system. To model foam film's thinning and thickening transitions, we conducted a second set of simulations at constant pressure but with varying water volumes in the system. All simulations consistently yielded the formation of a thin water film stabilized by the SDS surfactant monolayer at the air-water region. Despite the surfactant concentrations in the simulation being below the critical micellar concentration, so that we assume surfactants adsorb at the interface, we were surprised to observe the formation of SDS self-assemblies micelle-like within the bulk water phase under certain conditions. Our findings provide molecular insights on the morphology transitions of surfactant monolayers in confined system. Subsequently, a correlation was established between the system's bulk pressure and the simulation box's mechanical surface tension, with a correction applied for the inherent water surface tension. This correlation exhibited a trend like the experimentally measured disjoining pressure, signifying the system's response to the interplay between short-range repulsive and long-range attractive forces. This finding challenges the conventional understanding of the behavior of surfactants below critical micellar concentration in confined systems.

Keywords:

thin liquid fim, molecular dynamic, foams, surfactant, confinement

Reference:

Abdel-Azeim, S. (2020). Revisiting OPLS-AA Force Field for the Simulation of Anionic Surfactants in Concentrated Electrolyte Solutions. Journal of Chemical Theory and Computation, 16(2), 1136–1145. https://doi.org/10.1021/acs.jctc.9b00947

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BIOMATERIALS AND POLYMERS / 221

RECYCLED PET NANOFIBERS DECORATED WITH WO3 BY ELECTROSPINNING TECHNIQUE

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Polyethylene terephthalate (PET) is a synthetic polymer with which we have daily contact (packaging), becoming an important source of waste and pollution. The PET was from wasted beverage bottles, and, the polymeric solution precursor of the nanofibers was prepared by dissolving PET and WO3 in a solvent mixture of TFA and CHCl3 (1:3), stirring time (1 hour), spun sample volume (3 ml). The nanofibers were heated at 80℃ for 1 hour to remove organic residual, release residual stresses, and improve fiber stability. The nanofibers were fabricated by electrospinning technique under conditions of voltage (20 kV), the needle from the collector (15 cm), and relative humidity (38%). To observe the effect of WO3 particles, recycling PET fibers and other recycling PET fibers decorated with 6% WO3 were analyzed, SEM images of both samples reveal fiber morphology, showing that the decorated fibers have smaller diameters. Also, thermograms of the nanofibers show a rapid mass loss of 5% attributed to the moisture and the beginning of the thermal degradation followed by the highest percentage of mass loss represents the decomposition of PET around 368℃, final, it is observed complete decomposition process of PET nanofibers at 532.89 ℃. The nanofibers decorated with tungsten oxide show lower mass loss and slightly decrease the amount of carbonized residue, which is related to the fact that WO3 is stable at these temperatures. Reusing and recycling PET in the form of nanofibers contributes to the process of recyclability and also by decorating it with WO3 particles, it can increase near infrared photoabsorption and potentially be used in desalination, water evaporation, photocatalysis or gas sensing.

Keywords:

Recycled PET, Nanofibers, PET/WO3 nanocomposite, Electrospinning Technique.

Reference:

Chala T., Wu C., Chou M., Guo Z. Melt Electrospun Reduced Tungsten Oxide /Polylactic Acid Fiber Membranes as a Photothermal Material for Light-Driven Interfacial Water Evaporation. ACS Appl. Mater. Interfaces. 10 (2018) 28955 –28962. https://pubs.acs.org/doi/10.1021/acsami.8b07434

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BIOMATERIALS AND POLYMERS / 269

CHITOSAN-POLOXAMER SMART HYDROGELS AS A VEHICLE FOR CURCUMIN LOADING

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Curcumin is a natural polyphenol widely studied for its antioxidant activity, among other properties. The disadvantage in the use of this active pharmaceutical ingredient (API) is its poor solubility in water, so it is necessary to use nanovehicles, such as poloxamers, that have the ability to form micelles and to maintain the API in the lipophilic core and at the same time be in an aqueous solution. To further protect the loaded micelle, it can be encapsulated into a chitosan hydrogel. This double encapsulation helps to maintain the system stable for a longer period and potentially allows the prolonged release of curcumin. Furthermore, this double-encapsulation strategy allows the incorporation of liposoluble APIs such as curcumin in chitosan-based hydrogels, which otherwise would be dispersed as insoluble crystals; resulting in improved bioavailability of liposoluble APIs. Therefore, in this study, hydrogels were obtained by incorporating F 127 poloxamer micelles loaded with curcumin into chitosan crosslinked with citric acid. The concentrations of chitosan (0.5, 0.75 and 1%) and citric acid (0.05, 0.075 and 1%) were varied. Physicochemical characterization was carried out by FTIR-ATR, determining interactions between the poloxamer and chitosan, as well as evidence of effective cross-linking. After 6, 15 and 24 hours of cross-linking reaction, the hydrogel was still in the dispersed state, as confirmed by hydrodynamic diameter size. After testing several methodologies, freeze-drying and rehydration turned out to be the most efficient way to obtain consistent hydrogels. Samples with a higher percentage of chitosan displayed greater curcumin loading efficiency, achieving values up to 80%. The stimulus-sensitive pH property of the hydrogels was demonstrated following a sustained release of 75% at physiological pH, compared to 84% release at pH 5.5, achieved in 168 hours. This characteristic makes the system very attractive for a potential use as nanovehicle for loading and release of curcumin.

Keywords:

Chitosan, micelle, curcumin, double encapsulation

Reference:

Branca, C., Conti Nibali, V., Khouzami, K., Wanderlingh, U., & D'Angelo, G. (2021). Comparative study of pluronic-chitosan and pluronic-guar gum composite thermogels. International Journal of Polymer Analysis and Characterization, 26(2), 179–188.

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BIOMATERIALS AND POLYMERS / 355

Characterization and Application of Composite Materials Using Soursop (Annona muricata)

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This study explores the synthesis and characterization of composite materials using extracts from soursop (Annona muricata), aiming to enhance the mechanical properties of bioplastics, highlighting the importance of composite materials in various technological fields, particularly their role in improving the durability and strength of bioplastics, the objectives included synthesizing these materials through bio-reduction processes and characterizing their impact on bioplastics, employing plant extracts for a more sustainable and eco-friendly approach, characterization was performed using Scanning Electron Microscopy (SEM) to analyze the surface of the composites, which demonstrated increased rigidity and resistance in bioplastics containing the composite materials, the results indicated that composites synthesized from soursop extracts significantly improve the mechanical properties of bioplastics, making them suitable for various scientific and technological applications, contributing to the field of material science by providing a sustainable method for enhancing bioplastic properties and reducing environmental impact.

Keywords:

Composite materials, biosynthesis, characterization, bioplastics, soursop

Reference:

Shankar, S. S., Ahmad, A., & Sastry, M. (2003). Geranium leaf assisted biosynthesis of silver nanoparticles. Biotechnology Progress, 19(6), 1627–1631.

Stegemeier, J. P. (2015). Speciation matters: Bioavailability of silver nanoparticles to alfalfa. Environmental Science & Technology, 49(14), 8451-8460.

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CHARACTERIZATION AND METROLOGY / 256

Determination of Thermal Diffusivity in Thin Films Using Lock-in Thermography Technique

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Co-authors: Alberto Sebastián Villeda Patricio [1]; Angel Eduardo Cerda Frutis [1]; Araceli Flores Conde [2]; Francisco Gómez López [1]; José Luis Jiménez Pérez [1]; Misha Jessica Del Castillo Aguirre [1]

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This study presents an innovative methodology for determining the thermal diffusivity in thin films of metals and organic materials using advanced thermographic techniques. A diode laser pulse is employed to create a thermal contrast on the sample surfaces, with the resulting temperature evolution monitored by an infrared camera. The collected data is then processed using a MATLAB-developed algorithm, enabling precise calculations of thermal diffusivity. The methodology utilized two laser types: a 415 nm laser and a 910 nm infrared laser, with respective powers of 100 mW and 150 mW. This approach was applied to analyze a thin film of copper oxide and another consisting of Fe3O4 magnetic nanoparticles on glass. The developed technique is both effective and non-destructive, offering a highly accurate tool for the thermal characterization of materials.

Keywords:

magnetite, ferrofluids, ferromagnetic, thermal conductivity, TWRC

Reference:

[1] L. S. Ganapathe, M. A. Mohamed, R. M. Yunus, D. D. Berhanuddin, Magnetochemistr. 6, 68 (2020). https://doi.org/10.3390/magnetochemistry6040068.

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CHARACTERIZATION AND METROLOGY / 55

A DIFFERENTIAL THERMAL LENS SPECTROMETRY METHOD FOR TRACE DETECTION

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Thermal lens spectroscopy, reliant on the thermal lens effect, offers a sensitive and non-invasive means for analyzing samples through their light absorption-induced refractive index changes. We aimed to enhance sensitivity using a novel differential method. This involved measuring the signal at the center point of the probe beam spot and comparing it with the signal obtained through spatial filtering, termed the "eclipsed signal." Experimentation utilized Deyman's organic dye "Strawberry2143 v.7"dissolved in alcohol, with a periodically modulated solid-state laser (532 nm) for excitation and a HeNe laser (632.8 nm) for probing. Our approach showcased nearly a 50% enhancement in lowering the detection limit compared to conventional methods. Additionally, we developed a continuous-flow reactor for temperature control, facilitating experiments in photocatalysis and adsorption for water remediation. The described differential thermal lens spectrometry method presents a highly sensitive approach for trace quantification in liquid samples, promising significant analytical advancements.

Keywords:

Thermal lens, spectroscopy, sensitivity enhancement, differential method, trace quantification.

Reference:

Dobek K. "Thermal Lensing: Outside of the Lasing Medium". Appl. Phys. B. 2022. 128(2): 18–38

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Author approval:

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CHARACTERIZATION AND METROLOGY / 64

Chemical Analysis of the Interface between CsPbBr3 and Al2O3 deposited by ALD as Protector Layer.

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All inorganics halide lead perovskites have emerged as promising candidates for optoelectronic devices due to their exceptional properties, including high absorption coefficients, tunable bandgaps, and superior charge carrier mobilities. These attributes make them ideal for applications in solar cells, light-emitting diodes, and photodetectors. However, a significant challenge limiting their practical application is their instability under environmental conditions such as moisture, oxygen, and thermal stress. To address this issue, the implementation of Al2O3 directly on the top of the perovskite has been studied as a protective layer. This protective mechanism is crucial for extending the operational lifespan of CsPbBr3-based optoelectronic devices, potentially making them more viable for commercial use. Further analysis and optimization of the interface could lead to significant advancements in the development of stable, high-performance perovskite-based optoelectronics. This work focuses on the detailed in-situ deposited and chemical analysis of the Al2O3/ CsPbBr3 interface, where the perovskite has been deposited by Close Space Sublimation (CSS) and the Al2O3 deposited by Atomic Layer Deposition (ALD) and employing X-ray photoelectron spectroscopy (XPS), and others characterization techniques. A plausible growth mechanism of ALD Al2O3 on top of perovskite is presented.

Keywords:

All-Inorganic perovskite, Atomic Layer Deposition, Al2O3, X-ray photoelectron spectroscopy, In-Situ

Reference:

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CHARACTERIZATION AND METROLOGY / 75

Towards Self-healing Coating Based Polymeric Nanocomposite for Surface Protection

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The strategic integration of nanomaterials into polyurethane-based coatings offers considerable improvements with metal oxide nanoparticles providing enhanced properties to the coatings. This approach aims to contribute insights for developing materials in surface protection within demanding environments, fostering innovation in the design of materials with self-healing properties. To enhance the self-healing properties of nanocomposite coatings based on polyurethane by leveraging the influence of titanium dioxide and silicon nanoparticles (TiO2-SiO2) because they have proven to be an effective filler material to improve the mechanical properties of many polymeric systems[1]. Thus, coatings are engineered to bestow mechanical strength and self-healing properties, prolonging lifespan and enhancing performance in various industrial and technological applications[2].
In this research, polymeric nanocomposites were prepared and characterized to understand their performance for surface protection subjected to mechanical damage. The nanocomposites based on metal oxide nanoparticles and polyurethane were prepared using an in-situ process, and the coatings were deposited via spin coating. The chemical and surface properties guided the preparation of the nanocomposite coatings.

Keywords:

Coatings, Self-healing, Polymer Nanocomposite, Metal oxide nanoparticles

Reference:

1. Rahman, M. T. et al. Study on the mechanical, electrical and optical properties of metal-oxide nanoparticles dispersed unsaturated polyester resin nanocomposites. (2019).
2. Choi, K. et al. Properties and Applications of Self-Healing Polymeric Materials: A Review. Polymers (2023).

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CHARACTERIZATION AND METROLOGY / 154

Correlation between Oxidation Degree and Mechanical Properties in Graphene Oxide: A Comprehensive Analysis

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Two-dimensional materials, such as graphene, have acquired significant attention due to their unique electrical, optical, and mechanical properties, making them highly promising for various applications including electronics, optoelectronics, and energy storage. This study focuses on graphene oxide (GO) samples with varying degrees of oxidation, synthesized using a modified Hummers'method. These samples were investigated using force-displacement curve indentations with an MFP3D-SA Atomic Force Microscope (AFM). The study establishes a correlation between the mechanical response and the degree of oxidation, highlighting potential applications based on mechanical performance. Characterization techniques including Thermogravimetric Analysis (TGA), X-ray Photoelectron Spectroscopy (XPS), Raman Spectroscopy, Scanning Electron Microscopy (SEM), and AFM were employed to link the type and quantity of functional groups.

Keywords:

Graphene oxide, Mechanical properties, Atomic Force Microscopy, Material characterization

Reference:

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CHARACTERIZATION AND METROLOGY / 155

Flexible Electrospun Graphene-Polymer Electrodes for Supercapacitors

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With the increasing global population and advancements in portable technology, there is a growing demand for improved energy storage devices like supercapacitors, which offer high-power performance, rapid charge/discharge cycles, and longer service life than batteries despite storing less energy. To enhance supercapacitor performance, this study focuses on developing electrospun membranes composed of graphene family materials based on polymeric nanocomposites. These materials provide high specific surface area, optimal pore size distribution, low internal electrical resistance, and enhanced electrochemical and mechanical stability. Recent advancements in nanoscience highlight the potential of graphene and carbon nanotubes due to their superior properties, with reduced graphene oxide emerging as a cost-effective and scalable alternative to overcome graphene's limitations, making it a promising candidate for high-performance supercapacitors.
Incorporating graphene-derived materials into (i.e., cellulose acetate) matrices via electrospinning has practical implications, producing high-performance supercapacitor electrodes with enhanced capacitance. This project not only sets the stage for future research proposals and projects but also paves the way for designing prototypes that address the need for higher technological maturity. The findings underscore the potential for developing advanced, flexible energy storage devices, highlighting the importance of optimizing material composition and electrospinning parameters for further performance improvements.

Keywords:

Graphene Derivatives, Electrospun electrodes, Polymer Nanocomposites

Reference:

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CHARACTERIZATION AND METROLOGY / 73

SUBSURFACE MICROSCOPY USING THERMOREFLECTANCE ON MICROELECTRONIC TEST STRUCTURE CROSS-BRIDGE AND GREEK CROSS FOR SHEET RESISTANCE MEASUREMENTS: HIGH-TEMPERATURE IMAGING

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The discussion of this works is focus about the temperature field induced by thermal losses in these components, highlighting the standard form of heating in some regions of interest generated with

the method of Thermoreflectance images, using polysilicon Greek Cross and Cross-Bridge Test Structures. The generation of these images are obtained by a laser probe beam on the surface of the sample, in these images reveal the regions periodically heated by Joule effect, which are associated with the electric current distribution in the four terminals in Greek Cross structure and six terminals in Cross-Bridge structure using resistance measurements. The thermoreflectance microscopy provides a temperature distribution map of the operating device with high resolution. The technique is also useful for detecting and imaging defects, besides the temperature field, it is also sensitive to local electric field, the noncontact and nondestructive character of the technique is one of its main advantages, measure the uniformity of the current in the etching of polysilicon-metal, it is also tested by means of simulations by finite element.

Keywords:

Reflectance, Photothermal, Microscopy, Polysilicon, Joule effect.

Reference:

Almond, D. P., & Patel, P. (1996). Photothermal science and techniques (Vol. 10). Springer Science & Business Media.

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CHARACTERIZATION AND METROLOGY / 105

STUDY OF THE MORPHOLOGY, THERMAL AND OPTICAL PROPERTIES OF N-TYPE POROUS SILICON SAMPLES FABRICATED USING SHORT ELECTROCHEMICAL ETCHING TIMES.

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The study of porous silicon has gained prominence due to modifications in its thermal and optical properties stemming from the formation of a porous layer, expanding its applications from sensors development to solar energy conversion systems design. One of the most commonly employed techniques for its fabrication is electrochemical etching; where a mayor challenge lies in achieving uniformity in pore distribution and size. In this investigation, porous silicon samples were fabricated via electrochemical etching on N-type crystalline silicon substrates, utilizing hydrofluoric acid (40 %) and platinum plates. The samples were processed from 1 up to 10 minutes, studying the etched surface morphology, along optical and thermal properties of the samples, aiming to establishes a correlation between the etching conditions and the observed physical properties. The morphology of the etched surface was analyzed using scanning electron microscopy, evaluating the distribution of pore size in all samples. The optical characterization of samples was focused on the examination of absorption and reflection spectra, as well as photoluminescent response; while

the effective thermal properties have been determined from the analysis of the thermal response, obtained through time-resolved infrared photothermal radiometry and frequency-resolved photoacoustic detection technique. Upon prolonging the electrochemical etching time, an increase in pore area of up to 39.5% was observed. This led to a shift in the luminescence spectrum from 800 nm to 550 nm, alongside an increase in absorbance and a reduction in effective thermal diffusivity of up to 35.5%. These alterations were attributed to the increased incidence area and the formation of a SiO2 layer with Si nanoparticles. These modifications open new perspectives for their application in LED devices.

Keywords:

Porous silicon; Electrochemical etching; Morphology; Photoluminescence; Thermal diffusivity.

Reference:

Calderón, A., Alvarado-Gil, J. J., Gurevich, Y. G., Cruz-Orea, A., Delgadillo, I., Vargas, H., & Miranda, L. C. M. (1997c). Photothermal Characterization of Electrochemical Etching Processed n-Type Porous Silicon. Physical Review Letters, 79(25), 5022-5025. https://doi.org/10.1103/physrevlett.79.5022

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CHARACTERIZATION AND METROLOGY / 274

Inhomogeneous interference filters. A promising deposition technique

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Traditional optical interference filters have been manufactured with discrete thicknesses since the 1930s, when anti-reflection coatings were first introduced in Zeiss microscopes. In most standard applications, the theoretical calculation of the optical response of a given filter is achieved by propagating electromagnetic waves through a continuous medium, a procedure known as analysis. However, when more stringent requirements are imposed to achieve a complex transmittance filter profile, a synthesis process becomes necessary. Various approaches exist to address this challenge.
In this study, we focus on the approximate Fourier Transform method to determine the index profile for a specified transmittance. The resulting rugate filter exhibits a smoothly varying refractive index as a function of thickness. The challenge lies in growing and controlling these index variations. In this contribution, we utilize reactive sputtering controlled by optical emission spectroscopy (OES). We detail the entire process, including the synthesis of the filter, the cleaning and calibration procedures using spectral ellipsometry, and the deposition and characterization of the resulting filter. This work is part of a Cátedras CONAHCyT project, which encompasses designing and assembling

the deposition chamber, integrating the ellipsometer, creating the OES system, designing the electronics control, developing the programming for each stage, and studying the physics behind target poisoning, spectral line intensity ratios, and their relationship with the refractive index of the film to be grown. The ultimate objective is to acquire knowledge and technology that can be transferred to the industry. We present here our initial, promising results.

Keywords:

Rugate lters, Optical Emission Spectroscopy, Ellipsometry

Reference:

*J. A. Dobrowolski. (1974). Applied Optics, 17(19), 3039-3050.*P. G. Verly, (1989). Applied Optics, 28(14), 2864-2875
*Cheng, X.(2008). Optics Express, 16(4), 2315-2321.*Rodríguez López, R. (2023). Tesis de doctoral en CICESE
*Villa E. (2023), Tesis doctoral en CICESE

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CHARACTERIZATION AND METROLOGY / 84

Detection of diabetes biomarkers using a gas sensor array deposited with a polymeric and polymeric organometallic sensing films

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The diabetes is a chronic disease that is detected by measuring the glucose levels in the blood. A noninvasive alternative method was proposed for measuring the gas concentration emitted by individuals with this disease, where the compounds acetone (Ace) and ethanol (EtOH) are considered as biomarkers, and indicators of the disease. A gas sensor array was constructed using quartz crystal microbalance (QCM) with 30 MHz resonance frequency. Various sensing films with affinity for Ace, and EtOH biomarkers were deposited on the QCM electrodes. The polymers deposited over the QCM electrodes include ethyl cellulose (EC), poly[methylmethacrylate] (PMMA), Apiezon L, Apiezon T and poly[ferrocenylmethylphenylsilano] (PFS). The sensing films were deposited using the ultrasonic atomization method, where the QCM electrode was exposed to a micro-drops mist the polymeric solution. This mist was carried by an air flow of 100 mL/min until it reached the QCM surface, allowing the sensing film thickness to increase to approximately 200 nm on the QCM electrode. The gas sensor array was exposed to Ace and EtOH gases using volumes of 1, 5, 10, ad 15 µL injected into a static system for gas sensor response measurement at a temperature of 22℃, and 20 % relative humidity. We obtained gas sensor array sensitivity values ranging from 0.0018 to

0.810 Hz/ppm, and achieved a classification accuracy of 75 %, and 100 % for EtOH, and Ace gases, respectively.

Keywords:

Polymers, QCM, Diabetes

Reference:

M. Rodríguez-Torres, V. Altuzar, C. Mendoza-Barrera, G. Beltrán-Pérez, J Castillo-Mixcóatl, and S. Muñoz-Aguirre, Acetone Detection and Classification as Biomarker of Diabetes Mellitus Using a Quartz Crystal Microbalance Gas Sensor Array, Sensors (2023) 23, 9823. https://doi.org/10.3390/s23249823.

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CHARACTERIZATION AND METROLOGY / 92

Sensitivity enhancement in dual-beam mode-mismatched transient thermal lens spectroscopy by a differential approach

Author: Jorge Luis Mejorada Sánchez[1]

Co-authors: Adrián Felipe Bedoya Pérez [1]; Ernesto Marín Moares [1]; José Antonio Calderón Arenas [1]; José Bruno Rojas Trigos [1]; Lucio Rodrigo Vega Zuleta [1]; Ramón Enrique Cedeño Bernal [1]; Salvador Alvarado Ramírez [1]

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In dual beam, mode mismatched transient thermal lens spectroscopy (TLS), the evolution with time of the probe beam intensity after the sample´s excitation is measured at the far field and, in the conventional configuration, in the center of the beam. For samples with a negative temperature coefficient of the refractive index, a divergent thermal lens is formed after excitation, so that this intensity is a decreasing function of time. But at certain distances out of the axis of the probe beam at the detector plane, the probe beam intensity will increase with time [1]. In both cases, the total change of the intensity, measured with a photodiode as a proportional voltage difference (ΔV), determines the thermal lens signal that is proportional to the sample´s optical absorbance and thus to the concentration of the absorbing specie. Here, we use this effect to propose a differential configuration that enhances the sensitivity of the TLS method, as demonstrated by measurements performed in water solutions of a commercial dye, at different concentrations. The experimental configuration used is like that reported elsewhere [2], but the probe beam is divided so that two photodiodes can be used to measure simultaneously the increasing and decreasing signals, whose difference constitutes the differential signal. Calibration curves obtained by (a) the conventional TLS experiment and (b) using the differential configuration, showing the sensitivity enhancement and the lowering of the low detection limit (LOD) obtained with the latter.

Keywords:

Spectroscopy, thermal-lens, differential-measurements, calibration-curves, sensitivity, limit-of-detection

Reference:

C. Estupiñán-López, C. Tolentino Dominguez, and R. E. de Araujo, Eclipsing thermal lens spectroscopy for fluorescence quantum yield measurement, Opt. Express 21, 18592 (2013). https://doi.org/10.1364/OE.21.018592

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CHARACTERIZATION AND METROLOGY / 111

Simultaneous measurement of thermal conductivity and diffusivity of good thermal conductors using laser spot lock-in thermography.

Authors: Adrian Bedoya[1]; Alejandro Borges[1]; Ernesto Marín[1]; Gustavo Juarez[1]

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The application of the laser-spot active lock-in infrared thermography technique in a front detection configuration for the simultaneous measurement of the thermal conductivity (k) and diffusivity (D) of isotropic solids taking advantage of the heat losses by conduction from the sample to the surrounding air has been reported recently []. In this method, an intensity periodically modulated laser beam focused on the sample´s surface is partially absorbed and transformed into heat so that thermal waves are generated that propagate radially from the heating point. They are imaged using a thermographic camera at the same surface where the excitation took place. Video-thermograms are recorded at the light modulation frequency, from which amplitude and phase-shift profiles are obtained by lock-in processing as a function of the radial distance from the heating point. These profiles are then fitted with the help of a theoretical model to obtain k and D. However, the method is limited to thermal insulators for which a large mismatch between their thermal diffusivities and that of air exists so that for good conductors only the latter parameter can be recovered.

Keywords:

lock-in thermography diffusivity conductivity measurement

Reference:

Título: “Memory Technologies for Embedded Systems”
Capítulo: “Static Random-Access Memory (SRAM)”
Autores: Karen Panetta, Adam Hoskins
Fuente: Embedded Systems Design with Special Functions, CRC Press
Año: 2017

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CHARACTERIZATION AND METROLOGY / 172

CALCIUM CARBONATE NANOPARTICLES IN DRINKING WATER

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Drinking water is a vital resource. Assessing water quality is a health issue. Harmful substances such as heavy metals need to be in concentrations low enough for safe human consumption. It is also necessary to monitor other water characteristics. For instance, water hardness, related with calcium carbonate concentration, has an impact in detergent use and scale formation.
With the advent of nanotechnology concerns have arisen related to the effect of nanomaterials on health and the environment. Several studies have focused on the toxicology of nanoparticles. Water quality needs to be assessed not only to look for harmful substances in atomic or ionic states, but also in the form of nanoparticles.
The monitoring of water is of special importance in desertic or semi-desertic regions were water sources are scarce. There is also a need to study and improve water quality in the wake of environmental accidents or in polluted places.
In this work, we present an electron microscopy analysis of nanoparticles found in drinking water in two sites in Sonora, a state located in the Sonoran desert in Northwest Mexico. The chosen sites are along the Sonora river basin. A major mine spill in august 2014 is a source of concern regarding water quality in this region.
High-resolution transmission electron microscopy reveals the presence of a significant amount of amorphous calcium carbonate (ACC) nanoparticles in the studied water samples. Interestingly, these particles undergo a crystallization transition when illuminating with the electron beam. We also conducted a systematic experiment to study the effect of pH on the morphological changes of ACC. We varied the exposure time and the heat source using light and observed different agglomeration formations of particles on a substrate.
Finally, we discuss possible health and technological issues related to the existence of ACC nanoparticles in drinking water.

Keywords:

Calcium carbonate, nanoparticles, drinking water, Transmission electron microscopy

Reference:

The Physics and Physical Chemistry of Water, Felix Franks, ThriftBooks, 1995.

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CHARACTERIZATION AND METROLOGY / 289

MICROFABRICATION OF A PHOTO-SWITCH UTILIZING REDUCED GRAPHENE OXIDE (RGO) DECORATED WITH NICKEL (NI) NANOPARTICLES AS AN ACTIVE MATERIAL FOR OPTICAL COMMUNICATIONS

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This study presents the micro-manufacturing process and radio frequency (RF) evaluation of a Metal-Semiconductor-Metal (MSM) type photodetector, utilizing reduced graphene oxide (rGO) decorated with nickel nanoparticles as the photosensitive material for light detection. The photodetector was initially designed with a Ground-Signal-Ground (G-S-G) configuration to determine the spacing between these elements. The microfabrication process followed, including electron lithography, rGO deposition via the Langmuir-Blodgett method, and component metallization. During this stage, scanning electron microscope (SEM) micrographs were produced to verify the correct application of the nanomaterial and examine the details of the photodetector's manufacturing process. Finally, the RF characteristics were evaluated using a vector network analyzer (VNA) alongside a 1550 nm optical stimulus to determine the scattering parameters (S parameters) in terms of reflection (S11) and transmission (S21). These devices can be integrated into microwave systems, both passive and active, for control through optical excitation.

Keywords:

Langmuir-Blodgett method, Metal-Semiconductor-Metal (MSM), photodetector, optical, microfabrication

Reference:

R. Hui, "Photodetectors,"in Introduction to Fiber-Optic Communications, First., India: Academic Press, 2020, pp. 125–154.

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CHARACTERIZATION AND METROLOGY / 228

MICROSTRUCTURAL CHARACTERIZATION OF CONCRETE WITH GRAPHITE PARTICLE AGGREGATES

Author: Alejandro Flores Nicolás[1]

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Concrete is one of the most widely used materials in civil construction. It is a rock created artificially by mixing fine and coarse aggregate components, cement, and water. In this research work, the analysis of the interfacial transition zone in the concrete microstructure by adding different graphite contents, partially replacing the weight of cement, is presented. The morphology and microstructure of the paste/aggregate interface were analyzed using X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM) characterization techniques. It was determined that the concrete matrix with low carbon percentage addition acquired a more compact microstructure, with lower permeability and porosity. The graphite filled the pores of the paste and consequently increased the development of calcium silicate hydrate (CSH) in the cement hydration. These mechanisms accounted for the increase in the compressive strength of the concrete.

Keywords:

Concrete, graphite, microstructure, interfacial transition zone

Reference:

N/A

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CHARACTERIZATION AND METROLOGY / 215

Study of X-ray Photoelectron Spectra of Ag3d from salts and nanoparticles nanocomposites.

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The X-ray photoelectron spectroscopy technique has been applied to study compounds or oxidation states of elements with the principal objet of stablish whether correlations exists between electron binding energy and the formal charge. Natural polymer-based nanocomposites, silver nanoparticles act as nanofillers with potential in biomedical industry due to antimicrobial activity. Many methods for preparation, shapes or properties suggest the application. However, many references discrepancies of binding energy values for its most intense peak which refers the assignment of the

corresponding metal oxidation states. This reported values still controversy due to the large of spectra published with wrong interpretation information. In this work, we take the case of Ag3d peak, using silver salts from diverse companies, silver nanocompounds and using references spectra in literature. The main peak data are fitted simultaneously, with recognized methods using AAnalyzer software. In this work XPS data concerning the Ag-O bond in homogeneous systems are analyzed, then oxidation states of silver are investigated for the nature of chemical bonding.

Keywords:

X-ray photoelectron spectroscopy, silver nanoparticles, Ag3d peak fitting

Reference:

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CHARACTERIZATION AND METROLOGY / 236

STRUCTURAL CHARACTERIZATION OF NIFE/CU/NIFE TRILAYER FILMS: EFFECT OF COPPER LAYER THICKNESS

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In this study, we obtained films with the NiFe/Cu/NiFe strucure were obtained by cathodic erosion, with the NiFe layers maintaining a constant thickness of 100 nm and the intermediate copper (Cu) varying in thickness from 100, 200, and 300 nm. The structural characterization was carried out by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Consistent with previous literature [1], the XRD results demonstrated a face centered cubic (FCC) crystalline structure in all samples. Notably, as the thickness of the Cu layer increased, the intensity of the characteristic copper peaks also increased, indicating an enhanced crystallinity of the deposited layers. The SEM analysis shows that increasing the thickness of the Cu layer leads to an increase in the grain size of the films. These results suggest a relationship between the thickness of the Cu layer and the change in the structure of the trilayer systems. This characterization provides valuable information on how the thickness of the copper layer affects the microstructure of the systems, which is essential for potential applications in the fields of electronics and magnetism. A correlation between structural properties and electrical behavior is discussed.

Keywords:

Cu, NiFe, Films, XRD, SEM

Reference:

Liu, M., Wang, Z., Meng, Z., Sun, X., Huang, Y., Guo, Y., & Yang, Z. (2023). Giant Magnetoimpedance Effect of Multilayered Thin Film Meanders Formed on Flexible Substrates. Micromachines 14(5). (2023).

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CHARACTERIZATION AND METROLOGY / 318

Effect of uniaxial structural anisotropy of Al/Nb metamaterial on the superconducting transition temperature and magnetic response

Authors: F. Perez-Rodriguez[1]; F.J. Flores-Ruiz[2]; J. G. Medrano[1]

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Here, we have designed a metal/superconductor (Al/Nb) metamaterial to modulate its superconducting transition temperature Tc and response to external magnetic fields (Ha). The coherence length of the Cooper pairs of bulk Nb regulates the thickness of the Nb and Al layers; thus, the filling factor [fNb = dNb/(dNb + dAl)] of the metamaterial was set to 0.88 and 0.12, which were contrasted to a thick Nb layer, fNb = 1. Curves of magnetic moment vs. temperature allow observing the effect of anisotropy. The behavior of Tc and response of the metamaterial to the Ha is discussed in terms of uniaxial structural anisotropy and proximity effect.

Keywords:

hyperbolic metamaterial geometry, structural uniaxial anisotropy, Al/Nb multilayers, superconductivity.

Reference:

This abstract has no references

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Grants FOINS-CONACyT 2016-01-2488, CONAHCyT CF-2023-I-1429.

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CHARACTERIZATION AND METROLOGY / 311

Ellipsometry study of Cu3Se2 thin films growth by electrodeposition

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The study of the optoelectronic properties of films that compose a solar cell have significant impact in the optimization of the best configuration of a solar cell. Among these properties, the dielectric function of the materials is one of the most relevant. In this work, the study of the dielectric function <ε> of Cu3Se2 thin films growth over Glass/FTO by electrodeposition. The ellipsometric angles Ψ y Δ were measured and then a multilayered model composed by general oscillator general + Drude + Tauc-Lorentz. The energy band gap was calculated from UV-Vis measurements and used as fixed parameter in the ellipsometric model. The model allows to obtain the dielectric function of the films and to calculate the optical properties of the absorbent layer.

Keywords:

Cu3Se2, ellipsometry, absorbent layer

Reference:

no reference

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CHARACTERIZATION AND METROLOGY / 248

Characterization of reactive magnetron sputtering using a pulsed direct current power source

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Co-authors: Roberto Sangines [2]; Noemi Abundiz-Cisneros [2]; Juan Aguila-Muñoz [2]; Roberto Machorro-Mejia [1]

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Reactive sputtering is a very useful technique, particularly to prepare inhomogeneous interference filters, where refractive index changes smoothly during deposition. In such context, precise control over the involved parameters becomes imperative to obtain a good reproduction of the optical properties [1]. This study employed a pulsed direct current (pulsed DC) power source to investigate the influence of duty cycle on the target poisoning, sputtering plasma characteristics, electric signals, and the optical and morphological properties of synthesized films.
The experimental setup was characterized by analyzing the behavior of plasma emission via optical emission spectroscopy and voltage-current signals, while modulating parameters such as the oxygen content within the vacuum chamber. A set of thin films were coated on glass substrates, under different system conditions. The films underwent characterization employing spectroscopic ellipsometry to ascertain their optical constants, atomic force microscopy for surface morphology analysis, and X-ray diffraction for determination of crystalline structure.
The results indicate that longer duty cycles required higher oxygen levels to poison the target. Additionally, a detailed analysis of electrical signals revealed non-square waveforms, whose characteristics were influenced by both duty cycle and partial oxygen content within the sputtering chamber, resulting in higher effective voltages during the on-time of the pulsed current and voltage. Also, influenced the film characteristics, higher voltage during the metallic mode enhanced ion energy, promoting greater atom mobility and rougher surface morphology. Conversely, in the poisoned mode, limited atom mobility due to the oxide layer resulted in smoother surface morphology and slower grain growth.

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Keywords:

Reactive Magnetron Sputtering, Pulsed DC, Optical Emission Spectroscopy

Reference:

R. Sanginés, N. Abundiz-Cisneros, O. Hernández Utrera, C. Diliegros-Godines, and R. Machorro-Mejía, "Plasma emission spectroscopy and its relation to the refractive index of silicon nitride thin films deposited by reactive magnetron sputtering,"J Phys D Appl Phys 51(9), 095203 (2018).

This work was supported by:

This work was supported by the National Council of Humanities Sciences and Technology of Mexico, CONAHCYT [IxM CONAHCyT, 1081; CF-2023-I-704] and PAPIIT-UNAM [grant number BG101123] projects. E. Teran-Hinojosa acknowledges her Postdoctoral fellowship from CONAHCYT.

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CHARACTERIZATION AND METROLOGY / 331

ANALYSIS OF THE ELECTRO-PHOTONIC PROPERTIES OF SILICON-BASED LIGHT EMITTING CAPACITORS

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This work shows an electro-photonic characterization of light emitting capacitors (LECs) based on silicon rich oxide films (SRO) as active material. The LEC structure is based on metal-oxide-semiconductor (MOS) capacitor with polysilicon as top M-electrode and p-type silicon as semiconductor substrate. These devices exhibit a high current at low voltages with some current jumps/drops that produce the appearing/disappearing of electroluminescent (EL) spots on the surface of the top poly-Si contact [1]. These current jumps/drops are related to resistive switching (RS) events from low resistance (LRS) to high resistance states (HRS) through the competition of the formation/annihilation of preferential conductive filaments (CF) within the SRO films. This chaotic electro-photonic behavior can be annihilated by increasing the electric field to the LEC, which is dependent on the gate area of the devices. Once the CFs are annihilated the device emit a strong EL on the whole area of the devices. The electro-photonic characterization of these devices includes the current-voltage curves, EL spectra, optical power and endurance.

Keywords:

Electroluminescence, silicon rich oxide, conductive filaments, light emitting capacitors

Reference:

A. Morales-Sánchez; K. Monfil-Leyva; A. A. González; M. Aceves-Mijares; J. Carrillo; J. A. Luna-López; C. Domínguez; J. Barreto; F. J. Flores-Gracia,Strong blue and red luminescence in silicon nanoparticles based light emitting capacitors, Appl. Phys. Lett. 99, 171102 (2011). https://doi.org/10.1063/1.3655997

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CHARACTERIZATION AND METROLOGY / 249

Analysis of piezoresponse force microscopy signals obtained during force-distance curves

Authors: Eduardo Murillo Bracamontes[1]; J. J. Gervacio[2]; M. P. Cruz[1]; S.T. Hernandez-Marin[2]

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Piezoresponse force microscopy (PFM) is a unique technique that enables the study of ferroelectric properties at the nanoscale level. Scientific advancements and the proposal of new ferroelectric systems have encouraged the development of several variations of PFM. Specifically, for ferroelectrics with poor mechanical properties, hybrid-PFM (H-PFM) has been introduced.

Within force-distance curves, a time window of mechanical contact exists between the tip and the sample. In H-PFM, this time window can be leveraged to apply the AC bias used for PFM measurements, thereby avoiding the influence of lateral forces present in conventional contact PFM. Despite the utility of H-PFM in studying ferroelectric properties in mechanically soft samples, a thorough investigation of the H-PFM mode has not been conducted. The objective of this work is to analyze the amplitude and phase PFM signals during force-distance curves to gain a better understanding of the PFM results.

In this work, the amplitude and phase PFM signals will be analyzed during force-distance curves obtained on a periodically polarized sample of LiNbO3. The study will be divided into two parts: before contact and during tip-sample contact, in order to establish the optimal conditions for obtaining reliable PFM characterizations.

A developed protocol has determined that the PFM signals obtained before the contact of the force-distance curves can be utilized to discern the influence of electrostatic artifacts during PFM characterizations. Meanwhile, a procedure for obtaining the best amplitude and phase PFM images has been established during the contact in a force-distance curve.

Keywords:

AFM, PFM, Force-distance curves

Reference:

A. Kalinin, V. Atepalikhin, O. Pakhomov, A. L. Kholkin, A. Tselev, Ultramicroscopy 2018, 185, 49. https://doi.org/10.1016/j.ultramic.2

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CHARACTERIZATION AND METROLOGY / 290

Porosity percentage effect on porous silicon optical absorption

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An analysis of the reflectance spectra in porous silicon samples is reported to determine the effect of the percentage of porosity on their optical absorption capacity in the visible spectrum. Porous silicon (PS) samples were prepared by electrochemical anodization at 5, 10, 15, 20 and 30 minutes. A crystalline silicon (CS) wafer with orientation (100), phosphorus-doped n-type (thickness: 500 ± 15 μm), and resistivity of 1-5 Ωcm was used. A constant current density of 40 mA/cm2 and a 40% hydrofluoric acid (HF) solution were used in all cases. To measure the reflectance, an EDINBURGH INSTRUMENTS FS5 spectrofluorimeter was used as an optical energy source, which has a 150 W ozone-free xenon arc lamp and an excitation spectral coverage of 230 nm - 1000 nm and an R928P Photomultiplier, with spectral coverage of 200 nm - 870 nm, cooled and stabilized. Measurements were set in a range from 200 to 800 nm. The percentage of porosity changes significantly with anodization time, with an approximately linear increase as a function of the thickness fraction of the porous layer. The reflectance decreases noticeably for the PS samples, even for low anodization times, and reduces more for higher anodization times. From the reflectance results, the absorbance of each sample was obtained, showing a significant dependence on the percentage of porosity.

Keywords:

Porous silicon, porosity, reflectance, optical absorption.

Reference:

Nogal, U., (Master Thesis) Estudio de las Propiedades Ópticas y Térmicas en Silicio Poroso Elaborado Mediante Ataque Electroquímico, Mexico, (2012).

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CHARACTERIZATION AND METROLOGY / 350

EVALUATION OF HEMOGLOBIN IN URINE AS A BIOMARKER OF KIDNEY DAMAGE: IMPLEMENTATION OF CALIBRATION CURVES OBTAINED BY PHOTOACOUSTIC SPECTROSCOPY. TEST PILOT.

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Co-authors: Alfredo Cruz Orea [1]; Guadalupe Cleva Villaneva López [2]; Sergio Tomás Velazquez [1]

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The kidney damage present in septic shock is one of its most serious and irreversible symptoms. One of the key biomarkers of kidney damage is the presence of hemoglobin in the urine, which can indicate hematuria and acute kidney injury. Photoacoustic spectroscopy has shown its capacity and sensitivity as an alternative tool for the detection of hemoglobin in biological samples, including urine.

With this context, this work uses hemoglobin calibration curves obtained by photoacoustic spectroscopy. Hemoglobin has absorption bands at certain wavelengths (Soret band, 412nm and β and α peaks at 550nm and 580nm respectively), generating a photoacoustic signal that is proportional to the optical absorption spectrum and its concentration. The calibration curves were constructed using reference samples with known concentrations of hemoglobin (Sigma Aldrich hydrolyzed hemoglobin), which allowed establishing a relationship between the absorption of the measured photoacoustic signal and the concentration of hemoglobin in the sample, by using these specific calibration curves, the concentration of hemoglobin in urine of an animal group of Male Wistar rats, induced into septic shock at 0 and 6 hours of this, can be quantified, detecting an increase in said concentration. The above will facilitate early detection and monitoring of kidney damage in patients with septic shock.

Keywords:

photoacoustic spectroscopy, Urine, Damage, Hemoglobin, Kidney

Reference:

Chvojka, J., Sykora, R., Karvunidis, T., Radej, J., Krouzecky, A., Novák, I., & Matejovic, M. (2010). New developments in septic acute kidney injury. Physiological Research, 59(6), 859-69.

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CHARACTERIZATION AND METROLOGY / 343

TAILORED THIN FILMS FOR OPTICAL WAVEGUIDES AND FILTERS: EXPLORING ATOMIC LAYER DEPOSITED Al2O3, Y2O3, and TiO2-x.

Authors: Eder Lizárraga[1]; Diana Caballero[2]; Jorge Jurado[3]; Jorge Luis Vazquez Arce[4]; Carolina Bohórquez[5]; Bonifacio Can[5]; Javier Alonso López[6]; Oscar Edel Contreras López[7]; Nicola Nedev[8]; Mario Farías[5]; Eduardo Blanco[9]; Heriberto Márquez[10]; Hugo Tiznado[5]

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This study explores Atomic Layer Deposition (ALD) for engineering optical waveguides and filters. Al2O3-Y2O3 nanolaminates and Al2O3 thin films were fabricated using ALD, demonstrating their potential as waveguides with low propagation loss. The influence of the oxygen source (H2O vs. O3) in ALD Al2O3 waveguides was investigated, revealing lower losses for O3-based films. TiO2-x films with varying oxygen vacancy content were also explored, achieving a high refractive index (2.55) while maintaining good light propagation. Additionally, O3 annealing was examined for TiO2/Al2O3 multilayer filters, improving optical transmittance and etching resistance. Finally, waveguides were fabricated by ultrafast laser ablation of Al2O3 thin films, highlighting the potential of this technique. These findings showcase the versatility of ALD for creating advanced photonic devices using Al2O3, Y2O3, and TiO2-x materials.

Keywords:

optical waveguides, optical filters

Reference:

https://doi.org/10.1016/j.optmat.2020.109822
https://doi.org/10.1016/j.optmat.2020.110370

https://doi.org/10.1016/j.optlastec.2022.108880
https://doi.org/10.1021/acsami.3c07586
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CHARACTERIZATION AND METROLOGY / 61

MACHINE LEARNING IMAGE CLASSIFICATION ALGORITHM FOR THE DETECTION OF PERCOLATION THRESHOLD IN NANOCOMPOSITES.

Author: Giovanni Alejandro Cruz Ortiz[1]

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Machine learning algorithms have become indispensable tools across all branches of science in recent years. These algorithms, comprised of sets of neural networks, excel at identifying and classifying patterns within datasets, proving to be comparable to human capacity in classification tasks. Moreover, they offer the advantage of completing tasks much faster than a human could. In this study, we propose the use of an image classification algorithm to determine when nanoparticles within a nanomaterial dispersed in a matrix reach the percolation threshold. We evaluated nanocomposites with varying concentrations of metal nanoparticles and metal oxide nanoparticles for their electrical properties. Percolation in a nanocomposite occurs when its conductivity approaches that of the nanofiller dispersed within the matrix. To achieve this, we utilized a database of scanning electron microscope images capturing the cross-section of nanocomposites to train a convolutional neural network (CNN). Each image was associated with a percolation characteristic, either positive or negative, during the training phase. Image features were automatically selected by a non-supervised machine learning algorithm. Subsequently, this allowed us to identify the nanocomposites that had reached percolation without the need to characterize their electrical properties.

Keywords:

percolation threshold, convolutional neural network, nanocomposites, machine learning

Reference:

S. Mimar and G. Ghoshal, A sampling-guided unsupervised learning method to capture percolation in complex networks, Sci Rep 12, 4147 (2022). https://doi.org/10.1038/s41598-022-07921-x

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CHARACTERIZATION AND METROLOGY / 177

Graphene-based hydrogel electrolyte for supercapacitors

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Recent research has highlighted supercapacitors as promising candidates for energy storage applications due to their unique combination of rapid charge-discharge characteristics, low weight, flexibility, portability, and exceptional power density. These advantageous characteristics have facilitated their integration into emerging technologies within the aerospace sector, electric vehicles, and wearable electronics. However, specific applications often necessitate additional functionalities beyond energy storage, such as robust load-bearing capability, exceptional thermal stability, and enhanced corrosion resistance. To achieve this synergistic effect of simultaneous structural integrity and efficient energy storage, meticulous electrode and electrolyte materials selection is essential. In this regard, the utilization of solid or gel polymer electrolytes represents a highly promising approach for the development of high-performance supercapacitors. Graphene derivatives are particularly attractive because they provide exceptional mechanical reinforcement at the nanocomposite level while maintaining fast charge transport properties. This study investigates the implementation of gel electrolytes formulated with polyvinyl alcohol (PVA), and graphene derivatives possessing varying degrees of oxidation. These electrolytes were characterized using thermal and electrochemical techniques to elucidate the impact of incorporating graphene derivatives. These results will help to establish supercapacitor devices that achieve an optimal balance between mechanical properties and efficient energy storage capability.

Keywords:

supercapacitors, graphene, electrolyte, PVA, gel

Reference:

Xu, Jiaming, and Dong Zhang. "Multifunctional structural supercapacitor based on graphene and geopolymer." Electrochimica Acta 224 (2017): 105-112. DOI: 10.1016/j.electacta.2016.12.045

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LUMINESCENCE PHENOMENA / 294

PHOSPHORS FOR WHITE LED LAMPS

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In this work, the Li3Ba2La3(MoO4)8:(Eu3+, Tb3+) phosphor was investigated due to its excellent luminescence emission properties in the red spectral range (615~620 nm) under excitation with a blue LED (Light Emitting Diode). The phosphors were synthesized by the combustion and sol gel methods, at different Eu and Tb concentrations, in order to find the optimal luminescence conditions and nanostructural characteristics. Its physicochemical properties were studied by different analysis techniques. Subsequently, the optimized red material was mixed with a commercial YAG:Ce3+ phosphor at different concentrations to obtain white light. Then, a white light lamp was manufactured using a commercial blue LED as the excitation source for the combined luminescent powders. Finally, the emission spectra and the Color Rendering Index (CRI) of the lamp were reported. The proposed phosphor is a promising candidate for its application as a red-emitting component in lighting systems based on solid-state devices, particularly blue LEDs.

Keywords:

europium, terbium, energy transfer, LED

Reference:

1. Böhnisch, D., Baur, F., and Jüstel, T. (2017). "Photoluminescence and energy transfer behavior of narrow band red light emitting Li3Ba2Tb3(MoO4)8:Eu3+". Dalton Transactions, 47(5), 1520–1529.

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LUMINESCENCE PHENOMENA / 124

EVALUATION OF LUMINESCENT PROPERTIES OF CERAMIC POWDERS OF THE CEO2:EU2O3 SYSTEM

Authors: María del Rosario González García[1]; Antonieta García Murillo[2]; Felipe de Jesús Carrillo Romo[2]; Israel Donato Cabrera Ríos[2]

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In recent years, materials based on rare earth oxides have gained great importance in modern technology, due to the innovative properties they have. For application in different scientific-technological branches, ranging from the synthesis of hybrid materials to the development of new ceramic materials. The study of nanoparticles based on cerium oxides using the sol-gel method has become of great interest, because this method allows control through various parameters (lower temperatures than in other methodologies) such as: crystalline structures of materials, morphologies, sizes and obtaining products with a high degree of purity. This allows us to undertake a more complete study of the properties that this matrix has. In addition to the possible applications that can be developed, due to its unique properties. The focus of this work is the synthesis of undoped ceramic powders, with doping and mixtures with europium oxide using the sol-gel method, to obtain gels with molar concentrations (Ce:Eu= 100:0, 98 :2, 95:5, 92:8, 90:10, 70:30). The gels will be thermally treated at a temperature of 700 ℃ for 24 hours, to promote their crystallization and subsequently reveal the crystalline structure. Finally, the products obtained will be characterized structurally and morphologically. Its luminescent properties will be studied using infrared spectroscopy (IR), energy dispersive X-ray spectroscopy (EDX), scanning electron microscopy (SEM) and photoluminescence. These studies will allow establishing a correlation between their properties, revealing their structural and luminescent properties to understand the behavior of these materials and thus expand their field of application.

Keywords:

Rare-earths, Europium, Luminescence, Cerium, Sol-gel.

Reference:

E. Anne, D'Achille, R. Wallace, J. Coffer, Morphology-dependent fluorescence of europium-doped cerium oxide nanomaterials, Department of Chemistry and Biochemistry, Texas Christian University, (2021) , 3, 3563-3572, doi:0.1039/d1na00096a

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LUMINESCENCE PHENOMENA / 130

EMBEDDED METALLIC PATTERNS IN A HYBRID-MICROCAVITY USING E-BEAM LITHOGRAPHY.

Author: Eliseo García Ramírez[1]

Co-authors: Héctor Francisco Lara Alfaro [1]; José Antonio Cuevas Lara [1]; Miguel Ángel Vidal [1]; Edgar A. Cerda Méndez [1]

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Challenges in technology have been significant in reducing the size of components such as transistors, antennas, MEMs, LEDs, lasers, and many devices for biomedical and environmental improvement applications. Therefore, the concept of nanotechnology has played a significant role in the manufacturing and study of new materials at this scale. In the photonic area, the interaction between

light and matter has been researched for the polaritons behavior with metallic patterns embedded in a microcavity. A microcavity device is formed by two mirrors and an active medium, which, in our case, is composed of quantum wells. The mirrors, known as Distributed Bragg Reflectors (DBR), are made by stacking pairs of layers of two different materials, each with its own refractive index. The thickness of each layer is equal to a quarter of the resonance wavelength of the cavity. Polaritons are hybrid light-matter quasiparticles formed by the strong coupling between the cavity mode and the quantum well excitons.
In this work, we present the progress in the fabrication of a hybrid microcavity, where the two DBRs are made of different materials. Particularly, we report the development by e-beam lithography of metallic patterns using the INSPECT F50 equipment at Laboratorio Nacional de Ciencia y Tecnología de Terahertz (LANCYTT) within the Coordinación para la Innovación y Aplicación de la Ciencia y la Tecnología (CIACYT). In this project, we are endeavoring to create various patterns using circles to form lattices, such as the Lieb, kagome and moiré structures. Our objective is to produce strong confinement potentials for exciton-polaritons while simulating strain in these lattices by adjusting the separation between the lattice sites. Throughout this journey, we have achieved promising results, as we are currently presenting in this work.

Keywords:

DBR, microcavity, e-beam lithography

Reference:

E. A. Cerda-Méndez et al, Quantum fluids of light in acoustic lattices, J. Phys. D: Appl. Phys. 51 (2018). https://doi.org/10.1088/1361-6463/aa9ec7.

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LUMINESCENCE PHENOMENA / 166

MODEL BASED ON DIFFERENTIAL EQUATIONS TO EXPLAIN THE QUENCHING OF LUMINESCENT POROUS SILICON IN AN ETHANOL-WATER SYSTEM.

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Luminescence quenching in porous silicon has been widely employed due to its sensitivity to numerous molecular species acting as quenchers. Various molecular interactions can induce luminescence quenching, including excited state reactions, molecular rearrangement, energy transfer, complex formation in the basal state, and collisional quenching. Collisional inhibition, also known as dynamic process, occurs when the excited-state silicon is deactivated upon contact with another molecule in solution, called quencher. To explain the interaction of luminescent porous silicon with quenchers in an ethanol-water system, a model based on differential equations was proposed, which is a conventional tool for exploring luminescent processes. This method focuses on analyzing the population density of each energy level involved. Photoluminescence inhibition tests were conducted using ethanol and water. The amount of water was kept constant at 10, 11, and 12 mL, while the amount

of ethanol in each batch varied. Spectra were acquired using a fluorescence spectrometer (Varian-Agilent Cary Eclipse) with an excitation wavelength of 360 nm, employing a mount designed for liquids at room temperature. The collected measurements were analyzed and fitted to the proposed model. The findings indicate a strong alignment between the proposed model and the collected data.

Keywords:

Porous Silicon, photoluminescent, quenching, differential equiations, model

Reference:

Luis Octavio Meza Espinoza, "Estudio de la dinámica luminiscente en nanocristales de ZrO2 y Y2O3 dopados con Yb3+Er3+ por medio de ecuaciones de razón con un enfoque macroscópico y microscópico ,"Centro de investigaciones en óptica A.C., León, 2011.

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Instituto de Física ´Ing. Luis Rivera Terrazas´(IFUAP)

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LUMINESCENCE PHENOMENA / 117

STUDIES ON THE PHOTOLUMINESCENCE OF LUTETIUM OXIDE AEROGELS DOPED WITH EU3+

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Compounds synthesized from lanthanide elements have become indispensable due to their high efficiency in applications where their luminescent properties are taken advantage of. Among these can be found phosphors for illumination in screens or night vision, inks for security labels, lasers, photocatalysis, bioprobes, nanoscopy or in light-activated drug delivery. In the present work, through the sol-gel process, gels with different proportions of Eu3+ (0, 2, 5, 8 and 10 mol%) were synthesized in Lu2O3 host matrices, as well as an Eu2O3 matrix for comparative purposes. In the production of aerogels, the gels were dried with supercritical CO2 and subsequently subjected to a thermal treatment at 800 ℃ to induce crystallinity. The products were analyzed by infrared spectroscopy (IR), x-ray diffraction (XRD), scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS), transmission electron microscopy (TEM) and photoluminescence analysis. According to the results, it is indicated that the main absorption band (M-O-M), which is characteristic of the metal oxide compounds, is located around 560 cm-1 and did not present significant changes as the concentrations of the Eu3+ ion alter the composition of the aerogels. Furthermore, these materials are made up of type-C crystalline structures with crystallite sizes around 10 nm which, in turn, form three-dimensional networks of interconnected particles. Likewise, according to the luminescence studies, the emission bands around 580, 590, 612 and 650 nm were present due to the energy transitions 5D0⟶7F0, 5D0⟶7F1, 5D0⟶7F2 and 5D0⟶7F3 of the Eu3+ ions, respectively. The 10 mol% sample was the one that presented the best results in terms of intensity and quantum yield. In addition, the position of the color in the CIE diagram was calculated, establishing that the color emitted

by the aerogels is orange-red. This type of materials has a high potential to be used in biomedical as drug carriers or biomarkers.

Keywords:

Rare earths, Sol-gel, Supercritical drying, Aerogels, Luminescence

Reference:

M. Worsley, J. Ilsemann, Th. Gesing, V. Zielasek, A. Nelson, and M. Bäumer, Chlorine-free, monolithic lanthanide series rare earth oxide aerogels via epoxide-assisted sol-gel method, J. of Sol-Gel Sci. and Tech. 89 (2018) 1–13. https://doi.org/10.1007/s10971-018-4811-y

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LUMINESCENCE PHENOMENA / 191

Synthesis and characterization of Ca3(VO4)2 activated with Sm3+ for luminescent applications

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Recently, research on vanadates has generated genuine interest due to their high luminescent efficiency [1], resonant excitation with commercial NUV chips (λex = 350 nm) [2], high thermal stability [3], excellent chemical stability [4], and extraordinary dopant solubility. These qualities make vanadate matrices suitable for the incorporation of lanthanides to modulate their emissions to specific hues. In this regard, this work focuses on the synthesis and characterization of calcium orthovanadate (Ca2(VO4)2) activated with different contents of Sm3+. The compound is obtained through a double substitution synthesis using the solvent evaporation technique. The expected structure for Ca2(VO4)2 presents a trigonal symmetry [5]. The structural relationship was complemented by Raman spectroscopy, revealing that the main modes of symmetric and asymmetric vibrations correspond to [VO4]3- units. Scanning electron microscopy (SEM) micrographs show a loose aggregation morphology of the particles where smaller particles aggregate and form larger particles. By diffuse reflectance spectroscopy and the Kubelka-Munk algorithm, a forbidden band gap energy of 4.43 eV is determined [6]. The excitation spectra of Ca2(VO4)2 with different amounts of Sm was monitored at 646 nm, show the highest peak in the transition band (4G5/2⟶6H9/2) located at a wavelength of 406 nm. The emission spectra are obtained under direct and indirect excitation of the Sm3+ ion at excitation wavelengths of 275 and 406 nm, where characteristic emissions of Sm3+ 4G5/2⟶5H5/2, 6H7/2, 6H9/2, and 6H11/2 + 4G5/2 are observed. Additionally, an increase in local asymmetry is determined through the ratio of electric (ED) and magnetic (MD) dipole intensities.

Keywords:

Ca3(VO4)2, Sm3+, Raman, SEM, Kubelka-Munk algorithm,

Reference:

[1]https://doi.org/10.1021/jp910884c
[2]https://doi.org/10.1039/C8TC05110K
[3]https://doi.org/10.1021/acs.inorgchem.8b01808
[4]https://doi.org/10.1038/ncomms12012
[5]https://doi.org/10.1021/ic302333e

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LUMINESCENCE PHENOMENA / 118

YTTRIUM OXIDE AEROGELS CO-DOPED WITH EU3+;TB3+ AND FUNCTIONALIZED WITH TTA

Authors: Alan Daniel Alcantar Mendoza[1]; Antonieta García Murillo[1]; Felipe de Jesús Carrillo Romo[1]

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Aerogels are very novel materials due to the large number of potential applications that the scientific community is currently investigating. This is due to their extreme porosity and the ability to be synthesized using a wide variety of compounds. Although the excellent thermal and acoustic properties of aerogels are guaranteed by the interconnection of their particles at the nano and micrometer scale, they have a large window of opportunity for their production and study from rare earth elements. Therefore, through the sol-gel process and supercritical drying with CO2, in this work yttrium oxide (Y2O3) aerogels co-doped with europium oxide (Eu2O3) have been synthesized at different concentrations (Eu3+= 2, 4, 8% mol) and terbium oxide (Tb2O3) in low concentration (Tb3+= 0.075 mol%). In this type of system, Eu3+ and Tb3+ act as luminescence-activating and sensitizing ions, respectively. The products were heat treated at 800 ℃ to obtain crystalline materials. Subsequently, thenoyltrifluoroacetone (TTA = 9 μmol%) was added to study the so-called "antenna"effect provided by this compound. The crystallized aerogels and TTA functionalized powders were characterized by infrared spectroscopy (FT-IR), x-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive x-ray spectroscopy (EDS) and by a luminescent analysis. (FL). The materials exhibit the characteristic bonding of rare earth metal oxides (M-O-M); with coralliferous morphologies that are associated with extremely porous materials. Furthermore, the interconnected particles presented a suitable chemical composition created from type-C crystalline structures with sizes less than 20 nm. Finally, luminescent studies revealed emission bands located between 480 and 650 nm associated with the 5D0⟶7F0-4 energy transitions characteristic of the red emission of the europium ion that was modified when functionalized with TTA. This type of materials has a high potential to be used in optoelectronics.

Keywords:

Rare earths, Sol-gel, Supercritical drying, Aerogels, Luminescence

Reference:

A. García-Murillo, F. Carrillo-Romo and S. Díaz, Effects of Eu content on the luminescent properties of Y2O3:Eu3+ aerogels and Y(OH)3/Y2O3:Eu3+@SiO2 glassy aerogels, Ceramics Int. 43 (2017) 12196-12204. https://doi.org/10.1016/j.ceramint.2017.06.079

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LUMINESCENCE PHENOMENA / 28

Structural Rigidity and Blue Luminescence in a Lanthanum(III) Complex: A Case Study with 1,10-Phenanthroline

Author: Karla Scanda Raymundo Silva[None]

Co-authors: Christian Javier Salas Juárez [1]; Hiram Isaac Beltrán Conde [2]; Ismael Garduño Wilches [1]; José Guzmán Mendoza [3]; Raúl Erick Guzmán Silva [3]

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The search for sustainable and efficient solutions in the solid-state lighting field has gained significant importance due to its environmental impact. One such solution is light-emitting diodes (LEDs), which offer higher energy efficiency and durability than conventional lighting technologies such as incandescent bulbs and fluorescent tubes. Nowadays, LED technology has evolved to the development of organic LEDs (OLEDs), which have emerged in the technology industry due to their versatile optoelectronic applications, e.g., in a flat display of televisions and cell phones, as well as flexibility, low voltage, and fast response. In this work, a blue-emitting phosphor designed by lanthanum (III) coordinated with 1,10-Phenanthroline, [La(Phen)2(NO3)3], was obtained by an effective and low-energy precipitation method. Infrared spectroscopy (IR) and X-ray diffraction (XRD) revealed the compound coordination environment and crystal structure. The luminescence properties, absolute quantum yield (Φ), and luminescence lifetime decay (τ) were determined by photoluminescence spectroscopy. In addition, the chromatic coordinate CIE 1931 and color purity are reported. It is highlighted that the complex [La(Phen)2(NO3)3],] displayed a deep blue emission related to the electronic transitions of the 1,10-Phenanthroline, which is not perceptible in its free form as an organic ligand. This experimental observation is due to the structural rigidity caused by the coordination with the Lanthanum ion. The results will be discussed regarding a possible application as a blue-emitting phosphor, its organic nature, and the use of the promising material in OLED technology.

Keywords:

Luminescence, Photoluminescence, Lanthanide complex, Lanthanum, Blue light-emission

Reference:

S. Kim, “Design of fluorescent blue light-emitting materials based on analyses of chemical structures and their effects,”Materials Science and Engineering R: Reports, vol. 99. Elsevier Ltd, pp. 1–22, Jan. 01, 2016.

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LUMINESCENCE PHENOMENA / 37

LIGAND-SENSITIZED FLUORESCENCE OF EU(III) AND TB(III) USING AROMATIC CARBOXYLIC ACIDS)

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Lanthanide complexes are a new type of luminescent materials used for several optical applications, including biological fluoro-immuno assays, lasers, solid-state lighting, electroluminescent devices, and Light Emission Diodes (LEDs). The Direct excitation of Lanthanide ions inefficient absorption is due to forbidden transitions resulting in low quantum yield. However, it has been observed that organic ligands highly conjugated coordinated with lanthanide centers enhances luminescence immensely through an energy transfer mechanism also known as antenna effect.

In this work, aromatic ligands of carboxylic acids coordinated with Europium (III) and Terbium (III) were obtained by precipitation method. Photoluminescence spectroscopy (PL), Infrared spectroscopy (IR) and powder X-ray diffraction (PXRD) are reported to determine luminescence properties, coordination modes and crystal structure respectively. PL shows the direct excitation of the organic ligand which transfers energy towards the lanthanide ion, a process known as antenna effect. IR revealed coordination. In addition, the chromatic coordinate CIE 1931, color temperature, and color purity are presented.

Preliminary results indicate that coordination compounds with Eu(III) and Tb(III) sensitized with aromatic carboxyl ligands have promising applications as light-emitting phosphors in several technological fields.

Keywords:

Lanthanide complex, luminescent materials, aromatic carboxylic acids

Reference:

Wei, C.et al. Advances in luminescent lanthanide complexes and applications. Sci. China Technol. Sci. 61, 1265–1285 (2018).

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LUMINESCENCE PHENOMENA / 337

Properties study of TiO2 nanoparticle immobilized in a porous silicon template

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We report on the fabrication and characterization of TiO2 nanoparticles immobilized in porous silicon (p-Si) structures; p-si was obtained by chemical anodization using crystalline silicon (c-Si) substrates with varying resistivity. This study used two types of TiO2 nanoparticle nanoparticles to compare their properties: one synthesized by hydrothermal process and the other commercial. Structural characterization was conducted using X-ray diffraction (XRD), and the results were corroborated by Raman spectroscopy. Morphological characterization was performed using scanning electron microscopy (SEM) to determine the porous distribution as well as the shape and size of the TiO2 nanoparticles. The optical properties of the porous silicon were analyzed using luminescence techniques. Time-resolved photoluminescence (TRPL) was employed to determine the average lifetime of the carriers involved in the recombination processes.

Keywords:

Nanoparticles, Titanium dioxide, nanostructure, porous silicon

Reference:

Tank, C. M., Sakhare, Y. S., Kanhe, N. S., Nawale, A. B., Das, A. K., 2011). Electric field enhanced photocatalytic properties of TiO2 nanoparticles
Gupta, T., Cho, J., (2021). Hydrothermal synthesis of TiO2 nanorods: formation chemistry, growth mechanism, and tailoring

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LUMINESCENCE PHENOMENA / 103

SYNTHESIS AND LUMINESCENT PROPERTIES OF ZNO:ER3+

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Zinc oxide (ZnO) is a material with multiple electrical and optical properties, in this work we studied the incorporation of the Er^{3+} ion into the host of ZnO synthetized by the Sol-Gel. Changes in the luminiscent properties of ZnO:Er^{3+} are directly correlated with the incorporation of Er^{3+} ion (0.25, 1.25, 2.25, y 3.25 mol%). The Near-Infra Red (NIR) emission of ZnO:Er^{3+} was obtained excited at 980 nm with a pumping power around 370 mW, the maximum in the emission band at 1535 nm corresponding to $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition of the Er^{3+}. The Stark effect is appreciate in the NIR emission of ZnO:Er^{3+}, the splitting of the intra-electronic levels of Er^{3+} is caused by the crystalline structure associated to the ZnO. Near-infra Red photoluminescence is useful for applications in optoelectronics and solar-cell technologies, for such purposes ZnO:Er^{3+} is very promising.

Keywords:

Sol-gel, Near-infra Red photoluminescense, zinc oxide, erbium, crystalline structure.

Reference:

Han, H.L. & Yang, Liwen & Liu, Y.X. & Zhang, Y.Y. & Yang, Q.B.. (2008). Up-conversion luminescence switching in Er3+-containing ZnO nanoparticles through Li+ co-doping. Optical Materials. 31. 338-341. 10.1016/j.optmat.2008.05.003.

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LUMINESCENCE PHENOMENA / 116

Mn2+-Yb3+ Super-Exchange interaction in zinc phosphate glass

Author: Héctor Aníbal Félix Quintero[None]

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Zinc phosphate glasses with varying compositions of Mn2+ and Yb3+ were successfully synthesized using the conventional melt and quenching method. Mn2+ exhibits simultaneous green-orange emission through four- and six-fold coordination upon excitation at 350 nm, and via up-conversion when excited at 980 nm. Yb3+ shows its characteristic 976 nm emission due to the 2F5/2⟶2F7/2 transition when excited at 350 nm within the 6A1(S)⟶4E(D) Mn2+ energy level. This phenomenon is proposed to occur due to the presence of Mn2+-Yb3+ dimers or through charge transfer via oxygen bridges. An energy diagram is provided to illustrate the mechanism of this bidirectional energy transfer. Absorbance, excitation, and emission spectroscopic studies are presented.

Keywords:

Luminescence, Up-Conversion, Mn2+, Yb3+, Super-Exchange, Energy Transfer, Zinc Phosphate Glass

Reference:

H. Felix-Quintero, et. Al. J. Lumin. 230, 117733, 2021. DOI: 10.1016/j.jlumin.2020.117733

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LUMINESCENCE PHENOMENA / 121

EFFECTS OF EUROPIUM CONTENT ON STRUCTURAL, AND LUMINESCENCE, CHEMICAL PROPERTIES OF YPO4 POWDERS OBTAIN BY HYDROTHERMAL METHOD

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In this project, europium-doped yttrium phosphate powders (YPO4:Eu3+) with a concentration of 6 mol% were synthesized by the hydrothermal method. The hydrothermal reaction conditions were 190 ℃ for 3 hours. Heat treatment was carried out at 750 ℃ for 3 hours to form the crystal structure. The addition of glycerol as a cosolvent was to prevent agglomeration and promote dispersion of the particles. The pH was adjusted from an acidic medium (pH = 4) to a neutral medium (pH = 7), with the dropwise addition of sodium hydroxide. The powders obtained were characterized by X-ray diffraction (XRD), infrared spectroscopy (IR) and photoluminescence (PL), to study the structural, chemical, morphological, and luminescent properties with respect to the Eu3+ present in the YPO4 structure. The XRD results revealed the formation of the cubic phase without phase transformations 1or secondary phases. The lattice parameters were changed when YPO4 was doped with Eu3+, because the ionic radius of Eu3+ is larger than that of Y3+. Therefore, it is verified that Eu3+ was included in the YPO4 matrix. Using infrared spectroscopy, the bands attributed to the europium-doped yttrium phosphate were obtained, that is, the P-O and the O P-O at 1000, 642 and 618 cm-1 respectively. Photoluminescence analyzes showed the emission and excitation bands at 594 nm and 230 nm, respectively. The energy transitions of europium 3+ were observed: 5D0-7F1,

5D0-7F2, 5D0-7F3, 5D0-7F4 at 600 nm, 630 nm, 650 nm, and 700 nm, respectively. On the other hand, the chromatic coordinates were orange red, which agrees with the ultraviolet-excited Eu3+ emission. On the other hand, the quantum yield of Eu3+-doped YPO4 powders was 62.32%.

Keywords:

Phosphors, Rare-earths, Europium, Luminescence, Hydrothermal.

Reference:

J. Wu, C. Liu, H. Jia, Y. Qi, Optical properties, energy transfer and thermal stability of spherical nano-phosphor YPO4:Eu3+:Sm3+, College of Materials and Metallurgy, Inner Mongolia University of Sciences and Technology (2022) 22-2313. https://doi.org/10.1016/j.jlumin.2022.118791.

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LUMINESCENCE PHENOMENA / 208

LUMINESCENCE PROPERTIES OF CaMoO4 DOPED Dy3+

Author: Andrés Alfonso Saavedra Romero[1]

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Material Physics focuses on synthesis and characterization of materials for different applications, such like tunable color iluminants, LED applications, construction, and even medicine. Keeping this in mind, the incorporation of rare earths as crystal impurities in the host material is quite important, because it could change the electrical and optical properties in order to favor its emission. In particular, Dy3+ doped materials have been studied and proposed for modulable white LED applications, among these, CaMoO4: Dy has become of interest for many researchers due to its lumninescence and thermoluminescence properties. This work shows the synthesis and spectroscopic characterization of CaMoO4 doped with different molar concentrations of Dy3+, in order to determine which, one gives the best emission. The synthesis was performed by the solvent evaporation technique from appropriate solution of calcium chloride hexahydrate and sodium molybdate dihydrate, using deionized water as solvent, according to equation (1):

$$CaCl2 \quad 6H2O + Na2MoO4 \quad 2H2O \rightarrow CaMoO4 + 2NaCl + 8H2O \quad (1)$$

The solution was heated and stirred simultaneously at a temperature of 80 ℃ for 1 hour until the solvent was evaporated, leaving a precipitate of CaMoO4. At last, the sample was placed in a muffle oven at 700 ℃ for 8 hours in order to get the crystalline structure. XRD and Raman were used as characterization techniques for CaMoO4 doped with different concentrations of Dy3+ in order to verify that the compound was correctly synthesized. Photoluminescence emission was measured showing interesting results.

Keywords:

Luminiescence, Thermoluminescence, Crystalline, Raman, XRD

Reference:

Laguna, M. (et al.). Morphology control of uniform CaMoO4 microarchitectures and development of white light emitting phosphors by Ln doping (Ln = Dy3+, Eu3+). The Royal Society of Chemistry: CrystEngComm, Vol. 12, 1590-1600. (2017) doi: 10.1039/C6CE02611G

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LUMINESCENCE PHENOMENA / 223

Calcium molybdate impurified by Eu3+ for gas sensing

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To detect changes or events produced by physical phenomena in our environment, it is necessary to use sensors. The presence of some gases on high concentrations can be dangerous for the living beings and its early detection is of vital importance. Nowadays there are several sensing devices, among them those with luminescent properties represents an attractive option, because the interaction of the sensing material with the analyte is perceptible by naked eye, this due to that the guest molecules adsorbed by the material can change its color and/or its luminescent intensity.
On this work we synthetized calcium molybdate impurified by Eu3+ metallic ions by means of the solvohydrothermal microwave assisted method. We show results of structural and optical properties obtained by XRD, FTIR and photoluminescence. In a future this material will be evaluated as luminescent sensor.

Keywords:

microwave, sensing, gas, photoluminescence

Reference:

Hong, W. T., Lee, J. H., Jang, H. Il, et al. (2015). Orange-red light emitting europium doped calcium molybdate phosphor prepared by high energy ball milling method. 2015 20th Microoptics Conference (MOC), 1, 1–2. https://doi.org/10.1109/MOC.2015.7416428

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LUMINESCENCE PHENOMENA / 238

STUDY OF THE LUMINESCENT AND STRUCTURAL PROPERTIES OF CsVO3:Er3+ FOR INFRARED APPLICATIONS

Author: María Leonor Porras Sánchez[1]

Co-authors: Omar Soriano Romero [1]; Rosendo L. Lozada Morales [1]; Salvador Carmona Téllez [1]; Vicente Vargas García [1]

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Cesium metavanadate (CsVO3) materials have recently received extensive attention due to their out-standing luminescent properties.In this study, the synthesis of CsVO3 and CsVO3:Er3+ was conducted using the solid-state reaction method.Through a thermal treatment at 400℃ for 5 hours,the crystalline phase corresponding to PDF 00-70-0680 was obtained,achieving a phase purity ofapproximately 94% CsVO3.

CsVO3 was doped with erbium ions (Er3+) at varying concentrations ranging from 0.1 mol% to 6 mol%,and the structural and luminescent properties of CsVO3:Er3+ were investigated.The incorporation of Er3+ ions induced microstrains within the crystalline structure, altering the position of vanadium tetrahedra and consequently reducing the purity of the crystalline phase.

Excitation spectra of CsVO3:Er3+ were recorded from 200nm to 400nm, with emission monitored at 535nm.The obtained spectra revealed a peak at 355nm, corresponding to the 1A1⟶1T1 transition associated with (VO4)3−.Additionally, the emission spectra of CsVO3:Er3+ excited at 365 nm exhibited a broad band centered at 536nm,originating from the convolution of emission levels 3T1⟶1A1 and 3T2⟶1A1.Furthermore,sinks at 521nm (4I15/2⟶2H11/2) were observed in the emission spectra,indicating radiative energy transfer from [VO4]3− to Er3+. Moreover,near-infrared emisión under 980 nm excitation displayed a characteristic emission peak centered at 1534 nm, associated with the 4I13/2⟶4I15/2 transition.

Up-conversion emission peaks characteristic of Er3+, attributed tothe levels Er3+:2H11/2,4S3/2,and 4F9/2⟶4I15/2,are observed in UC emission spectra under λex=980nm diode laser excitation.The intensity of red emission is considerably higher than that of green.Integrated spectrum areas indicate an intensity growth with Er3+ content,with the 6.0% sample being the most intense.From UC emission spectra,color coordinates were evaluated using the CIE1931 protocol,observing a yellow hue with an average color purity of 98.7.

The optical properties of this material position it as an excellent candidate for enhancing the efficiency of solar cells.

Keywords:

Luminescence-Phosphors-Erbium-Cesium-Vanadate

Reference:

Espinosa-Cerón, M. Y., Meza-Rocha, A. N., Carmona-Téllez, S., Chacón, C., Soriano-Romero, O., Lozada-Morales, R. (2021). Effect of radiative energy transfer and direct excitation on the up-conversion and down-shifting emission properties of Er3+-doped Zn3(V O4)2. Journal of Luminescence, 238, 118239

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LUMINESCENCE PHENOMENA / 264

White emission of carbon quantum dots obtained from the avocado peel

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The aim of this work is to obtain fluorescent white light from quantum dots processed from avocado peel with different thermal treatments and mixtures.
The initial process consist in dehydrating the peel with sunlight for a week. After that, it is grounded and separated into three groups to apply different heat treatments in two of them, being 100℃ and 200℃.
Three suspensions containing concentrations of 0.2 g were prepared for each powder with different treatment and 30 ml of ethanol.
Finally, different mixtures were made between the suspensions with powder without heat treatment and with 200℃ in different proportions, being 25% - 75%, 50% - 50%, 75% - 25%.
Ultraviolet-visible absorption spectroscopy (UV-vis) and fluorescence spectroscopy were performed on all concentrations and mixtures. Two excitation sources were used for fluorescence spectroscopy, a UV lamp at 370 nm and a UV laser at 405 nm. X-ray diffraction spectroscopy (XRD) and infrared spectroscopy (IR) were performed on all powders obtained.
It was found that the flurescent color obtained closest to being white was the mixture of powder without heat treatment and 200℃ at a proportion of 25% - 75%.

Keywords:

White emission, quantum dots, fluorescence spectroscopy, UV, thermal treatments

Reference:

Kang, C., Huang, Y., Yang, H., Yan, X. F., & Chen, Z. P. (2020). A review of carbon dots produced from biomass wastes. Nanomaterials, 10(11), 2316.

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LUMINESCENCE PHENOMENA / 239

SYNTHESIS AND CHARACTERIZATION OF Er3+ DOPED 10Al2O3-60Li2O-30B2O3 INVERTED GLASSES

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In recent years, rare earth metals such as erbium have gained great importance in various technological applications. At the same time, borate glasses have emerged as another crucial material due to their ability to form glass even at relatively low cooling rates and under pressure alone[1]. B2O3 glasses facilitate melting, reduce viscosity and surface tension, which improves the material's workability and performance during processing. To analyze these materials, infrared (IR) spectroscopy [2] is used to identify the functional groups present in the sample. Subsequently, optical absorption spectroscopy reveals the main absorption bands, especially in the case of the Er3+ dopant ion, where electronic transitions from the ground state 4I15/2 to excited states such as 4I13/2, 4I11/2, 4I9/2, 4F9/2, 4S3/2, 4H11/2, and 4F7/2 are expected. To better understand the interaction between atoms and light in these systems, the Judd-Ofelt theory will be applied [4]. This theory allows the calculation of parameters such as Ω2, Ω4, and Ω6, which provide information about the local symmetry around the dopant ion (Er3+), as well as properties such as the viscosity and rigidity of the material. In addition, measurements such as the ratio of observed to predicted light emission (βexp, βcal), the probability of light emission instead of other forms of energy (AR) and the light absorption efficiency (σp), among others, will be employed. For a more detailed analysis of the dynamics of the systems, the theory developed by Inokuti and Hirayama will be used [3]. This will allow us to determine the lifetimes of the excited states, as well as to understand the predominant electrostatic interaction mechanisms, the critical interaction distance and the energy transfer efficiency between neighboring atoms.

Keywords:

Glass, Erbium-doped, Spectroscopy, Transitions.

Reference:

] J.M. Hollas. Modern Spectroscopy. Wiley, 2004. isbn: 9780470094716. url: https://books.google.com.mx/books?id=lVyXQZkcKKk

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LUMINESCENCE PHENOMENA / 245

Synthesis and characterization of carbon quantum dots from cucumber peel

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In this work, a synthesis process was carried out to obtain fluorescent quantum dots from cucumber peel in order to produce white visible light.
The production of quantum dots consisted in a dehydration process followed by a milling procedure to obtain powders of the dehydrated peels. Subsequently, two thermal treatments were carried out at 100 ℃ and 200 ℃ to equal quantity of powders. Afterwards, three suspensions were prepared by pouring 0.2 g of powder into 30 ml of ethanol. The first solution was without thermal treatment, the second contained the biomass treated at 100 ℃, and the third had the biomass treated at 200 ℃.
Alternatively, mixes were prepared between the suspension without thermal treatment and the suspension treated at 200 ℃ in proportions of 25% - 75%, 50% - 50%, and 75% - 25%, with the aim of exploring their optical properties in search of white emission.
The powders were characterized by X-ray diffraction (XRD) and infrared spectroscopy (IR), while the optical properties of the suspensions were measured by ultraviolet-visible absorption spectroscopy (UV-Vis) and fluorescence spectroscopy. For the latter, a UV lamp at 370 nm and a UV laser at 405 nm were used as excitation sources.
It was found that the closest white emission was generated by the obtained from the powder treated at 200 ℃ when excited with the UV laser.

Keywords:

carbon quantum dots, fluorescence, biomaterials, visible ligth emmision, sustainable materials

Reference:

Kang, C., Huang, Y., Yang, H., Yan, X. F., & Chen, Z. P. (2020). A review of carbon dots produced from biomass wastes. Nanomaterials, 10(11), 2316.

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LUMINESCENCE PHENOMENA / 275

Luminescent properties of Dy3+ doped Al2(WO4)3 for modular white light applications

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The present work synthesized Al2(WO4)3 activated with Dy, using the solvent evaporation methodology. Deionized water was used as a solvent, AlCl3, DyCl3 and Na2WO4 as reagents; Then it was subjected to heat treatment at 400°C for 2 hours. The X-ray diffraction patterns present high intensity peaks related to the orthorhombic phase of Al2(WO4)3, according to letter PDF-70-4478. With a crystallite size of 29.0 nm calculated using the Scherrer equation. Raman spectroscopy indicates that the main vibration modes are, located in, all related to the vibration modes of WO4 units. From

the Kubelka-Munk approximation, a direct and indirect forbidden gap energy was estimated with values of 4.61 and 3.38 eV, respectively. Excitation spectroscopy monitoring the emission at 575nm, exhibits an excitation band at 255 nm related to the 1A1⟶1T1+1T2 level associated with the WO4 units. In addition, the characteristic excitation bands of the Dy ion located at 325, 352, 366, 387, 424, 453 and 473 nm. From the excitation spectrum, the wavelengths 255 and 350 nm were selected as excitation lines to obtain the emission spectra. For the excitation wavelength of 255 nm, the emission spectrum presented an emission band related to the 1A1⟶1T1+1T2 level of WO4 units at 395 nm. Likewise, the characteristic emission bands of the Dy ion related to the levels can be seen. On the other hand, under an excitation wavelength of 350 nm the emission related to the 3T1+3T2⟶1A1 level of WO4 units at 395 nm is overshadowed by the high intensity of the Dy ion emissions described previously. Finally, from the emission spectra, the color coordinates are evaluated in the CIE1931 protocol. It starts with a bluish white emission for the matrix, followed by emission tones ranging from cold white, neutral white and concluding in yellow tones according to the increase in the Dy content.

Keywords:

: Luminiscence, lanthanide, WO4, Dy3+, CIE1931

Reference:

Batista, F. M. C., et al. "A joint experimental and theoretical study on the electronic structure and photoluminescence properties of Al2 (WO4) 3 powders." Journal of Molecular Structure 1081 (2015): 381-388.

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LUMINESCENCE PHENOMENA / 298

Photoluminescence and Judd-Ofelt analysis of Er3+ doped CdO-V2O5-ZnO-B2O3 inverted glasses.

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Er-doped CdO-V2O5-ZnO-B2O3 inverted glasses were synthetized by the melt-quenching method, using proportions of 80-5.0-2.5-12.5 mol% of CdO-V2O5-ZnO-B2O3, respectively, which were doped with different mol% of Er. The structural analysis, carried out by X-Ray diffraction patterns recording, showed an amorphous structure in all Er doping range. This fact was also verified by the line shape of Raman spectra, which revealed vibrational modes associated with borate, Zn2V2O7 and Cd2V2O7 in amorphous phases. By using optical absorption and the Tauc model, the direct optical

band gap (E_g^d) values were found around 2.74 eV, without tendency with Er mol% concentrations. The down-shifting emission spectra recorded under laser excitation at 980 nm exhibited the featured near infrared Er emission band centered at 1534 nm, which grows up to 2 mol% and remained oscillate for larger Er doping contents. The upconverting (UC) emission spectra registered under laser excitation of 980 nm, displayed the well-known green and red emission bands, related to relaxations of 2H11/2, 4S3/2 and 4F9/2 excited states to the 4I15/2 ground state, respectively. Such process is dominated by a linear decay mechanism, as revealed the dependence of the intensity versus the excitation laser power. The Judd-Ofelt (JO) parameters obtained by least-square method from the experimental and theoretical oscillator strengths, were found as Ω_2 = 6.43×10-20, Ω_4 = 0.96×10-20 and Ω_6 = 1.53×10-20 cm2 for the CVZB glass activated with 2.8 mol% of Er. Moreover, the emissions arisen by transitions from 4I13/2, 4I11/2 ,4F9/2, 4S3/2, 2H11/2, 4F7/2 states to 4I15/2 ground state, present radiative branching ratio (β_R) values higher than 0.6, and total radiative transfer probabilities A_T (4I13/2⟶4I15/2) = 782.46 s-1 and A_T (4S3/2⟶4I15/2) = 10248.56 s-1. Finally, for the 1533 nm emission, the stimulated emission cross section had a value of σem(λ) = 1.57×10-20 cm^2, and an effective bandwidth Δλem = 60.52 nm.

Keywords:

Luminescence, Inverted glasses, Judd-Ofelt, Laser, Upconversion

Reference:

Soriano-Romero, O., et al. “Spectroscopic evaluation a new and novel Nd3+/Yb3+ co-doped CdO-V2O5 glass system for 1 μm laser application.” Journal of Alloys and Compounds 777 (2019): 886-893.

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LUMINESCENCE PHENOMENA / 312

Synthesis and characterization of BiCa2VO6 doped Sm3+.

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Nowadays, vanadate-based materials have been a topic of studying due to their interesting structures and electronics, optics, and magnetic properties. In most cases, the structural characteristics are convenient to be impurified with trivalent lanthanide and/or transition metals, which opens the possibility of applications in deep-red LEDs, W-LED, among others [1]. Moreover, the vanadate intrinsic photoluminescence can serve to sensitize the lanthanide and transition metal emission, which in some cases suffers from an inefficient direct excitation, related to [VO4]-3. Based on these facts, the present work aims to study the photoluminescence properties of Sm3+-doped BiCa2VO6, which has not been studied. The vanadates mixed with Bi3+ promote chains of cations highly polarized or ions of mobile oxides [2-3]. Besides, it facilitates the incorporation of lanthanides by substitution

of ions of Bi3+. The synthesis of the phosphors Bi1-x Ca2VO6: xSm3+ (x=0.0 to 0.1) was carried out by the high-temperature solid-state method. The crystalline structure was analyzed from X-ray diffraction patterns. The vibrational modes were studied by Raman spectroscopy, showing their principal vibration modes [4-6]. The emission spectra, under 350 and 406 nm excitations, display four characteristic bands to Sm3+: 4G5/2⟶6H5/2, 4G5/2⟶6H7/2, 4G5/2⟶6H9/2 and 4G5/2⟶6H11/2 transitions, which enhances intensity with the doping content.

Keywords:

vanadate, sm3+, high luminescence, solid-state reaction, orange light.

Reference:

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LUMINESCENCE PHENOMENA / 319

Photoluminescence properties of Nd3+ activated novel CdO-ZnO-V2O5-B2O3 glasses for NIR laser applications

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There is a growing interest in the search for inverted glasses [1], which exhibit a low density of high-energy phonons. Due to the high energy phonons are the main source of non-radiative relaxations of lanthanide ions embedded in glasses, inverted glasses might show superior photoluminescence performance. Based on this issue, the present work aims to prepare and analyze the photoluminescence properties of inverted CdO-ZnO-V2O5-B2O3 glasses activated with Nd3+ ions. The glasses were prepared by melt-quenching method at 1200 ℃ for one hour. The glass host composition was 80, 5.0, 2.5, and 12.5 mol% of CdO, V2O5, ZnO, and B2O3, whereas the Nd3+ doping content was changed from 0.0 to 4.0 mol% regarding the host composition. The emission spectra under Nd3+ excitation at 808 nm displayed the Nd3+ emission bands at 880, 1060, and 1332 nm, associated with the 4F3/2 ⟶ 4I9/2, 11/2, 13/2 transitions, respectively, being that at 1060 nm the most suitable for NIR laser applications. The optimum emission was attained at 2.8 mol% of Nd3+. Beyond this concentration, the emission is quenched, as a consequence of cross-relaxation among Nd ions, dominated by an electric dipole-dipole interaction. The Judd-Ofelt (JO) theory was applied to the optimum emitting sample to evaluate laser parameters. The JO Ωi=2,4,6 parameters resulted to be Ω2 = 5.31×10-20, Ω4 = 2.81×10-20 and Ω6 =3.34×10-20 cm2, which lead to stimulated cross-section peak (σp) values of σp= 1.21×10-21 cm2(4F3/2 ⟶ 4I9/2) and σp= 3.50×10-20 cm2(4F3/2 ⟶ 4I11/2). The calculated quantum yield was 0.49. The Bandwidth (σem×Δλem) and optical gain (σem×τR), calculated from

the 4F3/2 ⟶ 4I11/2 emission cross-section peak, resulted to be 165×10-27 cm3 and 37×10-25 cm2s. Such values were better than some reported in phosphate and borate-based glasses.

Keywords:

Inverted glasses, NIR laser applications, Judd-Ofelt theory

Reference:

[1] Ahmed H.Hammad, Essam B.Moustafa, Ahmed R. Wassel, Emphasis of some physicaland dynamical properties of inverted barium phosphate base glass, J. Mater. Res. Tech. 15 (2021) 4813. https://doi.org/10.1016/j.jmrt.2021.

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LUMINESCENCE PHENOMENA / 327

CaWO4:Eu(III) based phosphors, characteristics and novel applications

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The synthesis and characterization of calcium tungstate-based micro-nanophosphors will be presented. These materials were prepared using the spray pyrolysis technique. Based on Scanning Electron Microscopy measurements, both CaWO4 and CaWO4:Eu (III) exhibit a quasi-spherical shape. CaWO4 displays blue luminescence originating from electron transitions within unperturbed WO4 complexes. In contrast, the luminescent properties of CaWO4:Eu (III) arise from the presence of Eu(III) ions, which emit light at wavelengths of 591, 615, 655, and 702 nm. These emissions stem from radiative transitions from the excited state 5D0 to 7Fj (j =1,4) inter-level transitions within the electronic energy states of Eu (III) [1].

These phosphors undergo testing in three different scenarios to explore potential and innovative applications. The first scenario involves blending them with a commercial 3D printing photocurable resin (Sain Smart 101-90-840TS) and infusing the resin with their luminescent properties, resulting in a 3D luminescent photocurable resin emitting red light. In the second scenario, the phosphors areincorporated into transparent glasses to create Phosphor in Glasses (PIGs), a concept currently under investigation for laser applications [2]. Finally, the third scenario involves utilizing the phosphors for the Visualization of Latent Fingerprint, leveraging the excellent powder luminescent characteristics
of CaWO4, which has been previously employed for this purpose [3].

Keywords:

CaWO4:Eu (III), 3D luminescent photocurable resin, Phosphor in Glasses (PIGs),

Reference:

[1] K.B. García-López, et. al.,Optical Materials 142 (2023) 114008
[2] Yueyuan Liang, et. al.,Journal of Materials Chemistry C, 2021, 9, 12751-12758
[3] Devidas S., et. al., Analysis Materials Horizons: From Nature to Nanomaterials. Springer (2023)143–155

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LUMINESCENCE PHENOMENA / 329

Synthesis and characterization of calcium phosphates and their effect on Daphnia Magna consumption

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The synthesis of hydroxyapatite and calcium phosphate of nanometric and micrometric sizes is carried out respectively. Were doped with erbium and ytterbium,with the aim of creating a biomarker who underwent chronic tests on Dania Magna. The synthesis and characterization of Ca5(PO4)3(OH) (hydroxyapatite or HAp) enriched with Er (III) and Yb (III) ions was carried out. The synthesis of calcium phosphate was carried out by means of the solvent evaporation technique using calcium chloride and phosphorus pentoxide as reagents supplied by Sigma Aldrich.The synthesis of hydroxyapatite was done byhydrosolvothermal.The luminescent properties of HAp:Er (III)/Yb(III) are activated by means of a continuous 980 nm laser producing two types of emissions, Stokes and Anti-Stokes.Stokes emissions occur in the near infrared area 1520 nm due to the interelectron transition 4I13/2 ⟶ 4I15/2. Anti-Stokes emissions also known as upconversion occur in two regions of the visible area of the electromagnetic spectrum, the first in the region from 515 to 565 nm due to the transitions 2H11/2 ⟶ 4I15/2 and 2S3/2 ⟶ 4I15/2 of the Er (III) ions while the second region that comprises from 640 to 680 nm corresponds to the 4F9/2 ⟶ 4I15/2 transition of the Er (III) ions. In the present work a comparison of calcium phosphate and hydroxyapatite as well as their clothing of erbium and Ytterbium, Europium and their reaction in Dafnia Magna is shown.

Keywords:

calcium phosphates,erbium, yterbium, daphnia Magna, europium

Reference:

Enhanced 1520 nm Photoluminescence from Er3+ Ions in Di-erbium-carbide Metallofullerenes (Er2C2)@C82 (Isomers I, II, and III), Yasuhiro Ito, Toshiya Okazaki, Shingo Okubo, Masahiro Akachi, Yutaka Ohno, Takashi Mizutani, Tetsuya Nakamura, Ryo Kitaura, Toshiki Sugai, and Hisanori Shinohara

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LUMINESCENCE PHENOMENA / 332

Discovering the potential of biomaterial-based mesoporous and magneto-luminescent nanohybrid (Nd-doped Hydroxyapatite/Fe3O4) for cancer theranosis

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Multimodality nanoplatforms play a crucial role in advancing medical interventions by integrating multiple functionalities into a single system. However, issues like intricate production processes and biocompatibility persist. Herein, a facile synthesis of a biomaterial-based mesoporous nanocarrier, HAp:Nd+SPIONs@mSiO2, loaded with the near-infrared (NIR) emitting dye indocyanine green (ICG) is reported.HAp:Nd nanoparticles were synthesized via combustion methods. Thereafter, commercial SPIONs and HAp:Nd were integrated within a mesoporous silica via a modified Stöber approach. HAp:Nd+SPIONs@mSiO2 nanoplatform was characterized for particle size, porosity, and luminescence using TEM, BET, and luminescence spectroscopy. The synthesized nanoplatform was further loaded with ICG dye and the loading efficiency was analyzed via UV-Vis spectroscopy. Photonic and magnetic thermal heating of the ICG-loaded nanoplatform was also analyzed along with the photo-stimulated ROS generation ability. Finally, cytotoxicity and therapeutic analysis was performed in vitro.The nanohybrid with ~100 nm average size, comprised of Nd-doped hydroxyapatite (HAp), Fe3O4 superparamagnetic iron oxide nanoparticles (SPIONs), and mesoporous silica, exhibiting magneto-luminescent properties. The mesoporous structure was loaded with ICG as a model drug (4.3 μg/mg of nanoparticles) where a pH-dependent release was observed. The nanocarrier demonstrated dual functionality by generating heat through magnetic and photonic stimulation, as well as producing reactive oxygen species (ROS) upon excitation with 808 nm light. In vitro bioevaluation on aggressive triple-negative breast cancer cells (MDA-MB-231) showed the high biocompatibility of nanohybrid with and without ICG and exhibited significant toxicity after irradiation of NIR light. Noticeably, the nanohybrids also exhibit the ability to monitor temperature changes via Nd3+ associated NIR luminescence. The nanoplatform integrates clinically relevant components, highlighting its potential for translation from the laboratory to clinical applications. The developed nanohybrids, with combined NIR-mediated photothermal and photodynamic effects, magnetic photothermal capabilities, and NIR/MR imaging, offer promise in addressing cancer heterogeneity and improving conventional treatments with reduced side effects.

Keywords:

luminescent materials, cancer theranostics, biomaterial, photodynamic therapy , magnetic hyperthermia

Reference:

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P. Sengar, K. Chauhan, and G.A. Hirata, Progress on carbon dots and hydroxyapatite based biocompatible luminescent nanomaterials for cancer theranostics, Transl Oncol 24 (2022) 101482. https://doi.org/10.1016/J.TRANON.2

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LUMINESCENCE PHENOMENA / 334

Eu3+ doped Al2(WO4)3 for red-emitting phosphors applications

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Since the discovery of the red light-emitting diode (R-LED) by Nick Holonyak in 1962, LEDs have become indispensable in many everyday applications, from lighting on display screens and smartphones, to laser diodes, even in specialized lighting in horticulture. In this direction, tungsten-based compounds are very attractive due to their high thermal stability greater than 800 ℃ and their high dopant solubility. Thus, in the present work reports the synthesis of Al2(WO4)3 doped Eu3+ through a double substitution reaction by solvothermal evaporation technique. The Structural characterization by X-ray diffraction patterns presents well-defined high intensity peaks related to the orthorhombic phase of Al2(WO4)3, according to chart PDF-70-4478, with a crystallite size of 29.0 nm calculated using the Scherrer equation. The Raman spectroscopy confirms that the main vibrational modes are located in 1052 cm-1 related at WO_4^(2-) units. The excitation spectrum monitoring the emission at 613 nm (5D0 ⟶ 7F2) presents seven excitation bands, one related to O-2 ⟶ W6+ charge transfer and the other six to the characteristic excitation bands of Eu3+: 7F0 ⟶ 5D4, 5L7, 5L6, 5D3, 5D2, 5D1 and 5D0. On the other hand, the emission spectrum was measured under an excitation wavelength of 394 nm (7F0 ⟶ 5L6). The emission spectra present five bands emission related to Eu3+: 5D0 ⟶ 7F0, 7F1, 7F2, 7F3 and 7F4. The intensity between the different J levels relies on the symmetry of the local environment of Eu3+ ion and is evaluated as described in the literature. Finally, the color purity is evaluated through emission spectra in the CIE1931 protocol, obtaining color purities above 97%. The correlation results indicate that the Eu3+-doped Al2(WO4)3 is suitable for LED applications.

Keywords:

Luminescence, Phosphors, Europium, Tungstate, Aluminium

Reference:

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LUMINESCENCE PHENOMENA / 271

LUMINESCENCE PROPERTIES OF CORDIERITE RED-EMITTING PHOSPHOR PREPARED BY COMBUSTION SYNTHESIS FOR APPLICATIONS IN WHITE-LIGHT ILLUMINATION LEDS

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There is a need to develop composite phosphors for white-emitting lamps based on blue LEDs that can be efficiently activated and generate light with high color rendering index (CRI). In particular, there are only few red-emitting luminescent materials excited with blue photons for CRI improvement of the illumination devices. In this investigation, we report a two-stage energy-efficient methodology to fabricate Eu-doped α-cordierite red-emitting phosphors. The first stage of the process consists in the preparation of a spinel-phase (MgAl2O4) and SiO2 mixture by using low-temperature combustion synthesis. Post-annealing treatment at 1350℃ for just 1 hour in a reducing atmosphere is employed as the second stage to obtain α-Mg2Al4Si5O18:Eu2+. When blue light (465 nm) was used as the excitation source the cordierite phosphor powders yielded a broad red emission peak centered around 617 nm making this material a robust red-emitting phosphor and a potential candidate for integration with YAG:Ce to improve CRI in white-emitting LED lamps. On the other hand, the photoluminescence spectrum of α-Mg2Al4Si5O18:Eu2+ displayed a broad blue emission band peaking at 465-488 nm under UV (365 nm) excitation.

Keywords:

Red-emitting phosphor, combustion synthesis, cordierite, LED, illumination

Reference:

no reference

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LUMINESCENCE PHENOMENA / 340

Nanographite: Detailed Analysis of its Optical Properties through Excitation Photoluminescence Spectroscopy

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Co-authors: Angel Adalberto Durán Ledezma [2]; José Luis Casas Espínola [3]; Karen Atzin Meza Martínez [2]; Margarita Lizeth Alvarado Noguez [2]; Raúl I. López Esquivel [2]

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Nanographite (NG), a nanoscale allotrope of carbon with sizes below 10 nanometers, has emerged as a fascinating material due to its unique properties in the optical and electronic fields. These nanostructures exhibit a series of intriguing characteristics that make them highly desirable for a variety of applications, ranging from advanced electronic devices to sensors and catalysts.

However, despite the growing interest in nanographite, there are still poorly understood areas, especially regarding its optical properties. Infrared shifts are a phenomenon that occurs in these nanoparticles and result from the quantum confinement effect, which occurs when the dimensions of the material are on the order of the wavelength of the incident light. Additionally, the structure and composition of nanographite play a crucial role in its optical properties. The presence of surface defects, as well as the interaction between electrons and lattice vibrations, can contribute to this phenomenon.

To address these uncertainties and advance our understanding of nanographite, various characterization techniques have been used, such as excitation photoluminescence spectroscopy (PLE), UV-Vis, Raman, infrared, and XPS.

Keywords:

Nanographite, Optical properties, Excitation Photoluminescence Spectroscopy

Reference:

Hoan, B.T., P.D. Tam, and V.-H.J.J.o.N. Pham, Green synthesis of highly luminescent carbon quantum dots from lemon juice. 2019. 2019.
Kundu, A., et al., Multicolor emissive carbon dot with solvatochromic behavior across the entire visible spectrum. 2020. 156: p. 110-118.

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LUMINESCENCE PHENOMENA / 365

Luminescent properties of mononuclear complexes from Eu(III) and variations of biphenyl carboxylic acid

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This project focuses on the study of europium due to its luminescent properties and various technological applications. The general issue with lanthanides is their low energy absorption,attributed to deficiencies in the ⊠–⊠ transition bands. Europium, dissipates energy through vibrations, which is not conducive to radiative processes. A solution is to add functional group bonds that generate an antenna effect, allowing the europium ion to capture energy and emit it as light.
The objective is to synthesize mononuclear complexes from Eu(III), create a precursor complex, add sensitizers, and evaluate the luminescent properties of three new mononuclear Eu(III) complexes using three variants of biphenyl carboxylic acid. Water is unfavorable for luminescent processes, biphenyl carboxylic acid was added, removing water molecules from the compound and resulting in a solvent-free complex, enabling luminescent processes. The resulting products are the compounds:$EuAB_3$-2N-Carboxylic, $EuAB_3$-3N-Carboxylic, and $EuAB_3$-4N-Carboxylic.
The luminescent properties of each compound were analyzed, with sensitization at wavelengths different from those of Eu^{3+} (393 nm and 464 nm). Emissions were generated from the $^5D_0 \longrightarrow {}^7F_1$ electronic transition producing photons at 590 nm and the $^5D_0 \longrightarrow {}^7F_2$ transition producing photons at 616 nm. The luminescence lifetimes were studied, identifying each compound as fluorescent due to their short emission times, emiting in the microsecond range. The color purity of each compound was simulated, and structural characterization was performed using XRD, demonstrating the development of unprecedented luminescent materials through new synthesis routes. The addition of the three biphenyl carboxylic acid variations optimized the molecules, providing new excitation and emission properties. Emission intensity varied with the non-centrosymmetry of the Eu^{3+},generating radiative processes by avoiding molecular resonance.

Keywords:

Europium, Luminescence, Mononuclear complexes, Antenna effect, Biphenyl carboxylic acid

Reference:

N/A

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LUMINESCENCE PHENOMENA / 25

EFFECT OF SILICA COATING ON THE STRUCTURAL AND LUMINESCENT PROPERTIES OF CSVO3

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This work studied the structural and luminescent properties of CsVO3 crystals synthetised by the Solid State Reaction, and the effect of the silica coated of the cesium metavanadate (CsVO3/SiO2) on the properties described above. The Solid State Reaction is a versatile and eco-friendly technique potentially applicable in the industry. The X-Ray Diffraction patterns shows that the crystalline structure is the characteristic of the CsVO3 for the crystals with and without silica coated. The excitation spectra of CsVO3 and CsVO3/SiO2 (from 200 nm to 400 nm) show that the band has the maximum at 323 nm, this absorption band corresponding to 1A1 ⟶ 1T2 transition associated to [VO4]3-. While the emission spectra from 400 nm to 800 nm, show that the band has the maximum at 535 nm, the band emission in the PL spectra is made up of 3T1 ⟶ 1A1 (548 nm) and 3T2 ⟶ 1A1 (486 nm) transitions.

Keywords:

Cesium Metavanadate, Solid State Reaction, Luminescent Properties

Reference:

Luo, J., Yang, A., Xie, Z., Huang, J., Zuo, X. (2021). Preparation, optical properties and first principle calculation of CsV O3. Journal of Luminescence, 229, 117658.

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LUMINESCENCE PHENOMENA / 19

Spectroscopic characterization of the inverted glass 10Al2O3-70Na2O-20B2O3 activated with Nd3+

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Recently, borate glasses have been widely investigated due to their unique qualities such as high optical transmission, low refractive index, and high thermal expansion coefficient [1]. Due to these characteristics, such glasses are suitable for being doped with trivalent lanthanides to explore potential laser applications. For this purpose, Nd3+, characterized for possessing near infrared emissions at 0.88, 1.06 and 1.34 μm, is a suitable ion to be embedded in a borate glass. Various theoretical and experimental studies show that it is possible to generate a 1.06 μm laser [1-3]. This work is devoted to study the spectroscopic and structural properties of a novel 10Al2O3-70Na2O-20B2O3 invert glass, activated with different contents of Nd3+. XRD patterns confirm the vitreous nature of the samples in all doping range. FTIR spectroscopy reveals that the main vibrational groups correspond to borate tetrahedra (BO4) and trihedra (BO3). The absorption coefficient spectra present bands related to Nd3+: 4I9/2 ⟶ 2P1/2, 2D3/2 + 2G9/2 + 4G11/2, 4G5/2 + 2G7/2, 2H11/2, 4F9/2, 4F7/2 + 4S3/2, 4F5/2 + 2H9/2 and 4F3/2 transitions. Within the framework of Judd-Ofelt theory, the experimental (fexp) and calculated (fcal) oscillator strengths are calculated, as well as the intensity parameters Ω2, Ω4, and Ω6, associated with the asymmetry, viscosity, and rigidity of the glass. Additionally, radiative parameters such as calculated (βcal) and experimental (βexp) branching ratios, radiative emission probability (AT), cross-section (σp), among other, are calculated to validate the potential

usefulness in 1.06 μm laser applications. The emission spectra, measured under 808 nm excitation, present three bands corresponding to the transitions 4F3/2 ⟶ 4I9/2, 4I11/2, and 4I13/2, being the 4F3/2 ⟶ 4I9/2 (1.06 μm) one the most dominant. Finally, the lifetime profiles are analyzed by using the Inokuti-Hirayama model, showing that the main interaction mechanism corresponds to a dipole-dipole interaction within the Nd3+-Nd3+ clusters.

Keywords:

Inverted glass, Neodymium, Luminescence, spectroscopy, oscillator strengths

Reference:

[1] https://doi.org/10.1016/j.jnoncrysol.2021.121085
[2] https://doi.org/10.1364/OE.468607
[3]https://doi.org/10.1016/j.jlumin.2021.118216

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LUMINESCENCE PHENOMENA / 20

Structural and Luminescent properties of CsVO3:Nd3+

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Co-authors: Abraham N. Meza Rocha [1]; Omar Soriano Romero [1]; Rosendo L. Lozada Morales [1]; Salvador Carmona Tellez [1]; Vicente Vargas García [1]

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This work studied the structural and luminescent properties of CsVO3 crystals synthetised by the State Solid Reaction doped with Nd3+ ion (0.5, 1, 1.5, 3, 4.5 and 6 mol%). The State Solid Reaction is a versatile and eco-friendly technique potentially applicable in the industry. The X-Ray Diffraction patterns shows that the crystalline structure is the characteristic of the CsVO3, the incorporation of the Nd3+ ion causes the structure to be modified. The excitation spectra of CsVO3:Nd3+ (from 200 nm to 400 nm) show that the band has the maximum at 323 nm, this absorption band corresponding to 1A1 ⟶ 1T2 transition associated to [VO4]3-. While the emission spectra from 400 nm to 800 nm, show that the band has the maximum at 535 nm, the band emission in the PL spectra is made up of 3T1 ⟶ 1A1 (548 nm) and 3T2 ⟶ 1A1 (486 nm) transitions. The Near-Infra Red (NIR) emission of CsVO3:Nd3+ was obtained excited at 808 nm with a pumping power around 370 mW, the maximum in the emission band at 1063 nm corresponding to4F3/2 ⟶ 4I11/2 transition of the Nd3+. Near-infrared photoluminescence is useful for applications in optoelectronics and photovoltaics and for such purposes CsVO3:Nd3+ is very promising.

Keywords:

Photoluminescence, Cesium vanadate, State solid reaction, Neodymium, Crystalline structure.

Reference:

T. Sun, A.H. Li, C. Xu, Y.H. Xu, R. Wang, Energy transfer properties of Nd3+⟶Yb3+ in Nd:Yb:LiNbO3 crystals, Opt. Laser Technol. 56 (2014) 322–325. https://doi.org/10.1016/j.optlastec.2013.09.010.

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LUMINESCENCE PHENOMENA / 123

SYNTHESIS AND PHOTOCATALYTIC EVALUATION OF ELECTROSPUN TIO2 NANOFIBERS DOPED WITH EUROPIUM FOR THE DEGRADATION OF ORGANIC POLLUTANTS.

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The importance of water treatment cannot be ignored, especially now that the distribution and availability of this resource have been negatively affected, and it is essential for our survival. Photocatalysis is a technique used to degrade the organic pollutants present in industrial water. Titanium dioxide (TiO2) is extensively utilized as a photocatalyst due to its chemical stability, easy production and benign impact on human health and the environment further enhance its appeal as a photocatalytic agent. However, the adsorption of organic pollutants is poor, due to its low ability to harvest sunlight. Enhancing photocatalytic performance can be achieved by doping with europium. The TiO2:Eu3+ with 7.5% and TiO2 nanofibers were fabricated by electrospinning technique. Both nanofibers were calcined at 600℃ in an air atmosphere. The nanofibers were characterized by SEM, EDS, XRD, and DRS. SEM images demonstrated that the nanofibers look like network randomly oriented, with some areas with high material density and some empty spaces. From EDS spectra, we confirm the presence of europium in the doped nanofibers. The TiO2 and TiO2:Eu3+ shown the anatase phase. The bandgap was similar in both samples. The photocatalytic test was performed in the degradation of Rhodamine B (RhB) solution at 2.5 ppm and acetaminophen (AMF) at 7 ppm. With a pollutant-photocatalyst ratio of 1mL:1mg. After 6 hours of reaction, 25% of the AMF was degraded with TiO2, but with TiO2:Eu3+ 60% of the AMF had already been degraded. For RhB, in the same 6-hour time, with TiO2 80% of the dye had already degraded, and with TiO2:Eu3+ 90% of the RDB had already degraded. It can be conclude that the presence of europium enhances the photocatalytic response.

Keywords:

Photocatalysis, Titanium dioxide, europium, electrospinning, acetaminophen

Reference:

Wang H, Li X, Zhao X, Li C, Song X, Zhang P, et al. A review on heterogeneous photocatalysis for environmental remediation: From semiconductors to modification strategies. Chinese Journal of Catalysis. 43 (2022) 178-214.
https://doi.org/10.1016/S1872-2067(21)63910-4

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MICROELECTRONICS AND MEMS / 202

DESIGN AND FABRICATION OF MICROFLUIDICS PLATFORMS USING 3D PRINTING FOR EASY MIXING OF SUBSTANCES

Authors: Tamara Jennifer Crisóstomo Rodríguez[1]; Miguel Ángel Alemán Arce[2]; Luis Alfonso Villa Vargas[2]; Marco Antonio Ramírez Salinas[2]; Verónica Iraís Solís Tinoco[2]

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Microfluidic platforms have become essential in manipulation substance due to their significant advantages. These platforms allow precise fluid control, minimize sample contamination risks, and reduce volumes. Applications of microfluidics include various areas such as water parameter monitoring, controlled cellular microenvironments, and polydispersion index measurement. Thanks to advances in microfabrication techniques, protocols such as soft lithography1, laser ablation, micromilling and thermoforming have been proposed. However, those requires sophisticated installations and expensive materials. Additionally, if one seeks to acquire a microfluidic chip, its geometry, materials and consequently its application, is defined by the company that manufactured it, limiting its utility, and thereby increasing the cost of research. Therefore, it is necessary to design simple, reproducible, large-scale fabrication protocols that can be implemented in any laboratory. In this study, we present a low-cost experimental methodology, which involves (1) designing various microfluidic channel geometries using CAD software, followed by (2) printing a resin master mold with the desired geometry using 3D printer. (3) The resin mold is replicated using the properties of the biocompatible polymer polydimethylsiloxane, and (4) subsequently permanently bonded to a glass substrate through a combination of corona plasma treatment and temperature techniques. With this strategy, it is possible to design different geometries and replicate them effectively up to 20 times, having a minimum resolution of 100 μm. To examine the behavior of laminar fluids, water solutions are combined with vegetable dye and mixed within the microchannels. The results showed that the microfluidic chips work at pressures ranging from 0.5 kPa to 103.4 kPa with flow rates from 913.2 μL/min to 6734.4 μL/min respectively, without any leakage. With this work, researchers, new or not in the field of microfabrication will be able to leverage the advantages of microfluidics across various scientific domains.

Keywords:

microfluidics, fabrication, 3D printer, mixing substances

Reference:

V. I. Solis-Tinoco, et al. Building of a flexible microfluidic plasmo-nanomechanical biosensor for live cell analysis. Sensors and Actuators B: Chemical 291, (2019) 48–57. https://doi.org/10.1016/j.snb.2019.04.038

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MICROELECTRONICS AND MEMS / 95

A RAPID AND SIMPLE MICROWAVE-ASSISTED SYNTHESIS MoO3 FOR THE POTENTIAL DEVELOPMENT OF 2D SEMICONDUCTOR APPLICATIONS

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Molybdenum trioxide (MoO3) has been widely investigated for applications in semiconductor devices due to its structural, morphological and optical properties. In this regard, different techniques have been reported to obtain MoO3, but these involve a thermal processing above 200℃ or high vacuum conditions (< 4mPa) and a long synthesis time. Currently, the challenges consist in the design of synthesis processes without using toxic chemicals, reducing the reaction time and the required synthesis energy. In this sense, the microwave-assisted synthesis method provides a simple and highly controlled methodology for the nanomaterials formation with a uniform distribution of particle size. In this work, MoO3 was synthesized from a dilution of metallic molybdenum powder in ethanol and hydrogen peroxide, and assisted by microwaves (MW) during 5 min. Subsequently, a thermal annealing at 600℃ with a 10℃/min rate was carried out. The phase confirmation and crystal structure, the vibrational behavior of chemical bonds, its morphology, the energy bandgap, and the oxidation states were determined by XRD, FT-IR, SEM, UV-Vis spectroscopy, and XPS spectroscopy characterization techniques, respectively. Through the liquid-phase synthesis process assisted by MW and the calcination temperature, a nanobelts morphology with a stable orthorhombic α-phase was obtained. Furthermore, the presence of vibrational modes of molybdenum-oxygen bonds in the wavenumber range of 500 to 1000 cm−1 were determined. Finally, an energy bandgap of 3eV was extracted from a Tauc plot and only the characteristic oxidation states of Mo6+3d5/2 and Mo6+3d3/2 were determined from XPS spectrum. The results presented here provide the evidence of a sustainable synthesis process of functional MoO3 for the potential development of applications through 2D materials.

Keywords:

MoO3, microwave-assisted synthesis, nanobelt, oxidation states.

Reference:

Kumar, A., Kuang, Y., Liang, Z., & Sun, X. (2020). Microwave chemistry, recent advancements, and eco-friendly microwave-assisted synthesis of nanoarchitectures and their applications: a review. Materials Today Nano, 11, 100076.

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MICROELECTRONICS AND MEMS / 246

INFLUENCE OF DEPOSITION CYCLES OF ZNO THIN FILMS BY SILAR FOR CO GAS SENSING ASSESSMENT

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Zinc oxide (ZnO) as thin film is a versatile semiconductor material, which is very applicable for devices as sensors, transistors, and solar cells. In this work, ZnO thin films as n-type semiconductor with a wurtzite structure were prepared by Successive Ionic Layer Adsorption and Reaction (SILAR), which is a solution process that allows control characteristics as grain size, bandgap energy, and electrical resistance by adjusting parameters as molar concentrations, pH, times, and temperatures during the deposition. The SILAR deposition is by following four sequential steps: first, a glass substrate is immersed in a cation precursor of zinc chloride complexed with ammonia, a second step is rinsing the substrate in deionized water, a third step is rinsing the same substrate in hot deionized water at 90℃ as anionic precursor, and a fourth step is newly rinsing the substrate in other deionized water to complete a cycle of the ZnO thin film formation. The thin films were prepared at 50 and 100 cycles of deposition. Then, the thin films were characterized by X-ray diffraction (XRD), Ultraviolet-Visible spectroscopy (UV-Vis), Scanning Electron Microscopy (SEM), and current-voltage (I-V) measurements to study the structural, optical, morphological, and electrical characteristics. The top surface of the ZnO thin films was patterned by an interdigital arrangement through a lithographic process to sense the electrical resistance by passing different carbon monoxide gas concentrations in ppm, and it is to evaluate the lowest possible gas sensing condition.

Keywords:

Keywords: zinc oxide, thin films, SILAR, gas sensing

Reference:

T.R. Acharya, D.K. Chaudhary, S. Gautam, A.K. Singh, R. Shrestha, B.C. Adhikari, P. Lamichhane, B. Paudyal, N.K. Kaushik, E.H. Choi, Sensors and Actuators A: Physical, Volume 351, 2023, 114175,

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MICROELECTRONICS AND MEMS / 235

DESIGN AND FABRICATION OF ELECTRODES WITH FRACTAL GEOMETRY FOR A MoO3 GAS SENSOR

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Co-authors: Ariel Guzman Vargas [2]; Francisco Javier Hernández Cuevas [3]; María de la Luz Olvera Amador [4]; Norberto Hernandez Como [5]

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A gas sensor was fabricated using a sensitive MoO3 film with the Si-SiO2/Cr-Au/MoO3 structure and CO (carbon monoxide) as the analyte gas. The manufacturing process involved cleaning the Si-SiO2 substrate, followed by Cr and Au deposition (75 nm) using electron beam metal evaporation. Electrodes were designed using fractal geometry, specifically employing a 4th-order Hilbert curve. This curve served as the basis for tracing the two electrodes without them coming into contact. Interdigitated electrodes were also fabricated to compare their behavior with the fractal geometry electrodes. The purpose of using fractal geometry is to increase the contact area between the electrodes and the sensitive film, thereby enhancing the sensitivity of the device. Electrodes was defined through photolithography, and the lift-off photolithography technique was employed to define the active area. Subsequently, a MoO3 film (120 nm) was deposited by sputtering with a reactive O2 atmosphere. Characterizations of the MoO3 films were conducted using XPS to confirm the formation of MoO3, XRD was used to identify the phase of the material, UV-Vis spectroscopy and the Tauc method were utilized to calculate the band gap of 2.84 eV. SEM images of the MoO3 film surface revealed a uniform surface, and the four-point probe test showed a resistivity of 8.93 x 103 Ωcm. Finally, the device was evaluated with IV curves to calculate its resistance, and a dynamic CO sensing test resulted in a sensitivity of 25% for 500 ppm of CO. The sensitivity was calculated using a dynamic sensing test, and the device with interdigitated electrodes was compared to the device with fractal geometry electrodes.

Keywords:

Sensor, chemiresistive, MoO3, gas, fractal, electrodes

Reference:

J. Zhang, Z. Qin, D. Zeng, and C. Xie, "Metal-oxide-semiconductor based gas sensors: Screening, preparation, and integration,"Physical Chemistry Chemical Physics, vol. 19, no. 9. Royal Society of Chemistry, pp. 6313–6329, 2017. doi: 10.1039/c6cp07799d.

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MICROELECTRONICS AND MEMS / 265

EFFECT OF DENSITY OF STATES IN ELECTRICAL SIMULATION OF AMORPHOUS INDIUM-GALLIUM-ZINC-OXIDE THIN FILM TRANSISTOR

Author: Arturo Torres-Sanchez[1]

Co-authors: Isai S. Hernandez-Luna [1]; Francisco Hernandez-Cuevas [1]; Cuauhtemoc Leon-Puertos [1]; Norberto Hernandez-Como [1]

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Amorphous oxide semiconductors (AOS) used as channel in Thin Film Transistors (TFTs) have extended their applications not only as switching devices in display technologies, but also as main elements in logic circuits such as inverters, logic gates, etc. In addition, materials such as amorphous Indium-Gallium-Zinc-Oxide (a-IGZO) due to their optical transparency and low deposition temperatures are used in low-cost flexible electronics, which gives the possibility of a-IGZO TFTs in portable electronics for healthcare sensing. The electrical performance of amorphous and microcrystalline transistors made of organic, inorganic and metal oxides materials is determined by the density of states (DOS) in the bandgap of the semiconductor material. In materials such as a-IGZO the DOS is composed of two exponentials describing the tails of acceptor/donor states and two Gaussians representing the deep acceptor/donor states. In this work, simulations were carried out on the density of the deep donor states related to the oxygen vacancies in the a-IGZO and how those affects the output and transfer graphs of the a-IGZO transistors.

Keywords:

amorphous oxide, a-IGZO, thin film transistor, oxygen vacancies, Silvaco

Reference:

T. Fung, et al. , “Two-dimensional numerical simulation of radio frequency sputter amorphous In–Ga–Z–O thin-film transistors,”November, 2009.

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SIP-IPN under grant 20240507 and 20241809. Arturo Torres-Sanchez and Isai S. Hernandez-Luna would like to thank the program “Estancias Posdoctorales Académicas”by CONAHCYT

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MICROELECTRONICS AND MEMS / 266

Evaluation of various topologies of NMOS inverters based on flexible TFTs

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Bottom gate top contact flexible thin-film transistors (TFT) were fabricated with In-Ga-Zn-O (IGZO) and hafnium oxide (HfO2) as semiconducting and gate dielectric films. The transistors have a threshold voltage of 0.5 V, a field effect mobility of 40 cm2/V-s, a subthreshold slope of 170 mV/dec, and an Ion/Ioff ratio of 4x107. This TFT technology has a minimum channel length and width of 5um. Four different inverter topologies were designed, fabricated and tested: 1) resistive load, 2) diode load, 3) depletion load, and 4) pseudo-E. Each inverter was electrically characterized with the voltage transfer characteristics (VTC) at different supply voltages (VDD). From the VTC, the following parameters were extracted: the gain, high and low noise margins, the output voltage high and low levels, and the input voltage high and low levels. The gain turned out to be around 4, 4, 40 and 3 for the 1), 2), 3) and 4) inverter topologies, respectively. The ac response was also evaluated for each topology in a frequency range from 10Hz to 10kHz. The results of the different inverter topologies are of interest for further development of a digital standard cell library.

Keywords:

TFT, IGZO, inverter

Reference:

Phys. Status Solidi B 2024, 2300493

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MICROELECTRONICS AND MEMS / 295

COMPLEMENTARY INVERTER WITH N-TYPE IGZO AND P-TYPE SNO THIN FILM TRANSISTORS DEPOSITED BOTH BY SPUTTERING RF

Author: Isai S Hernandez Luna[1]

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Thin film transistors (TFTs) based on oxide semiconductors have been of continued interest due to their promising potential in the future of wearable, transparent and flexible electronics. Current applications have been carried out with unipolar nMOS TFT circuits, based on materials such as IGZO, this has achieved interest in the study of p-type oxide semiconductors, to achieve the characteristics of complementary logic circuits. This work presents the complementary inverter fabricated with TFTs of IGZO and SnO oxide semiconductors to obtain transistors with n and p type conductivity, respectively. The deposit method for both semiconductor layers is by radio frequency sputtering at room temperature and then thermal annealing at 150 oC and 250 oC for n and p type, respectively. IGZO TFTs show an electron mobility of 10 cm2/Vs, a threshold voltage of around 2 V, a subthreshold slope of 210 mV/decade. SnO TFTs have a hole mobility close to 1 cm2Vs, threshold voltage of 0.5 V. The characteristics of the semiconductor layer depend on the deposition methods used, the use of low fabricating temperatures makes it compatible with low-cost processes and the use of high k

dielectrics helps to reduce the operating voltage of the devices. Preliminary results demonstrate complementary inverters with a voltage gain of 2 for 5 V supply and a low static power consumption of 0.4 uW. The development of materials and devices p-type oxide semiconductor continues with lower performance than of n-type oxide semiconductor, which restricts the development of circuits and logic complementary for now. These results show good application prospects for electronics based on TFTs.

Keywords:

CMOS, TFTs, SnO, IGZO, RT-sputtering

Reference:

S. -M. Hsu, D. -Y. Su, F. -Y. Tsai, J. -Z. Chen and I. -C. Cheng, "Flexible Complementary Oxide Thin-Film Transistor-Based Inverter With High Gain," DOI: 10.1109/TED.2021.3052443

This work was supported by:

SIP-IPN under grant 20230982 and 20231952, and Isai S Hernandez-Luna and Arturo Torres-Sanchez would like to thank the program "Estancias Posdoctorales Académicas"by CONAHCYT

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MICROELECTRONICS AND MEMS / 308

CHARACTERIZATION OF MOS2 DEPOSITED BY RF SPUTTERING IN A MIS STRUCTURE AS 2D MATERIAL FOR TFTS

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For the last years, Thin Film Transistors (TFTs) based on dichalcogenides materials have raised special interest since these materials are expected to be immune to Short Channel Effects (SCEs). Currently, 2D MoS2 is the most studied semiconductor material due to it possess peculiar characteristics which make it one of the best alternatives to be part of the next generation of electronics. In this work it is presented the electrical characterization by capacitance-voltage (CV) and by current-voltage (IV) measurements of Metal-Insulator-Semiconductor structures (MIS) and Metal-Semiconductor structures (MS), using Mo as the contact and gate metal, HfO2 as dielectric and MoS2 as semiconductor layer. The three layers are deposited at room temperature by RF magnetron sputtering, from Mo, HfO2 and MoS2 targets. The effect of a thermal annealing on the resistivity of the semiconductor layer is studied and an improvement was found to be in more than two orders after the annealing at 300 ℃. The deposited MoS2 layer presented P-type conductivity in CV measurements of MIS capacitors (Mo/HfO2/MoS2/Mo), which seems to be related to plasma etching used during the fabrication processes. The calculated resistivity of the MoS2 layer is in the order of 4.6x104 Ω-cm, by the four-probe method, the resistivity of the metal layer was calculated to be around 4x10-2 Ω-cm and the contact resistance in the MS interface is around 3x109 Ω. IV measurements from a MIM structure revealed a good quality dielectric layer. The CV characteristics revealed bias stability, an operating range of -1 to 1.5 V and a VFB of 0.5 V, results that indicate that 2D TFTs can be obtained by using this structure.

Keywords:

2D materials, MoS2, CV and IV characterization, resistivity of MoS2

Reference:

Chhowalla, M., D. Jena, and H. Zhang, Two-dimensional semiconductors for transistors. Nature Reviews Materials, 2016. 1(11): p. 1-15.

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MICROELECTRONICS AND MEMS / 342

Conductive TiO2 thin films growth using reactive pulsed laser deposition monitored by insitu XPS.

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TiOx thin films are of great importance in recent decades, in all fields of science, including in electronics (2). Herein, TiO2 thin films were deposited in a multi-chamber Riber LDM-32 ultra-high vacuum system utilizing Reactive Pulsed Laser Deposition of a 99.993% purity Ti target. Ultra-high purity O2 was used, which was introduced into the deposition chamber through a mass flow controller (purchased from Aalborg). A 1064 nm wavelength Nd:YAG pulsed laser system (Continuum Surelite SLI-10) was used as the laser beam source. The laser beam was focused with an 8 cm focal distance lens positioned close to the deposition chamber's Quartz viewport. The laser beam incidence angle was 45° to the target surface.
A series of TiOx thin films was deposited by varying an O2 flow into the deposition chamber. Immediately after depositing, samples were moved to the analysis chamber(background pressure of 5×10-10 Torr), where in situ XPS measurements were performed between the first 10 minutes after deposited. Electrical parameters were investigated the same day of the deposition, revealing conductive, insulating and ambipolar properties of the films. Surface morphology and thickness estimation was obtained by Atomic Force Microscopy (AFM) in an XEI-70 Park system. Cathodoluminescence measurements was performed on selected samples. Spectrum's from 200 nm to 800 nm with 1 nm step resolution was recorded.

Keywords:

conductive TiO2, pulsed laser deposition, in situ XPS

Reference:

(1) https://doi.org/10.1016/j.stam.2004.06.003

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MICROELECTRONICS AND MEMS / 91

HfO2/PVP-PMMA/In2O3 solution-processed flexible thin film transistors

Authors: Gouri Syamala Rao[1]; Javier Meza Arroyo[1]; Julia Hsu[None]; Rafael Ramírez-Bon[1]

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Flexible thin-film transistors have garnered great interest because their potential applications in wearable electronics, bendable displays, and Internet of Things (IoT) devices. However, achieving high-performance flexible transistors depends on the development of dielectric layers that are flexible, of high quality, and capable of being processed at low temperatures while maintaining excellent electrical and mechanical properties. In this study, we investigate an organic-inorganic hybrid dielectric film created by blending HfO2 with the copolymer PVP/PMMA. The organic phase aims to enhance flexibility, substrate adhesion, and processability, while the organic one enhances the dielectric properties. The hybrid films were synthesized on a flexible PEN substrate using a straightforward spin-coating method at a low temperature of 200℃. We further examine the impact of the hybrid layer as dielectric gate on the electrical performance of In2O3-based TFT flexible devices. The flexible TFTs exhibited mobilities of around 10-2 cm^2/Vs with minimal changes under mechanical stress at a bending radius of 75 mm. Notably, the devices demonstrated excellent stability with a saturation mobility of 5 × 10-2 cm^2/Vs, a threshold voltage of 1 V, a subthreshold swing of 1.1 V/dec, and an Ion/Ioff ratio of 10^3. In conclusion, the solution-derived HfO2-PVP/PMMA hybrid layers represents a promising alternative for gate dielectrics in flexible TFTs, suitable for applications in wearable sensors, biosensors, and other flexible devices.

Keywords:

transistors

Reference:

Arroyo J M, Rao M G S, Ventura M S de U, Martínez-Landeros V H, Daunis T B, Rodríguez O, Hsu J W P and Bon R R 2023 J. Mater. Chem. C 11 1824–41

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MICROELECTRONICS AND MEMS / 230

FABRICATION AND CHARACTERIZATION OF NiOx/ZnOx DIODES VIA REACTIVE PULSED LASER DEPOSITION FOR THEIR IMPLEMENTATION IN GAS SENSORS

Authors: Ivonne Julieta Silva Contreras[1]; Oscar Edel Contreras López[2]; Wencel De La Cruz[2]

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A novel application of p-n junctions is the selective detection of different gases with the same device only by changing the external bias voltage. Nickel oxide and zinc oxide are two stable semiconductors tested as gas detector materials independently; it is possible to obtain p-n heterojuctions with both, which can selectively detect between methane and hydrogen. To obtain thin semiconductor films, we have chosen the reactive pulsed laser deposition method because it is a technique that allows the thin films to be synthesized at room temperature and modulate their physical properties by modifying their stoichiometry. In this work, diodes have been manufactured using photolithography. NiOx and ZnOx thin films were grown by RPLD at room temperature under oxygen pressures of 25 mTorr and five mTorr, respectively. The chemical composition of the thin films was obtained through X-ray photoelectron spectroscopy. Additionally, the electrical resistivity of the semiconductors was measured by the Van der Pauw technique. An estimate of the band gap was calculated from transmittance measurements using UV-vis spectroscopy and the Tauc method. Grazing X-ray diffraction measurements have been carried out to identify whether the thin films obtained have crystallinity. Finally, the diodes manufactured in this study were electrically characterized employing I-V measurements. The results of the chemical analysis showed a stoichiometry of NiO1.4 and ZnO0.94. The electrical resistivity was 4.88 Ω cm for nickel oxide and 0.036 Ω cm for zinc oxide. Their respective energy band gaps were 3.25 eV and 3.20 eV. Both semiconductors were polycrystalline with FCC and HCP crystalline structures for NiOx and ZnOx, respectively. The electrical evaluation of the diodes showed that a rectifying behavior was obtained. This result is promising for the implementation of this heterojunction for selective gas detection.

Keywords:

NiO/ZnO heterojunctions, RPLD, thin films, p-n diode

Reference:

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MICROELECTRONICS AND MEMS / 321

DESIGN, SIMULATION, AND FABRICATION OF OPERATIONAL AMPLIFIERS BASED ON AMORPHOUS INDIUM-GALLIUM-ZINC-OXIDE THIN FILM TRANSISTORS

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Thin Film Transistors (TFTs) based on amorphous oxide semiconductors (AOS) like amorphous Indium-Gallium-Zinc-Oxide (a-IGZO) have extended their applications to portable electronics for healthcare sensing. This work focuses on the design, simulation and fabrication of operational amplifiers (OPAMPs) a-IGZO TFTs. The OPAMP is based on n-type TFTs, which were designed using a 5 um manufacturing process. Furthermore, the different materials that comprise the IGZO TFTs were deposited with techniques of up to 150° C, allowing their integration into low-cost flexible substrates. Preliminary simulations were performed to optimize the design of the OPAMPs, followed by experimental fabrication and characterization. The devices were evaluated in terms of voltage gain and bandwidth. The results showed that OPAMPs based on IGZO TFTs achieved a voltage gain and a bandwidth similar to reported in the literature.

Reference:

Cheng J. R., et al., "A 50 dB high gain operational amplifier integrated with metal oxide TFTs", Semicond. Sci. Technol., 2022.

Keywords:

amorphous Oxide, a-IGZO, TFTs, OPAMPs

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MICROELECTRONICS AND MEMS / 317

STUDY OF IGZO-BASED RESISTORS AS SENSING DEVICES

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The use of indium gallium zinc oxide (IGZO) as an active layer material in TFTs continues to be studied and used in electrical devices due to its good uniformity in large areas, obtaining at low temperatures, high mobility, and good compatibility with transparent and flexible substrates. In addition to being used mainly as a controller in thin displays and in the design of integrated circuits, IGZO has been demonstrated as sensing material and be easily integrated into circuit systems with TFT technology. In this work, the study of resistors based on IGZO for sensing temperature and environmental agents was carried out. The IGZO layer was deposited by sputtering at room temperature and then thermal annealing were carried out. To isolate the active layer, the IGZO was protected

with PMMA. Au or Mo is used as contact material with the IGZO, where interdigitated electrodes of different lengths and separations are included. The resistors were electrically characterized and subjected to temperature changes. Studies continue to obtain sensors with good sensitivity, good stability, low response time, developed with a simple fabrication process.

Keywords:

IGZO, sensor, thermal, resistors, electrodes

Reference:

H. Jeong et al., "Temperature Sensor Made of Amorphous Indium–Gallium–Zinc Oxide TFTs," in IEEE Electron Device Letters, DOI: 10.1109/LED.2013.2286824.

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MICROELECTRONICS AND MEMS / 131

EFFECT OF THE pH ON THE SYNTHESIS OF Ni(OH)2 THROUGH THE HYDROTHERMAL METHOD.

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Over the past few years, the scientific community has focused on nanoscale materials due to their diverse physical and chemical properties, which have presented remarkable improvements compared to bulk materials. Thus, the characteristics that considerably influence these properties are the particle size and the morphology. Regarding this last case, the nanoparticles preparation has developed different morphologies, such as spheres, rods, or plates. In recent years, one material that has offered this advantages diversity at nanoscale is the nickel hydroxide (Ni(OH)2), which has enhanced the development of applications, including batteries, supercapacitors, and catalysts. One important factor in size control of particle and morphology is the pH level; however, it has not been examined in detail its influence on obtaining Ni(OH)2. In this study, the Ni(OH)2 was hydrothermally synthetized, where the reaction time and temperature were maintained constant, while the solution pH was fine-tuned in a wide values range between 7 and 12. After a drying process at 100℃ for 24 h, the obtained powders were characterized by Fourier Transform Infrared spectroscopy, where the vibration modes of Ni(OH)2 were determined. X-ray diffraction patterns agreed with the brucite-like hexagonal structure of β-Ni(OH)2. By Scanning Electron Microscopy, hexagonal nanosheets (side=204nm) were observed for the lower pH values, while high pH synthesis resulted in a spheres (diameter=91nm) morphology. The versatility on shapes and dimensions of the obtained Ni(OH)2

particles, only by the fine-tuning of solution pH in the hydrothermal synthesis, promotes its use in several applications.

Keywords:

nickel hydroxide, hydrothermal synthesis, nanostructures, particle size control, morphology versatility.

Reference:

Y. Khan, S. K. Durrani, M. Mehmood, A. Jan, & M. A. Abbasi, pH-dependant structural and morphology evolution of Ni (OH) 2 nanostructures and their morphology retention upon thermal annealing to NiO, Materials Chemistry and Physics, 130.3 (2011) 1169-1174. https://doi.org/10.1016/j.matchemphys.2011.08.052

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MULTIFUNCTIONAL AND MAGNETIC MATERIALS / 369

A COMPREHENSIVE APPROACH IN MATERIALS SCIENCE FOR GRADUATE STUDENTS

Authors: Jesús Leonardo Heiras Aguirre[1]; Juan Guillermo García Posada[2]

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Today students with a variety of academic backgrounds are pursuing a graduate degree in different areas on Materials Sciences. The wide spectrum of undergraduate training ranges from biology, chemistry, physics, and engineering with several specialties. Some of these students are not familiar with modern concepts in Quantum Mechanics, Statistical Mechanics; Thermodynamics, and Physisc and Chemistry of Solids. Some of them are not even proficient in Mathematics. In some cases students need to deepen or refresh their knowledge with a new perspective. We are proposing a curse with curricula that includes: I. Basic concepts in quantum mechanics, chemistry and solid state physics, statistical mechanics and thermodynamics. The necessary mathematical background will be addressed, in detail, particularly differential equations. II. Types of chemical bonding.in condensed matter: origin and mechanisms. III. Oxides: types and applications. IV. Semiconductors: carriers, conductivity, density of states, and applications. V. magnetic moments ordering (this gives different types of magnetism: ferro, dia, para, frerri, antiferro, superpara and heli), interchange mechanisms, and applications. This last topic is usually the last to be covered, and in most cases, it is not covered in depth. The course may be covered in one semester or two four month period curses and will provide a fundamental and comprehensive background for all students involved in any field of condensed mater sciences and it must be a compulsory second year course.

1. "Solid State Chemistry and Its Applications", Anthony R. West, Ed. Wiley 2007.

2. "Solid State Physics", R. J. Singh, Ed. Pearson 2012.
3. "Core Maths for Advanced Level", L. Bostock, S. Chandler, Ed. Nelson Thomas Ltd, 2000
4. "Statistical Mechanics: a set of lectures", Richard P. Feynman, Ed. Addison-Wesley, 1972
5. "Introducción a la Termodinámica Clásica, L. García Colín, Ed. Trillas, 2008.

Keywords:

Reference:

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MULTIFUNCTIONAL AND MAGNETIC MATERIALS / 386

Nickel concentration effect on Curie temperature in FeCoNi multi-principal element alloys

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Four new alloys were synthesized using an electric arc melting furnace with the following atomic ratios between Fe:Co:Ni = 25:25:50, 20:20:60, 15:15:70, 10:10:80. The samples were characterized using X-ray diffraction, and thermogravimetric assay. The thermodynamic calculations for low entropy multi-principal elements alloys suggest the formation of a single-phase FCC solid solution in the samples. The XRD pattern confirm that the samples exhibit a pure FCC structure, the red parameter 'a'and cell volume reduced as the nickel concentration increased, also, the Curie temperature has the tendency to reduce as nickel increase from the mass percentage of 50 % to 80 %. Finally, the Curie temperature reduction can be attributed to the Ni content increment due to its lowest magnetic exchange interaction strength among iron and cobalt, driving the alloy to a lower magnetic order strength under temperature changes.

Keywords:

Low entropy alloy, Curie temperature, FeCoNi alloy, FCC structure

Reference:

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MULTIFUNCTIONAL AND MAGNETIC MATERIALS / 122

"CORE-SHELL NIFE2O4@CEO2 NANOPARTICLES WITH HIGH PHOTOCATALYTIC PERFORMANCE FOR THE REMEDIATION OF TOXIC PHARMACEUTICAL WASTE IN WASTEWATER"

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Water contamination by pharmaceuticals, even at low concentrations, is a growing environmental problem affecting aquatic organisms and humans. The photodegradation of organic contaminants is a key solution, and wide bandgap semiconductors, such as CeO_2, are prominent photocatalysts in this process. Recently, semiconductor composites made of metal oxides with heterojunctions have been developed, which improve the recombination of electrons and holes and generate radicals capable of decomposing organic compounds into water and carbon dioxide. Ferrites, due to their magnetic properties, are promising among low bandgap nanomaterials as they facilitate the recovery of the photocatalyst [1]. This research evaluated the effect of the synthesis method on the morphological and photocatalytic properties of the $NiFe_2O_4@CeO_2$ compound in the degradation reactions of two emerging contaminants: ibuprofen and oxytetracycline. Samples prepared by solid-state and sol-gel methods were compared. The structural, morphological, and optical properties were characterized using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), transmission electron microscopy (TEM), thermogravimetric analysis (TGA), Fourier-transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-Vis), and Raman spectroscopy.The active species generated during the degradation of ibuprofen and naproxen were studied using UV-Vis spectroscopy and liquid chromatography (HPLC), and the transformation products were identified using gas chromatography-mass spectrometry (GC/MS). Both synthesis methods showed good photocatalytic activity, but the solid-state method was more effective in degrading the pharmaceuticals. The kinetic model indicated that, under visible light, 90% of the pharmaceuticals degrade within 60 minutes with the photocatalyst, compared to 65% without CeO_2. Additionally, the material could be recycled at least five times using the magnetic separation capability of the nanocomposite, and during the cycle, the rate of drug degradation remained almost unchanged. These new nanocomposites are expected to have potential applications for the degradation of organic pollutants in wastewater.

Keywords:

Niquel ferrite, Core–shell, Magnetic properties, Photocatalyst, dye degradation

Reference:

[1] Hebah Sami Jarusheh, Ahmed Yusuf, Fawzi Banat, Mohammad Abu Haija, Giovanni Palmisano, Integrated photocatalytic technologies in water treatment using ferrites nanoparticles, Journal of Environmental Chemical Engineering, Volume 10, Issue 5, 2022, 108204, ISSN 2213-3437, https://doi.org/10.1016/j.jece.2022.108204.

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MULTIFUNCTIONAL AND MAGNETIC MATERIALS / 309

STUDY OF THE INFLUENCE OF CARBON DOTS CONCENTRATION ON THE HETEROSTRUCTURE OF CDS/TIO2 ON THEIR PHOTOCATALYTIC ACTIVITY IN THE DEGRADATION OF ORGANIC DYES.

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The fast fashion industry has significantly increased aquifer pollution due to the excessive use of organic dyes for coloring fabrics. The photocatalysis has proven to be a viable option for degrading organic compounds such as textile dyes. In this study, the photocatalitic activity of Carbon Dots (CDs)/Titanium Dioxide (TiO2) samples was evaluated with Rodamine B solution. For the synthesis of CDs, 5 ml of precursure aqueous solution of urea and citric acid was deposited in the microwave-asisted solvothermal, the product obtain was purified with ethanol and it was heated to evaporate the solvents. A pechini solution was prepared with a titanium isopropoxide, ethylene glicol and citric acid mixture at 1:16:4 molar ratio that was heated and stirred until get a traslucent solution. TiO2 nanoparticles (Sigma-Aldrich, >21mn, purity 99.5) and CDs were dispersed separately in ethanol varying the porcentaje of CDs in 0, 10 y 15%, they were integrated with pechini solution by ultrasonic. The solvents were evapored by heat treatment, the dry mixtures were pulverized in a vibrating mil for 7 hours. The morphology of the CDs was characterized using SEM. From SEM, it was observed that the synthesized CDs have a quasi-spherical morphology with a diameter of less than 20 nm. The photocatalytic activity was evaluated with the degradation of Rhodamine B solution at 5ppm. With 5 mg of each sample. Under ultraviolet light during 195 minutes. The sample with 0% CDs achieved 80% degradation; the sample with 10% CDs degraded 86%, while the sample synthesized with 15% CDs. In conclusion the increase in CDs in the CDs/TiO2 heterostructure increases the degradation percentage of the Rhodamine dye.

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Keywords:

arbon dots, Photocatalysis, Titanium dioxide, heteroestructure,degradation.

Reference:

N. U. M. Nor, E. Mazalan, C. Risko, M. Crocker, and N. A. S. Amin, "Unveiling the structural, electronic, and optical effects of carbon-doping on multi-layer anatase TiO2 (1 0 1) and the impact on photocatalysis,"

MULTIFUNCTIONAL AND MAGNETIC MATERIALS / 97

ROLE OF THE IN-PLANE APPLIED CURRENT DIRECTION IN MAGNETOTRANSPORT PROPERTIES OF MN3GA THIN FILMS.

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Materials with topological spin textures have attracted attention in recent years due to their potential technological applications as the next-generation of non-volatile magnetic memories. The compounds with hexagonal crystal structure and kagome spin structure, $D0_{19} - Mn_3X$ (X = Ga, Ge, and Sn), are promising topological structures for this purpose. Most of the topological Hall effect studies in Mn_3X have been focused on single crystals and polycrystals in bulk, and only few works have been devoted to thin films. In this work, magnetotransport properties of hexagonal $D0_{19} - Mn_3Ga$ (Mn_3Ga) epitaxial thin films grown on GaN (0001) were studied. Starting from the premise that the interaction of the direction on which the electric current (*I*) is applied within the triangular spin structure will affect its magnetotransport responses, three different azimuthal directions for I with respect to the [1-100] direction of Mn_3Ga were employed to measure magnetoresistance (MR) and Hall resistivity. By rotating the azimuth in which *I* is applied, a higher Hall resistivity is obtained for *I* at 45° from those obtained along [1-100] and [1100] directions. In the case of MR, it is observed that *I*, perpendicular and parallel to the [1-100] direction lead to asymmetric curves, whereas symmetric curves are obtained at 45°. These changes are attributed to the interaction of the electric current considering the symmetry and antisymmetry planes of the kagome structure.

Keywords:

Magnetotransport, Magnetoresistance, Topological Hall Effect, Thin Films

Reference:

M. Raju, et al., Anisotropic anomalous transport in the kagome-based topological antiferromagnetic Mn3Ga epitaxial thin films, Phys. Rev. Mater.8 (1), 014204 (2024), https://doi.org/10.1103/PhysRevMaterials.8.014204

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NANOSTRUCTURES / 205

ROOM TEMPERATURE STRONG POLARIZED EMISSION IN SELF-ASSEMBLED GAAS NANOWIRES

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One-dimensional quantum semiconductor arrays are intriguing systems for exploring fundamental physical properties and potential electronic and optoelectronic applications [1]. In particular, such nanowire arrays exhibit anisotropic effects in their electronic transport and light emission properties [2]. Here, we report the dependence of polarization in the photoluminescence (PL) emission due to this anisotropy in GaAs nanowires grown by self-assembly between AlGaAs barriers, synthesized by Molecular Beam Epitaxy (MBE) on a high-index GaAs substrate. Strong emission was obtained from PL and micro-PL measurements, even at room temperature. Furthermore, anisotropic behavior was observed in the emission intensity of the quantum wires, achieved from linearly polarized measurements, indicating good 1D confinement. Polarization degrees as high as 0.4 (40%) were obtained, confirming significant polarization dependence. Applications related to this high degree of polarization at room temperature, such as the fabrication of Vertical-Cavity Surface-Emitting Lasers (VCSELs) for use in various laser products including fiber optic communications are highlighted. [1] Jia, C., Lin, Z., Huang, Y. & Duan, X. Nanowire Electronics: From Nanoscale to Macroscale. Chem Rev 119, 9074–9135 (2019). [2] Cruz-Hernández, E. et al. Photoluminescence study of self-assembled GaAs quantum wires on (631)A-oriented GaAs substrates. Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures 30, 02B111-5 (2012).

Keywords:

Polarized, Nanowires, MBE, GaAs, Photoluminescence

Reference:

Cruz-Hernández, E. et al. Photoluminescence study of self-assembled GaAs quantum wires on (631)A-oriented GaAs substrates. Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures 30, 02B111-5 (2012).

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NANOSTRUCTURES / 134

Pressure tuning the density of states in one-dimensional photonic crystal

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In this work, we calculate the local density of states using dyadic Green's functions for a defective one-dimensional photonic crystal of finite size composed of polymeric layers. The spatial periodicity of the crystal is broken when infiltrating a cavity to detect a cancer cell. This work considers that the refractive index of polymeric materials changes with the applied pressure. We determined the existence of a confined mode within the cavity with a maximum value of the local density of states. The results show that, as pressure increases, the local density of states decreases within the confined mode.

Keywords:

one-dimensional photonic crystal, cavity, pressure, dyadic Green's functions

Reference:

Local density of states in a one-dimensional photonic crystal with a semiconducting cavity, Results in Physics 33 (2022) 105129.

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NANOSTRUCTURES / 234

Electron beam lithography. Analysis and control of process variables through testing and verification by SEM images.

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Electron beam lithography is an essential tool for fabricating micro and nano-scale devices, and an unlimited number of devices can be developed, such as sensors, MEMS, NEMS, and antennas, among others. These designs can modify the electrical, magnetic, optical, thermal, and mechanical

properties of some materials; to achieve this, it is necessary to use this lithography technique, requiring exceptional control of the different variables that influence the whole process. The resist, the electron beam, the etching area, the exposure times, the shape and direction of the beam, and the development of the resist are some issues that involve one or more variables to be controlled in this process. In this work, we show the different designs created by this means in the SEM laboratory of CIACYT, the control of each of the variables, and how they individually affect our designs through SEM images. One of the objectives of this work is to obtain the most accurate parameters for each situation, depending on the shape and size of the designs, seeking to standardize a method of evaluating designs prior to lithography to improve the structures created in terms of quality and reduce manufacturing times, as well as reduce unnecessary waste of resources. The second objective is to achieve the smallest structures that our equipment allows. It was possible to obtain images demonstrating how each of the controlled variables influences the engravings, and by controlling these, it was possible to correct and obtain more defined and better-quality structures. Results are shown for simple circle-shaped, ranging from 86nm to 3µm, 40 nm thin lines, as well as more complex structures in the shape of asterisks or interdigitated circuits and the arrays in the shape of a matrix of some of those designs that can work as antennas and sensors.

Keywords:

nanotechnology, Lithography, Electron Beam, SEM, nanofabrication

Reference:

Mohammad, Mohammad & Muhammad, Mustafa & Dew, Steven & Stepanova, Maria. Fundamentals of Electron Beam Exposure and Development.(2012). https://doi.org/10.1007/978-3-7091-0424-8_2

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NANOSTRUCTURES / 287

HETEROGENEOUS PHOTOCATALYSIS OF TIO2 NANOSTRUCTURES IMMOBILIZED ON GLASS SUBSTRATES FOR THE DECOLORIZATION AND DEGRADATION OF TEXTILE DYES

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The elimination of dyes in the effluents of the textile industry currently represents a technological challenge in wastewater treatment processes, the present study reports on the evaluation of the photocatalytic properties of TiO2 nanostructures with controlled crystalline structure and immobilized on glass substrates. Using the dipping technique, electrospun TiO2 nanofibers were deposited on the glass substrate. Scanning electron microscopy (SEM) allowed us to corroborate the presence of the films formed by the nanostructures. Furthermore, Raman scattering and X-ray diffraction confirmed that the phase present is anatase. Azo-type reactive dyes were used to evaluate the photocatalytic properties under UV light exposure. FTIR spectroscopy was used to monitor the bands assigned to the dye chromophore, which decreased as a function of time. The kinetics of the reaction were also followed by UV-vis spectroscopy, measuring the intensity of the main absorption bands. The absorbance spectra showed a gradual decrease in this band, obtaining discolorations close to 100% in a time of approximately 70 min, which can be attributed to its high surface area and the incorporation of impurities that benefit the photocatalysis process.

Keywords:

Titanium dioxide, Immobilized TiO2 nanofibers, Textile dyes

Reference:

L. Núñez, J. García-Hortal, and F. Torrades, Study of kinetic parameters related to the decolourization and mineralization of reactive dyes from textile dyeing using Fenton and photo-Fenton processes. Dyes and Pigments, 75 (2006) 647-652. https://doi.org/10.1016/j.dyepig.2006.07.014

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NANOSTRUCTURES / 69

LITHIUM/SODIUM EFFECTS ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF TITE2 MONOLAYERS FOR BATTERIES

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The demand for portable electrical energy is growing due to the use of mobile devices which satisfy daily needs. In that context the dichalcogenide TiTe2 has demonstrated a charging voltage of ~ 0.7 V (Zn2+/Zn) and a reversible capacity of 225 mAh/g [1]. Currently, it has been possible to synthesize the 1T-TiTe2 monolayer [2]. In this work, a systematic study was made of the Li/Na effect

on the TiTe2 monolayer in the different adsorption-sites on the structural and electronic properties; This was carried out using DFT implemented in the CASTEP code. Structural properties show increments for the monolayers in lattice parameters a and b due to the insertion of Li/Na in the different adsorption-sites. Besides, it is observed that the Top- and Hollow-sites could be the most stables for adsorption of Li/Na atoms. Furthermore, the electronic properties for the TiTe2 bulk compound and Pristine monolayer shows a metallic behavior in the similar way for the monolayers with Li/Na on the different adsorption-sites. This behavior is due to the interaction of *p*-Te and *d*-Ti orbitals. Finally, the voltage obtained indicates that this material can be used as an anode in ion batteries.

Keywords:

Batteries, TiTe2, DFT, Monolayers, Electronic properties.

Reference:

[1] Y. Du, et al., J Mater Chem A Mater 10 (2022) 16976–16985. [2] P. Chen, et al., Nat Commun 8 (2017) 516.

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NANOSTRUCTURES / 70

SI/LATIO3 SEMICONDUCTOR-OXIDE INTERPHASE: A DFT THEORETICAL STUDY

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LaTiO3 (LTO) perovskite is a Mott-Hubbard insulator; however, its electronic and magnetic properties can be modulated by substitutional defects, quantum confinement or heterojunction with a semiconductor material such as Si. For this work, these effects were investigated using density functional theory (DFT). The model used consisted of cutting a slab from the LTO bulk phase so that the system is two-dimensionally (2D) confined, the free surfaces are parallel to the (001) crystallographic planes and have a TiO2 termination. Then, to form a Si monolayer on the LTO slab, Si atoms were placed at highly symmetric absorption sites as follows: top sites for Ti and O atoms and hollow sites in the center of the ring formed by O and Ti atoms. Another nanostructured model was created by substituting La with Li atoms in the LTO bulk phase. Similar to the Li-free case, this forms a 2D confined perovskite system; in addition, Si atoms were positioned at the aforementioned absorption sites. Results shown that the electronic and magnetic properties of each system notoriously depend

on the confinement and the substitutional Li defects. For all cases, Si atoms interact strongly with O and Ti atoms; this fact was evidenced by means of the electronic density difference analysis and there are suggestions of covalent and ionic Si-Ti and Si-O bonds, respectively.

Keywords:

Li-batteries, DFT, nanostructured systems, perovskites

Reference:

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NANOSTRUCTURES / 302

DEVELOPMENT OF SERS SUBSTRATES FOR THE DETECTION OF DIFFERENT ANALYTES INCLUDING RHODAMINE B AND RHODAMINE 6G

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The identification of different chemical compounds and molecules is crucial, especially when they are toxic and humans are in direct contact with them, like Rhodamine B and Rhodamine 6G, that can be potentially toxic. Therefore, it is essential to employ sensitive techniques such as surface-enhanced Raman scattering (SERS), which can detect these compounds without damaging the sample and offers easy reproducibility, reliability, and high sensitivity. In this study, we utilized the SERS technique to detect Rhodamine B and Rhodamine 6G. We developed and implemented three SERS substrates: the first one comprised Ag nanoparticles deposited on Si wafers by spin coating, the second system involved Ag nanoparticles deposited on Si wafers using a Teflon ring, and the third one consisted of SiO_2 particles covered with Au and deposited on Si wafers by spin coating. Raman spectroscopy showed SERS signals of Rhodamine B and Rhodamine 6G for all three systems. The results revealed that the substrate prepared with SiO_2 particles covered with Au produced the largest enhancement of the Raman signal. However, the SERS substrate deposited using a Teflon ring on Si wafers detected more signals of Rhodamine B and Rhodamine 6G, as the Teflon ring facilitated the formation of clusters of Ag nanoparticles, increasing the presence of hot spots. The SERS substrate deposited by spin coating on Si wafers provided well-defined signals due to the homogeneous distribution of the Ag nanoparticles, as demonstrated scanning electron microscopy (SEM). In contrast, the Au coating on SiO_2 particles was non-homogeneous.

Keywords:

SERS, detection, Rhodamine 6G, Rhodamine B.

Reference:

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NANOSTRUCTURES / 303

IMPACT OF THE GRAPHENE BUFFER LAYER ON THE GROWTH OF ANTIMONIDES FOR NEAR AND MID-INFRARED OPTOELECTRONIC DEVICE INTEGRATION

Author: Nayeli Colin Becerril[1]

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Due to its favorable electrical, structural, and optical characteristics, including high electron mobility and a direct band gap, the antimonide family provides an excellent alternative for developing more efficient and high-speed optical devices. Antimonide-based devices, such as light emitting and detection systems, operate in the near and mid-infrared region. Recently, significant interest has emerged in improving the crystal quality of the antimonides, leading to investigation into their coupling with 2D materials such as graphene (G)[1]. The interaction between antimonides and graphene occurs through van der Waals forces, which are inherently weak, facilitating the transfer of growth from the graphene substrate. Therefore, in this work, we grew gallium antimonide (GaSb) on G/Si (111) using the close space vapor transport (CSVT) technique. GaSb was grown at temperatures ranging from 510 to 610℃. The GaSb compound was characterized by Raman spectroscopy, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). As results, we were able to observe by Raman the LO and TO phononic modes corresponding to GaSb at 231 and 226 cm^-1, respectively. Additionally, SEM revealed the formation of 3D GaSb structures in the form of islands and nanocolumns. Finally, we could confirm the presence of Ga—Sb and O—Sb bonds in the structures by XPS.

Keywords:

graphene, antimonides, CSVT, van der Waals forces, optoelectronic device

Reference:

Y. Alaskar et al., "Towards van der Waals Epitaxial Growth of GaAs on Si using a Graphene Buffer Layer,"Adv. Funct. Mater., vol. 24, no. 42, (2014), pp. 6629–6638, doi: 10.1002/adfm.201400960

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CONAHCYT, IPN, Project CONAHCYT-Frontier Science 2023 CF-2023-I-1117

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NANOSTRUCTURES / 71

ADSORPTION OF ALKALI, ALKALINE-EARTH AND TRANSITION METALS ON ZR2C STRUCTURE

Authors: Héctor Muñoz González[1]; Jaime Eugenio Antonio Pallares[2]; José Miguel Cervantes Cervantes[3]; Raúl Omar Escamilla Guevara[1]; José Antonio López Aranda[3]; Martin Romero Martínez[2]; Raúl Escamilla Guerrero[3]; Eliel Carvajal Quiroz[1]

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This study describes the structural and electronic properties of alkali (Li, Na and K), alkaline earth (Be, Mg and Ca) and transition (Cu, Ag and Au) metal adsorption on ZR2C structure. First-principles calculations based on the Density Functional Theory (DFT) were performed, using the SIESTA code with the generalized gradient approximations (GGA). The structure was generated parallel to the (1 1 1) crystallographic plane. The metals were adsorbed on the Zr atom (top T site), on the C atom (down D site), on the bond between C and Pb (bridge Ba and Bb sites) and above the hexagonal figure formed (hollow H site) of ZR2C. The transition, Na and Ca atoms are adsorbed preferentially on the H site; while Li, Be and Mg are adsorbed at the D site; and K atom is adsorbed at the T site. The results indicate that the adsorption of transition and Be atoms could have applications in storage of hydrogen, whereas Li and Na atoms for ion batteries.

Keywords:

DFT, Zr2C, adsorption

Reference:

SN

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This work was partially supported by the projects IPN-SIP 20201114, 20210203, and 20220567, and the UNAM-DGAPA-PAPIIT Program under Grants IN103923, IN100222, and IA103923. R. O. Escamilla and H. Muñoz acknowledge the scholarship granted by CONACYT.

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NANOSTRUCTURES / 93

CVD REDUCED GRAPHENE OXIDE: ELECTROCHEMICAL PLATFORM FOR ANALYTE SPECIFIC DETECTION

Author: Ramón Gómez Aguilar[1]

Co-authors: Gerardo Ortega Cervantez [1]; Gabriela Leticia Araujo Bernal [2]; Juan Pablo Gonzalez Aguilar [3]

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This study presents the characterization of ethanol-assisted chemical vapor deposition (CVD) reduced graphene oxide and its application as a platform for electrochemical sensors. Using CVD, graphene oxide thin films were reduced on quartz substrates by varying the temperature and reduction time with ethanol to improve the electrical conductivity and electron exchange capacity of the material. The structural, morphological and electrochemical properties of the resulting films were characterized using techniques such as scanning electron microscopy, Raman spectroscopy and four-point spectroscopy. The results indicate an effective reduction of graphene oxide with a significant improvement in electrochemical activity. The platform was developed for the immobilization of bacteria (E. coli O157:H7), glucose and even the binding of antibodies to recognize antigens (P53 Elisa Kit - MBS355295). The platform demonstrated high sensitivity and selectivity for the detection of these specific analytes when coupled to a TFT that acts as a transducer and allows us to analyze the analyte concentration on the platform by observing changes in the TFT output currents, making the platform a promising alternative for applications in biosensors and biological detection devices. This work highlights the potential of CVD-reduced graphene oxide as a versatile and effective platform for a wide range of electrochemical sensing applications.

Keywords:

CVD, graphene, oxide, platform, electrochemical

Reference:

N. Alzate-Carvajal y A. Luican-Mayer, «Functionalized Graphene Surfaces for Selective Gas Sensing», ACS Omega, vol. 5, n.o 34, pp. 21320-21329, sep. 2020, doi: 10.1021/acsomega.0c02861.

This work was supported by:

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NANOSTRUCTURES / 13

SYNTHESIS AND CHARACTERIZATION OF MAGNETIC LUMINESCENT CORE-SHELL NANOPARTICLES

Authors: Arturo Rodriguez Paredes[1]; Margarita Lizeth Alvarado Noguez[2]

Co-authors: Nidia Esther Moreno Cabrera [3]; Ángel Adalberto Durán Ledezma [4]; Ciro Falcony Guajardo [2]; Jaime Santoyo Salazar [2]; Vicente Vargas García [5]

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In clinical analysis, the use of contrast medium is of great importance because it allows the visualization of specific structures in cells and tissues, facilitating the detection of anomalies in the body and contributing to more precise and early diagnoses (1). However, current contrast medium methods have certain disadvantages, so developing new methods is an important area of research. In this work, magnetite nanoparticles doped with neodymium (Nd) and ytterbium (Yb) were synthesized using the iron salt co-precipitation method. Subsequently, they were coated with silicon dioxide (SiO2) and Nd, improving their luminescence and biocompatibility. The core-shell nanoparticles were physicochemically characterized, determining the crystalline structure of their core with an approximate size of 15nm, as well as their luminescence with absorption and emission at 656nm and 990nm, respectively. The results show these nanoparticles are possible candidates for contrast medium in biomedical applications.

Keywords:

Biosensor, Luminescence, Nanoparticles

Reference:

(1) Geng, Y., Zou, H., Li, Z., and Wu, H. Recent advances in nanomaterial-driven strategies for diagnosis and therapy of vascular anomalies. Journal of Nanobiotechnology, 22, 1 (2024) 120.

This work was supported by:

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NANOSTRUCTURES / 17

ANTIOXIDANT AND ANTIFUNGAL EFFECT OF NANOPARTICLES FUNCTIONALIZED WITH ORGANIC EXTRACTS.

Authors: Jocelyn Arleth Lopez Martinez[1]; Margarita Lizeth Alvarado Noguez[2]; Plácido Rojas Franco[2]

Co-author: Dulce María Andrade Pavon [2]

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Curcumin is the main polyphenol in turmeric, which is a root from the Zingiberaceae family. Both have been widely reported to exhibit strong antioxidant and antifungal activities, demonstrating a high capacity to neutralize free radicals and protect against oxidative damage. Magnetite nanoparticles have been used in the biological field as nanocarriers for pharmaceuticals and other health-beneficial substances, finding applications in the food, pharmaceutical, and cosmetic industries. In this study, the antioxidant and antifungal potential of magnetite nanoparticles coated with turmeric and curcumin extract is investigated. The nanoparticles were synthesized and coated using a modified iron salt coprecipitation method. The nanoparticles were synthesized, characterized, and their antioxidant capacity was evaluated through in vitro assays, including free radical scavenging. Additionally, the antifungal activity of both types of nanoparticles against the Candida albicans fungal strain was analyzed using mycelial growth assays and growth inhibition tests.

Keywords:

Antifungal, Antioxidant, Nanoparticles, Magnetite, Turmeric

Reference:

Alvarado-Noguez, M. L., Matías-Reyes, A. E., Pérez-González, M., Tomás, S. A., Hernández-Aguilar, C., Domínguez-Pacheco, F. A., Arenas-Alatorre, J. A., Cruz-Orea, A., Carbajal-Tinoco, M. D.Processing and Physicochemical Properties of Magnetite Nanoparticles Coated with Curcuma longa L. Extract. Materials 16(8), 3020. https://doi.org/10.3390/ma16083020

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Instituto Polítecnico Nacional "Escuela Nacional de Ciencias Biológicas"
Departamento de Física, Centro de Investigación y de Estudios Avanzados-IPN,

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NANOSTRUCTURES / 43

SELF-ORGANIZED GOLD NANOPARTICLES ON SIO2 SURFACE NANOPATTERNS INDUCED BY MEV ION IMPLANTATION

Author: Cristian Felipe Cruz García[1]

Co-authors: Erick Flores-Romero [1]; Jorge Rickards [1]; Miguel Angel Garcia [2]; Luis Ricardo De la Vega [3]; Jaqueline Cañetas-Ortega [1]; Juan Gabriel Morales-Morales [1]; Luis Rodríguez Fernández [1]

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The MeV ion implantation leads to the formation of surface ripple nano-patterns on diverse kind of materials, as metals, dielectrics, and semiconductors. Also, under oblique irradiation, the implanted ions are preferentially deposit on the crests of such patterns. Based on the previous experimental facts, this work shows the formation of gold nanoparticles arranged on surface nanopatterns induced on SiO2 by 1.8 MeV Au ion implantation and at impinging angle of 60°. To promote the nanoparticle nucleation the samples were followed by a thermal annealing at 1000℃. During implantation, the

ionic current was kept constant (400 nA) while the ionic fluence (proportional to implantation time) was between 0.4-2.0×10^17 cm-2. The surface morphology of the implanted substrates was analyzed by atomic force microscopy (AFM) and scanning electron microscopy (SEM). For the lowest fluences (0.4-0.8×10^17 cm-2), the formation of isolated surface structures on a flat background was observed whose morphology mimics the exoskeleton of a bug. According to a SEM-EDS analysis, the formation of gold nanoparticles on the exoskeleton of the bugs was observed. In the intermediate fluences (0.8-1.4×10^17 cm-2), a ripple background now appears and begins to surround the bugs. Finally, in the highest fluences (1.4-2.0×10^17 cm-2), the surface shows a ripple pattern without traces of the bugs. In this last case, the gold nanoparticles are formed along the crests of the surface ripples. The optical absorption of the samples show the presence of a Surface Plasmon Resonance (SPR) in the 511-555 nm wavelength region, suggesting the presence of plasmonic gold nanoparticles. The results obtained here may be of special interest for the manufacture of SERS-type sensors based on plasmonic metal nanoparticles organized according to a surface periodic nanopattern.

Keywords:

ion implantation, surface ripple nanopatterns, plasmonic gold nanoparticles

Reference:

C F Cruz-Garcia et al 2023 Phys. Scr. 98 105956

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NANOSTRUCTURES / 189

On the mechanisms of InAs quantum dots AlGaAs capping: strain, shape and intermixing.

Authors: Daniel Lopez Vilchis[1]; Leticia Ithsmel Espinoza Vega[2]; Irving Cortes[3]; Maria Fernanda Mora Herrera[4]; José Pablo Olvera Enríquez[5]; D. Corte-Ponce[6]; K.L. Marquez-Antonio[7]; A. Hernandez-Reyna[7]

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Throughout the years the semiconductor nanostructures like the quantum dots (QDs) have taken relevance in the industrial and academic fields due to the electron confinement properties they uphold, allowing for the harvesting of a wide range of the solar spectrum in photovoltaic technology, giving the user superior versatility and efficiency on devices such as TV screens for vibrant colors, photodetectors with enhanced sensitivity, etc. To properly tailor the absorption range, the full control of the synthesis process by modifying their size, composition, and arrangement in multi stacked heterostructures should be propitiated. In this study we present a method to control the morphology of the QDs by encapsulating them in asymmetric composition AlGaAs/GaAs layers by Molecular Beam Epitaxy (MBE). For sake of guaranteed reproducibility in the experiment, it was verified that prior to the capping all the QDs grown on GaAs showed the same diffusion parameters, critical thickness, and pyramidal shapes with 50° vortex angle. When encapsulating in asymmetrical AlGaAs barriers the InAs lattice mismatch is nearly maintained for any Al composition (%Al) in the ternary alloy. Nevertheless, reflection high-energy electron diffraction (RHEED) patterns of the QDs revealed consistent changes on their shape to truncated and tip rounded pyramids. GaAs capping (0%Al) conduces to a sudden flattening of the surface in such a way that the faceted growth is lost at 1.2nm. On the contrary, for high %Al alloys capping the vortex angle progressively diminishes to 20°, and its observed up to 7nm. These results prove that despite the similar lattice mismatch, the surface diffusion tailored by %Al plays a key role when capping the QDs. Numerical simulations were run to explain the ternary alloy strain effect, accounting for the morphological shapes of the pyramids, and intermixing processes.

Keywords:

Molecular Beam Epitaxy, QDs, Strain, RHEED, encapsulation

Reference:

J.P. Olvera-Enriquez, L.I. Espinosa-Vega, I.E. Cortés-Mestizo, C.A. Mercado-Ornelas, F.E. Perea-Parrales, A.Belio-Manzano, C.M. Yee-Rendón and V.H. Méndez-García, Journal of Vacuum Science & Technology A 41, 042714 (2023)

This work was supported by:

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NANOSTRUCTURES / 300

Condensation of water from the atmosphere with a Peltier cell through nanostructured materials

Author: Julio Cesar Cruz Cardenas[1]

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The amount of fresh water on the planet is decreasing, however, in the atmosphere that amount is approximately 1.4 x 10^19 liters, which makes the atmosphere an almost inexhaustible source. This project, uses the dew point temperature to condense water on different nanostructured surfaces

and configurations, to increase the condensation area. The study was developed using a Peltier cell, which had a water-cooling system and was supplied with energy through a voltage source. The temperature of the cold face was measured with a type J thermocouple. The entire system was controlled with ARDUINO, to ensure a constant temperature close to the dew temperature of the cold face in real-time. The materials used were copper and porous copper (50 m pore size), porous carbon, deposited by the magnetron sputtering technique, and aluminum and porous aluminum. The results indicate that the amount of condensed water is a function s of the temperature and humidity values of the environment. Contact angle values of said surfaces are also shown. Moreover, there was a variation in water condensation between pristine materials and those that are porous. Regarding the contact angle, there were minor variations between one material and another.

Keywords:

water condensation, nanostructured surfaces, Cu surfaces, Al surfaces

Reference:

Ankit Nagar, et al., ACS Nano 2020 14 (6), 6420-6435

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PAPIIT-IG101123 project

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NANOSTRUCTURES / 159

Ion exchange synthesis of NiY zeolite. Diffuse reflectance spectroscopy (DRS) and inductive coupling plasma (ICP) temporal analysis

Authors: Andrés Josué Reyes Solis[1]; Victor Soto[1]

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The controlled growth of Ni nanoparticles supported in zeolite Y (NiY) is of great interest, for example, by the petroleum industry due to its bifunctional characteristic (C-C bond breaking and hydrogenation-dehydrogenation function). Although there are several methods of NiY synthesis (precipitation, coprecipitation, solid state, among others), the method of synthesis by ion exchange and subsequent reduction by hydrogen is more convenient due to the ease implementation and growth control compared to the other methods previously mentioned. In this project, temperature-controlled growth of Ni nanoparticles supported in a Y zeolite (with Si/Al molar ratios of 15 and 40) was carried out using the aqueous ion exchange (first experimental stage) and reduction method with hydrogen gas (second experimental stage), characterizing each stage of the process both qualitatively and quantitatively. In the first experimental stage, the exchange time was varied from 15 to 60 days, carrying out a qualitative follow-up of the exchange by diffuse reflectance spectroscopy (DRS) and quantitative by spectroscopy with inductive coupling plasma (ICP). From the DRS, it was possible to determine the characteristic bands of nickel in the SI' and SII cationic zones of zeolite, finding a certain relationship with those reported by other authors (Lepetit & Che, 1996). On the other hand, through ICP analysis, it was possible to quantify the concentration of nickel in the exchanged samples, increasing proportionally with respect to the exchange time.

Keywords:

zeolite Y, nickel, ionic, exchange, nanoparticles,

Reference:

Lepetit, C., & Che, M. (1996). Discussion on the Coordination of Ni 2+ Ions to Lattice Oxygens in Calcined Faujasite-Type Zeolites Followed by Diffuse Reflectance Spectroscopy. J. Phys. Chem., 100, 3137–3143.

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NANOSTRUCTURES / 161

FAST ADSORPTION OF COPPER IONS USING MESOPOROUS SILICA FUNCTIONALIZED WITH THIOL AND AMINO GROUPS

Author: Jaret Wendolyn Varela Pérez[1]

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Mesoporous materials have the potential to be used in various areas, such as catalysis, adsorption of contaminating agents, controlled release of drugs, among others. In this work, the synthesis of mesoporous silica functionalized with thiol groups and amino groups is reported. Mesoporous silica was synthesized using the sol-gel method; tetraethyl orthosilicate (TEOS) was used as a precursor and pluronic P123 as a surfactant at concentrations of 1, 2 and 4%. The material obtained was functionalized by the grafting method; (3-mercaptopropyl)trimethoxysilane and (3-aminopropyl)trimethoxysilane were used as precursors of thiol and amino groups, respectively. The synthesis of an amorphous silica was confirmed by X-ray diffraction. Fourier transform infrared spectroscopy showed that thiol and amino functional groups are present in mesoporous silica, with absorption bands at 2565 cm-1 and 1567 cm-1, respectively. By SEM, the morphology of the mesoporous silica reveled, structures of 3 μm in the form of corrugated tubes, after functionalization with MPTMS and APTMS, were found structures of 4 μm long tubes and 4 μm diameter spheres were observed, respectively. Finally, the pore size of each sample was determined using the BET technique. Mesoporous silica functionalized with thiol and amino groups was used in the removal of Cu2+ ions by performing adsorption experiments. Metal quantification was performed using atomic absorption spectroscopy; the data were fitted to the Langmuir and Freundlich isotherms. It was found that mesoporous silica functionalized with amino groups has greater adsorption capacity, since it removed up to 99.7% of the Cu2+ ions.

Keywords:

Mesoporous silica, adsorption, copper

Reference:

Houmei Liu, Hui Yu, Pian Jin, Preparation of mesoporous silica materials functionalized with various amino-ligands and investigation of adsorption performances on aromatic acids, Chemical Engineering

Journal. 379 (2020) 122405. https://doi.org/10.1016/j.cej.2019.122405.

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NANOSTRUCTURES / 163

PAIR DISTRIBUTION FUNCTION ANALYSIS FOR PT-PD-CO ATOMIC MOBILITY IN NANOPARTICLES

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Through in situ monitoring of fuel cells in oxidation-reduction processes with high-energy X-ray diffraction for ternary systems (Pt-Pd-Co), the PDF is created through the Fourier transform of the diffraction pattern of a sample. It has been seen that the lattice strains in nanostructures are reflected in the oscillation of the peaks of the atomic pair distribution function (PDF). The analyses have revealed that there is atomic mobility within the ternary nanoparticles. Thus, it is sought that atomic structural models reproduce the oscillation of the PDF peaks at a certain moment, to have the average atomic distribution of the nanoparticles in the fuel cell. Different atomic structural models were created and these were applied molecular dynamics simulations using LAMMPS with second neighbor MEAM potentials. And the pair distribution function of the models was calculated trying to reproduce the experimental PDF. It is shown that a non-uniform distribution of the elements of the ternary system within the structures is the cause of the lattice strain oscillations for the nanostructures, mainly the radial distribution of Co turns out to have a greater effect on the peaks of interest in the PDF altering the general structure of the nanoparticles.

Keywords:

Nanoparticles, Pair-Distribution-Function, Strains, Ternary, Diffusion, Simulation, MEAM.

Reference:

Z.-P. Wu, D. T. Caracciolo, Y. Maswadeh, J. Wen, Z. Kong, S. Shan, J. A. Vargas, S. Yan, E. Alloying–realloying enabled high durability for Pt–Pd-3d-transition metal nanoparticle fuel cell catalysts, Nat. Commun. 12 (2021) 859. https://doi.org/10.1038/s41467-021-21017-6.

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NANOSTRUCTURES / 167

SYNTHESIS OF DOUBLE-WALLED CARBON NANOTUBES BY THE PEADSA METHOD

Author: José Luis Jiménez Pérez[1]

Co-authors: Carlos Couder-Castañeda [2]; Cornelio Ramos [1]; David Saucedo-Jiménez [2]; José Luis Luna Sánchez [1]; Verónica Hernández Rosas [1]

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The double-walled carbon nanotubes can be synthesized using the pulsed electric arc discharge with the spinning anode method (PEADSA). With this method, the frequency of the pulsed discharge can be controlled, as well as the discharge onset, which directly affects the nucleation and growth of carbon nanotubes. In this work, the experimental diameter of the double-walled carbon nanotubes (DWCNTs) was calculated employing an empirical equation that considers the quantum coupling between inner and outer carbon nanotubes and compared with the theoretical diameter (1% error). From these results the chiral indexes were calculated. The following parameters were used: current discharge at 150 A DC with a carbon disc as anode divided into eight sectors an catalytic mixture C/Ni/Fe/Co/S 95/0.6/1.4/2.8/0.3 mole fraction and angular velocity of 360 rpm. The electrode configuration was point-to-plate, and the cathode was a graphitic rod with a triangular point. The discharges and idle state durations were 20 ms and 22 ms, respectively. The synthesis was done under hydrogen atmosphere at 200 Torr. Scanning (SEM) and transmission (TEM) electron microscopy and Raman spectroscopy were for characterization. The obtained double-walled carbon nanotubes had an internal diameter of 0.82 –1.52 nm and an external diameter of 1.52 –2.33 nm.

Keywords:

DWCNTS, Arc Discharge method, Carbon nanotubes characterization

Reference:

No references

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NANOSTRUCTURES / 169

MWCNT DECORATED WITH CS2 FOR ENERGY STORAGE SYSTEMS, SYNTHESIZED BY THE PEADSA METHOD

Author: José Luis Jiménez Pérez[1]

Co-authors: Alejandro Gonzalez Cisneros [1]; Alejandro Pisil Carmona [1]; Carlos Couder-Castañeda [2]; David Saucedo-Jiménez [2]; Diego Padilla Pérez [1]; Isaac Medina [2]; José Luis Luna Sánchez [1]

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An in-depth study of previously data for the synthesis of new carbon nanostructures is made. The Raman spectra and electron microscopy images obtained were analyzed to give a physical interpretation and a possible application related to electrical charge in storage systems. By using the experimental pulsed electric arc discharge method with a spinning anode (PEADSA), pulsed discharge was performed. The angular velocity and the geometric configuration of the spinning anode were controlled and using these parameters, the electric discharge frequency, the length of the discharge time and no discharge time were regulated. Elemental sulfur powder in a sulfur rich catalytic mixture containing 93.84/2.56/1.43/0.69/1.48 of C/Ni/Fe/Co/S in mole fraction was used. A low-pressure hydrogen atmosphere (100 Torr), an angular velocity of 600 rpm and a discharge frequency of 80 Hz were employed. The catalytic mixture was disposed in sixteen alternating cavities, eight filled, eight empty. Two types of multi-walled carbon nanotubes deposited depending on the electrode were found. Mainly multi-walled carbon nanotubes (MWCNTS) with an average diameter of 60 nm and few microns in length were observed at the anode. On the other hand, MWCNTS of smaller diameters and lengths of several microns were found at the cathode. Both nanotubes were decorated with carbon disulfide. The disulfide that decorated the nanotubes had an oval shape with an average dimension of 15 nm along the surfaces of carbon nanotubes.

Keywords:

Energy storage systems, MWCNT, Arc discharge method.

Reference:

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NANOSTRUCTURES / 173

PREPARATION AND CHARACTERIZATION OF NEW MULTIFUNCTIONAL TEXTILES CONTAINING TIO2 NANOFIBERS

Authors: Josefina Aguila López[1]; José Francisco Sánchez Ramírez[2]

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This work presents the preparation of multifunctional cotton textiles using TiO2 nanofibers. The obtaining of single-crystalline TiO2 nanofibers with high specific surface area synthesized by electrospinning technique with controlled crystal structure and morphology. The nanofibers were annealed at 500 ℃ in a controlled atmosphere in the presence of air for two hours to achieve crystalline phase transformation. The cotton fabrics were functionalized with different concentrations of TiO2 nanofibers by ex situ method. The surface energy of the cotton fabric was modified using hexadecyltrimethoxysilane. Fabrics with superhydrophobic, antibacterial, UV protection and photocleaning properties were obtained. In this research, the results of the characterization of the samples using SEM, EDS, transmittance spectroscopy and contact angle measurement techniques are presented. The results showed that the modified cotton has potent antibacterial activity against Staphylococcus epidermidis bacteria. Modification of the textile surface composition was successfully carried out. Ultraviolet light blocking was measured by transmittance data at 280-400 nm and showed a higher ultraviolet protection factor than pristine cotton, it also presents a static contact angle with water ˃ 150° for a 5 µl droplet.

Keywords:

Textile, Nanofibers, Multifunctional, Electrospinning

Reference:

[1]Shateri Khalil-Abad M, Yazdanshenas ME. Superhydrophobic antibacterial cotton textiles. Journal of Colloid and Interface Science. 351 (2010), 293–98. https://doi.org/10.1016/j.jcis.2010.07.049.
[2] Rashid MM, Simončič B, Tomšič B. Recent advances in TiO2-functionalized textile surfaces. Surfaces and Interfaces. 22 (2021), 100890. https://doi.org/10.1016/j.surfin.2020.100890.

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NANOSTRUCTURES / 175

PREPARATION OF NEW CONTROLLED RELEASE SYSTEMS FOR METAL NANOBIOHERBICIDES

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The results of the encapsulation of a nanobioherbicide formulation of *Puccina* sp.- Ag NPs using the drip extrusion technique and chitosan as encapsulating polymer are presented. The synthesis of Ag nanoparticles was obtained by chemical reduction method. The Ag NPs were characterized by visual inspection, ultraviolet-visible spectroscopy and transmission electron microscopy (TEM).

The nanobioherbicide precursor solutions containing sodium tripolyphosphate (TPP) as a gelling agent were prepared under ambient conditions and rigorous stirring. By varying the percentage of TPP 4.0, 3.0, 2.0 and 1.0% in the precursor solution containing the nanobioherbicide, it was possible to prepare nanobioherbicide capsules with sizes of 4 mm and to control the porosity of the shells. Characterization by optical microscopy showed the formation of well-defined and homogeneous microcapsules. SEM analysis revealed the formation of different morphologies in the cross section of the shells depending on the TPP concentration. UV-Vis spectroscopy results revealed the presence of the nanobioherbicide in the capsules. Finally, the nanobioherbicide *Puccina* sp.- Ag NPs was applied on Amaranthus retroflexus in order to observe the herbicidal effect.

Keywords:

Ag nanoparticles, Encapsulation, Nanobioherbicides

Reference:

G. L. Zabot, F. Schaefer Rodrigues, L. Polano Ody, M. Vinícius Tres, E. Herrera, H. Palacin,J. S. Córdova-Ramos, I. Best y L. Olivera-Montenegro, Encapsulation of Bioactive Compounds for Food and Agricultural Applications, Polymers, 14 (2022), https://doi.org/10.3390/polym14194194

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NANOSTRUCTURES / 184

Fabrication of nanofibers from PET using a solution of $CHCl_3$ and $C_2HF_3O_2$ acid.

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The production of polyethylene terephthalate (PET) nanofibers by electrospinning is a modern and efficient method that uses the electric field for the production of fine fibers, allowing the fabrication of porous and versatile structures called scaffolds, organized by nanofiber units. This method has aroused great interest in the materials industry due to the unique properties they offer, such as their high mechanical strength and their potential applicability in fields such as regenerative medicine and tissue engineering. In this study, we propose an innovative approach using electrospinning for the fabrication of PET nanofibers. During the development of this project, we have created the initial solution necessary for the production of recycled PET nanofibers using the electrospinning technique. For this purpose, we have used the following materials: recycled PET from bottles and a solution composed of $CHCl_3$ and $C_2HF_3O_2$ acid. Once manufactured, the nanofibers exhibited a

uniform and homogeneous structure, characterized by high porosity and excellent interconnection between the fibers. This reflects the high quality of the production process and the desired properties for various advanced uses. The processing of PET nanofibers by electrospinning has proven to be an efficient and promising method. The results obtained in this study indicate that it is possible to produce high quality nanofibers using recycled PET, which not only retains the desired mechanical and structural properties, but also promotes sustainable practices in the materials industry.

Keywords:

high quality,recycled materials,various applications,modern method,homogeneous

Reference:

J., Said I., Manaf A., Suhad A., Zeravan A., Ahmed H. Electrospinning of polyethylene terephthalate (PET) nanofibers: optimization study using Taguchi design of experiment. IOP Conf. Ser.: Mater. Sci. Eng. 2018; 454: 0121130-0121145.

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NANOSTRUCTURES / 190

METHYLENE BLUE DEGRADATION UNDER VISIBLE LIGHT EXPOSURE USING TiO2/Au NANOCOMPOSITES SYNTHESIZED VIA LASER ABLATION OF SOLIDS IN LIQUIDS

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Co-authors: José Guadalupe Quiñones-Galván [1]; Laura Patricia Rivera-Reséndiz [1]; Enrique Campos-González [2]; Enrique Camps [2]

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Under the premise that TiO2 and Au nanoparticles exhibit good photocatalytic properties for the degradation of chemical contaminants in water, nanocomposites of TiO2/Au were synthesized in a 30% H2O2 and H2O solution using the laser ablation of solids in liquids technique. A Ti target was ablated with an energy of 475 mJ/pulse for 120 s, and in the same solution, an Au target was ablated applying the same energy while varying the ablation times, aiming to induce changes in Au concentration for each sample. The solutions containing the nanocomposites, along with samples of TiO2NPs and AuNPs synthesized under the same parameters used for the nanocomposites, were characterized using UV-VIS spectroscopy, grazing incidence X-ray diffraction (GIXRD), Raman spectroscopy, and transmission electron microscopy (TEM). Utilizing the obtained samples, photocatalytic degradation of methylene blue (MB) dye was conducted using TiO2/Au nanocomposites and TiO2NPs in the visible light range, with the incidence of an LED lamp for a total of 150 minutes, measuring solution absorbance with UV-VIS spectroscopy at intervals of 0, 15, 30, 45, and 60 minutes.

Keywords:

TiO2/Au, methylene blue, visible light, photocatalysis, water

Reference:

V. Verma, M. Al-Dossari, J. Singh, M. Rawat, M. G. M. Kordy and M. Shaban, "A Review on Green Synthesis of TiO2 NPs: Photocatalysis and Antimicrobial Applications," Polymers, vol. XIV, no. 7, 2022.

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NANOSTRUCTURES / 194

LASER EFFICIENCY AND EXTENDED DYNAMICS OF NANOEMITTERS EMBEDDED IN CARBON NANOFIBERS

Author: JESÚS JONATHAN MARTÍNEZ OCAMPO[1]

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We investigated how nanoemitters randomly distributed in single-walled carbon nanotubes (SWCNTs) can enhance laser emission when excited by plasmon-polariton (PP). We found that when the plasmonic frequency of the carbon nanotubes exceeds a critical value, the plasmon-polariton is macroscopically excited throughout the entire SWCNT. The laser generation time of the nanoemitters is strongly influenced by this plasmonic frequency. This leads to a reconnection of the fields in the nanoemitters and a significant coupling between the emitter radiation and the plasmon-polariton fields. We demonstrated that the resonant change in the spatial field structure is related to an increase in PP excitation, which is evidenced by a strong and narrow peak in the inverse participation ratio of the optical field. This phenomenon has implications for the design of active devices in contemporary nanoelectronics.

Keywords:

nanotubes,nanoemitters,plasmon,polariton,laser

Reference:

Gennadiy Burlak, Gustavo Medina-Ángel,Extended dynamics and lasing of nanoemitters enhanced by dispersing single-walled carbon nanotubes,Journal of Quantitative Spectroscopy and Radiative Transfer,Volume 296,2023,108463,https://doi.org/10.1016/j.jqsrt.2022.108463

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NANOSTRUCTURES / 211

Optimization of Conditions for Controlling the Size of Iron Nanoparticles through Ultrasonic Cavitation in Water

Authors: Jorge Aguilar Fabela[1]; Julio Cesar Cruz Cardenas[2]; Marco Antonio Martinez Fuentes[2]; Roxana Marisol Calderón Olvera[3]; Stephen Muhl[2]; Verónica Cristel Vázquez De la Cruz[3]

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Ultrasonic cavitation is the process of growth and collapse of vacuum cavities in a liquid when subjected to high-intensity ultrasonic waves. The ability to control the size and distribution of these particles is crucial for various industrial and technological applications, such as catalysis and regenerative medicine.
The objective is to establish a set of conditions that allow for more precise control over the size and structure of the nanoparticles produced, utilizing advanced characterization techniques such as Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM), which enable us to obtain images where the shape, size, and crystallinity of the nanoparticles can be observed.
In this study, operational conditions were investigated to optimize ultrasonic cavitation in the production of iron nanoparticles. The systematically varied parameters included cavitation time (2, 4, and 6 hours) with 10-second breaks every 10 seconds of ultrasonic activity, temperature (20, 30, 40, 70, 80, and 90℃), and ultrasound amplitude (50% and 100%).
The results indicate that it is possible to generate nanoparticles ranging from 3 nm to 500 nm, with changes in morphology and crystallinity. Additionally, spike-shaped nanoparticles with a crystalline composition can be generated, with resultant sizes between 4 and 8 nm.

Keywords:

Ultrasonic cavitation, iron nanoparticles, electron microscopy, size control, crystallinity.

Reference:

https://www.hielscher.com/es/acoustic-vs-hydrodynamic-cavitation-for-mixing-applications.htm

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NANOSTRUCTURES / 217

STRUCTURAL PROPERTIES OF HYDROXYAPATITE AND REDUCED GRAPHENE OXIDE COMPOSITES TO ENHANCE ELECTROCHEMICAL BIOSENSOR PERFORMANCE

Author: José Javier Ruíz Osorio[1]

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The hydroxyapatite/reduced graphene oxide (HA/rGO) composite has great versatility in applications because it exhibits a synergistic effect of its properties due to the unique characteristics of its components, such as biocompatibility, chemical and thermal stability, high surface area, excellent mechanical properties, and electrical conduction. Nowadays, there are several synthesis methodologies for this material. However, in this work, we synthesized HA/rGO composite through the microwave hydrothermal method because it combines the benefits of the hydrothermal and microwave methods, allowing us to reach ideal temperature and pressure conditions, thus reducing the synthesis time. The synthesized material was subjected to prior characterization by X-ray diffraction, Raman spectroscopy, FTIR, Scanning Transmission X-ray microspectroscopy (STXM), and SEM to elucidate the structural and morphological properties. Rietveld refinement was performed from XRD data, a Rwp value of 8.33 was obtained, and the presence of hexagonal crystalline phase of HA in HA/rGO composite was confirmed. No diffraction peak of rGO was observed in the XRD pattern because the characteristic rGO (002) peak is much weaker and broader than HA (002) peak owing to the amorphous nature of rGO. Thus, the rGO peak is covered by the highly intensified HA (002) peak with high crystallinity. Raman spectroscopy confirmed the formation of HA/rGO composite; Raman spectra show bands attributed to characteristic Raman active modes of each composite precursor. NEXAFS spectra of composite exhibit peaks associated with electronic transitions from C 1s level to $\sigma and\ \pi$ high energy levels of rGO, and transitions corresponding to Ca and O L-edge and P K-edge of HA. From SEM analysis, it is concluded that HA possesses nanorod morphology and is well distributed along the surface and edges of the graphitic layer of rGO.

Keywords:

Composite, hydroxyapatite, reduced graphene oxide, electrochemical biosensing.

Reference:

G. Barath, R. Madhu, S. Chen, and V. Veeramani. Enzymatic electrochemical glucose biosensors by mesoporous 1D hydroxyapatite-on-2D reduced graphene oxide. J. Mater. Chem. B (2015) 3, 1360-1370. 10.1039/c4tb01651c.

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NANOSTRUCTURES / 273

SYNTHESIS OF IRON AND TITANIUM NANOPARTICLES BY THE CAVITATION METHOD

Authors: Julio Cesar Cruz Cardenas[1]; Stephen Muhl Saunders[1]; Hugo Alejandro Hinojosa Novales[2]; Paula Irán Diego Villegas[2]; Iván Camps-Balabanov[3]

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Currently, bimetallic nanoparticles are of great interest due to their optical, electronic and magnetic properties, since these can be improved compared to their monometallic counterparts. The applications of this type of nanoparticles in industry are of great relevance. For example, in medicine they are used for the treatment of cancer and are also used for water treatment through photocatalysis. In this work, the synthesis of titanium and iron nanoparticles was carried out using the ultrasonic cavitation method, with the purpose of analyzing their properties and composition. For this, three different types of characterization were carried out: TEM to know its composition and structure, RBS to rectify composition and XRD to rectify structure. According to the results obtained from TEM, a composition of iron and titanium oxide nanoparticles was found, with iron found in nanowire structures of approximately 100 nm. This result was corroborated by RBS analysis using a proton beam at 1.5 MeV and also by XRD analysis, where peaks corresponding to different crystal phases of iron and titanium oxides, like ferrite, were detected. Once the properties of the nanoparticles were established, they were subjected to an annealing process, at a temperature of 800℃ for 1 hour, to see the effect of a thermal treatment. Thanks to a new XRD analysis, it was observed that after annealing, a simple tetragonal phase was reached for titanium, known as rutile.

Keywords:

Bimetalic nanoparticles, Ultrasonic cavitation, TEM, RBS, XRD

Reference:

R. Kawassaki, M. Romano, and N. Dietrich, Titanium and Iron Oxide Nanoparticles for Cancer Therapy: Surface Chemistry and Biological Implications, Front. Nanotechnol 3 (2021) 1-24. https://doi.org/10.3389/fnano.2021.735434.

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SYNTHESIS OF NANOSTRUCTURED MATERIALS FOR THE PRODUCTION OF CLEAN FUELS

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Due to a need for obtaining energy from non-fossil sources, the use of dimethyl ether (DME) as a high-efficiency fuel is a promising alternative. Its use implies zero emissions of CO2 and other toxic compounds. In this study, we propose the synthesis and characterization of nanostructured materials based on transitions metals (W oxide), supported on alumina, to be used in the methanol dehydration reaction to produce DME. The materials were prepared by the precipitation method and characterized by X-ray diffraction (XRD), temperature-programmed desorption (TPD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). The activity was discussed in terms of methanol conversion and selectivity towards DME. A tungsten oxide load at submonolayer coverage on alumina (Al2O3) renders highly dispersed dimeric polytungstate and isolated monotungstate species with tetrahedral, octahedral, and distorted octahedral coordination, whose proportion increases as it approaches a monolayer. Crystalline WO3

nanoparticles emerge at higher loads. All species displayed hexavalent oxidation. The 5 wt % sample showed the highest percentage of W-O-Al species, correlating with the highest methanol conversion. This is also attributed to the appearance of weak acid sites revealed by temperature-programmed ammonia desorption.

Keywords:

Tungsten, Polytungstate and monotungstate, Nanomaterials, Submonolayer coverage

Reference:

F. Aguilera, et al, A. Olivas*. Tungsten oxide nanomaterial interactions below monolayer coverage. J. Ovonic Research, Vol. 20 (3), May-June 2024. M.A. Armenta, et al, A. Olivas. Highly dispersed Ag2O-CuO nanospheres for methanol dehydration to DME. Fuel 358 (2024) 130268

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NANOSTRUCTURES / 279

Molecular beam epitaxial growth and properties of InAs quantum dots in asymmetric (Al)GaAs matrices.

Authors: José Pablo Olvera Enríquez[1]; Leticia Ithsmel Espinoza Vega[2]; Irving Cortes[3]; Maria Fernanda Mora Herrera[4]; D. Lopez-Vilchis[5]; Cristian Alejandro Mercado Ornelas[6]; C.M. Yee-Rendon[7]

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Currently, one of the most outstanding advances in cutting-edge science is the self-assembly of quantum dots (QDs), a promising process in the field of nanotechnology. These nanostructures restrict the degrees of freedom of electrons, phonons, and photons, allowing the creation of optical and electronic devices with exceptional characteristics.To achieve devices with the unique properties offered by QDs,it is essential to successfully stack multiple layers of the barrier/QDs/barrier structure vertically. This project focused on understanding and controlling the morphological characteristics of InAs quantum dots, such as their shape, size, and spatial distribution, analyzing the biaxial strain (εxx) based on theoretical understanding from numerical simulations [1].In this work, the growth

of InAs QDs in asymmetric (Al)GaAs matrices using the MBE technique was analyzed.Experiments were conducted with systematic variations in growth parameters (GP) such as temperature, deposition rate, and matrix composition. Before encapsulation of the QDs, the GPs were adjusted until reaching an InAs nano average island density, height and base of 5x10^10 cm^-2, 5nm and 40 nm, respectively. Better spatial distribution of QDs conduced to low noise photoreflectance spectra,where a transition close to 1.12eV was observed attributable to the quantum electron confinement of the QDs. These QDs were later capped with GaAs, Al(30)Ga(70)As and Al(40)Ga(60)As. When covering the QDs the rate of flattening of the surface strongly depends on the concentration of Al, as analyzed by reflection high-energy electron diffraction (RHEED) patterns. On this respect, several encapsulation models are proposed in this work. It is noteworthy that in spite of the intrinsic roughness of the QDs containing samples, high resolution x-ray diffraction pattens showed uniform Pendellösung fringes through which heterostructure properties were attained.Furthermore, computational simulations and theoretical models were developed to support the experimental results and provide a deeper understanding of the growth and formation mechanisms of QDs in asymmetric (Al)GaAs matrices.

Keywords:

MBE, self-assembly, QDs, numerical simulations, encapsulation

Reference:

J. P. Olvera Enríquez, L. I. Espinosa Vega, I. E. Cortés Mestizo, C. A. Mercado Ornelas, F. E. Perea Parrales, A. Belio Manzano, C. M. Yee-Rendón and V. H. Méndez García, J. Vac. Sci. Technol. A Vol. 41 (2023). https://doi.org/10.1116/6.0002674

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NANOSTRUCTURES / 297

Effect of the metal M (M: Au, AuAg, AuCu, Ag and Cu) in CeO2 catalysts, effective in the reduction of toxic 4-NP and MO

Authors: Brenda Jeanneth Acosta Ruelas[1]; Carlos Eduardo Niño González[2]

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CeO2 catalysts have been widely explored in oxidative reactions [1] however, in reductive reactions they have also been attractive for their redox properties. The synthesis of compound catalysts is usually long and multi-stage, resulting in core-shell or yolk-shell morphologies. In the present work, the microwave radiation-assisted one-pot synthesis of M@CeO2 catalysts is presented. The effects of the metal on the structure of the hollow and porous spheres of CeO2 were studied by XRD, TEM and N2 physisorption techniques, as well as the optical properties by UV-Vis spectroscopy where

the presence of the metal was confirmed by the appearance of the plasmon peak. It was also evidenced that the catalytic performance is affected by the metal in question both in the reduction of 4-nitrophenol (4-NP) and in methyl orange (MO) of which, the bimetals were more active due to the synergistic effect between metals. Regarding catalytic stability, catalysts were found to be effective in at least 10 consecutive reaction runs (4-NP reduction) with a decrease in activity. This loss of activity was attributed to a transformation in CeO2 induced by the reductive environment of NaBH4 which was evidenced by Raman spectroscopy, it was found that both the incorporation of the metal and the rich environment of H2 induce oxygen vacancies in CeO2 as well as the agglomeration of the metal to nanoparticles of larger diameters which are less active.

Keywords:

One-step, Nanoreactors, bimetal, Oxygen-vacancies, nitrophenol-reduction

Reference:

[1] sun, xuan; Wang, Xiuxiu; Chen, Beibei; Chen, Guozhu (2016). Oxygen vacancies dependent Au nanoparticle deposition and CO oxidation RSC Adv., 2016, 6, 87978–87987

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NANOSTRUCTURES / 241

Computational Simulations Applied to Kagome GdV6Sn6

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In this talk, I will present a recent computational study applied to Kagome GdV6Sn6 nanomaterials. We compared results about the Fermi surface and the Haas van Alphen quantum oscillations with experimental data. The spin-orbit effect and high electron correlation due to f-orbitals are mandatory to reach a good agreement with the experiment. The angle-dependent dHvA oscillation frequencies indicate that the smaller pockets of the Fermi surface have almost 3D character, whereas the bigger pockets are mostly two-dimensional. The comparison of the observed frequencies with the electronic structure calculations indicates that the heavier masses correspond to saddle point-like features of electronic structure at M point contributed by □ and □ bands. Our work reveals the features of the Fermi surface containing heavier fermions originating from saddle points in the electronic structure at the M point inherent to the Kagome lattice.

Keywords:

Kagome, Flat bands, Spin-orbit coupling

Reference:

C. Dhital, et al., Accepted for publication in Physical Review B, 2024.

This work was supported by:

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NANOSTRUCTURES / 338

COMPARATIVE STUDY OF TWO DIFFERENT LACASSE ENZYMES IMMOBILIZED IN NTC'S USED AS BIOSENSOR TO DETECT CATECHOL

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Carbon nanotubes (NTC´s) are novel artificial structures that have good mechanical, electrical and thermal properties. These properties have made the NTC´s object of application in the immobilization of enzymes for the manufacture of biosensors. In the present study, NTCs were used as support for the immobilization of the laccase enzyme to develop an amperometric biosensor for the determination of phenolic compounds in solutions. The enzyme used was obtained from two sources: commercial laccase enzyme from Trametes versicolor (Sigma) and crude enzymatic extract from Trametes versicolor (TA-CMU). The NTC´s were purified and oxidized by acid treatment with a solution of concentrated HNO3 and H2SO4 (1: 3) to leave the surface charged with the carboxyl group and carry out the immobilization of the enzyme. Subsequently, they were characterized by SEM, X-ray diffraction, FTIR and Raman spectroscopy. Electrodes modified with NTCs and both either enzyme or the extract were prepared, later characterized by Electrochemical Impedance Spectroscopy (EIS) techniques, identifying the interface formed on the surface of the electrode, showing the impedance or resistance to the passage of ions that the enzyme presents itself. Alone and by the presence of NTCs bound to the enzyme, was improved the process of electron transfer. Finally, cyclic voltammetry tests were performed in the presence of catechol to evaluate their detection. Values of the oxidation peak were determined in 715,624 μA and 709,224 μA for E-NTC-GA and EXT-NTC-GA, respectively, showing that the extract was capable to detect the phenol compounds.

Keywords:

Carbon nanotubes, enzyme

Reference:

[1]Guadarrama-Fernández L., Chanona-Pérez J., Manzo-Robledo A., Calderón-Domínguez G., Martínez-Rivas A., Ortiz-López J., and Vargas-García J.R. (2014) Microsc. Microanal. 20, 1479–1485.
[2]Trojanowicz, M. (2006). TrACTrends Anal Chem 25, 480–489.

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NANOSTRUCTURES / 348

NANO-STRUCTURED MG2(B2O5) AND MG2(B2O5):DY THERMOLUMINESCENT MATRIXES AND THEIR POTENTIAL APPLICATIONS AS TLDS.

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The thermoluminescence dosimeter (TLD) is a passive radiation detector whose response is proportional to the absorbed dose. Magnesium borate-based TLDs have an effective atomic number close to that of human tissue, making them useful in personal dosimetry. In the field of thermoluminescence dosimetry, the synthesis of new materials with a response to ionising radiation similar to that used in medical radiotherapy is important. Magnesium borates have the relevant physical and chemical properties, including a simple glow curve, low fading, high sensitivity, chemical and thermal stability, etc., which make them suitable for possible application as personal TLDs. This work focused on the synthesis of $Mg_2(B_2O_5)$ in both its pure form and doped with rare earth $Mg_2(B_2O_5) : Dy$ in nanometric sizes by hydrothermal synthesis. The concentration of Dy was varied from 0.01 to 1.5 molar. To determine the sensitivity of the material to gamma radiation, a Cs-137 source was used on different radiation doses. X-ray diffraction analysis determined that the samples had a pure phase of $Mg_2(B_2O_5)$ with a triclinic structure. The refinement Rietveld method indicates that the reported cell parameters a=6.149 Å, b=9.221 Å, c=3.121 Å, α=90.29o, β=92.230o, γ=104.3o changed by 0.1 to 0.7% as the Dy concentration increase. At the same time, the grain size varied from 15 to 25 nm. Finally, SEM and EDS techniques were used to obtain the morphology of nanoparticles and to determine their chemical composition. A dosimetric study and analysis of the thermoluminescence response will be carried out. The results of this research will provide a solution to improve the safety of medical personnel involved in the application of radiotherapy to cancer patients through the use of personal TLDs appropriate to the type of radiation used in this type of therapy.

Keywords:

Nanostructures, thermoluminescence, dosimetry, magnesium borates, hydrothermal synthesis

Reference:

J. Kumar,A. Yadav, P. A. Alvi, S. Kumar, & A. Vij, Combustion synthesis and thermoluminescence response of near ultra-violet irradiated Mg2B2O5 nanophosphors.
AIP Conference Proceedings 2093, 020025 (2019); https://doi.org/10.1063/1.5097094

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NANOSTRUCTURES / 364

VIRUS- LIKE NANOPARTICLES FOR SMART MEDICINE

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Enzyme replacement therapy (ERT) has been used to treat a few of the many existing diseases which originate from the lack of, or low enzymatic activity. Exogenous enzymes are administered to contend with the enzymatic activity deficiency. Nanotechnology has significantly impacted the development of medicine; a significant research effort is currently focused on the use of nanoparticles (NPs) for drug delivery, nonetheless, NPs can also be used as nanocarriers for enzymatic activity. Enzymatic nanoreactors based on enzyme encapsulation inside virus-like particles (VLPs) are excellent delivery vehicles for therapeutic enzymes as they are biodegradable, uniformly organized, and porous nanostructures that transport and can protect the biocatalyst from the external environment without greatly affecting their bioactivity.

On the other hand, endocrine disruptors (EDs) are exogenous compounds with the potential to alter hormonal synthesis and regulation, consequently affecting health and reproduction in animals and humans. On the other hand, the superfamily of cytochrome P450 enzymes (CYP) play important roles in the biosynthesis of steroids and prostaglandins. CYPs are also involved in the detoxification of a wide range of compounds such as pharmaceuticals or chemical pollutants (including EDs), and it has been established that these enzymes produce the initial biotransformation of many EDs.

In this work, we discuss ongoing research being conducted in our lab concerning the use of virus-based enzymatic nanoreactors for the treatment of lysosomal storage diseases, as well as potential therapies for galactosemia. In addition, a bionanoreactor based on the encapsulation of an enhanced peroxygenase CYPBM3 "21B3"inside the capsid of bacteriophage P22 VLPs was designed and characterized. VLPs were covered with glucose oxidase (GOx) in order to generate hydrogen peroxide necessary to activate the transformation of different Eds such as bisphenol A (BPA), nonylphenol (N2), 17 beta-estradiol (E2) and triclosan (TCS).

Keywords:

virus, nanoparticles, smart-medicine

Reference:

[1] Chauhan K., Olivares-Medina C.N., Villagrana-Escareño M.V., Juárez-Moreno K.O., Cadena-Nava R.D., Rodríguez-Hernández A.G. and Vazquez-Duhalt R. (2022) Targeted enzymatic VLP-nanoreactors with β-glucocerebrosidase activity as potential enzyme replacement therapy for Gaucher's disease. ChemMedChem 17: e202200384

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NANOSTRUCTURES / 244

From Graphene oxide to N-doped Graphene: Understanding the doping process

Authors: José Israel Paez Ornelas[1]; José Manuel Ruiz Marizcal[1]; Héctor Noé Fernández Escamilla[2]; Noboru Takeuchi[3]; Jose Manuel Romo Herrera[1]

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Various approaches are available for the nitrogen (N) doping of graphene oxide, but there needs to be more understanding of the N insertion mechanism using melamine as a precursor. N-doped graphene is widely recognized for its applications in oxygen reduction reactions (ORR). This study explored the mechanism of N insertion into graphene layers and investigated the influence of oxygen in this process. Furthermore, we examined the mechanisms of N doping and desorption at different temperatures (700, 800, 900, and 1000 ℃). After thermal treatment at 900 ℃ for 2 hours, we assessed the selectivity of nitrogenated species and their impact on ORR effectiveness. Three types of materials were analyzed: a raw sample treated at 700 ℃ for 30 minutes, a sample treated at 900 ℃ for 30 minutes, and a sample subjected to sequential treatment first at 700 ℃ for 30 minutes, followed by heating at 900 ℃ for 2 hours. The total nitrogen content in each sample was approximately 21, 9, and 8 nitrogen atoms per 100 carbon atoms, respectively. Notably, the samples treated at 900 ℃ had similar nitrogen and nitrogen species content, but the NP species specifically decreased compared to the other samples, suggesting a potentially significant role in the activity. Density functional theory (DFT) calculations were performed to elucidate the O and N variations upon the insertion mechanisms.

Keywords:

graphene oxide, N-doping, ORR, DFT

Reference:

Hector Noe Fernandez-Escamilla, et.al. Understanding the selectivity of the oxygen reduction reaction at the atomistic level on nitrogen-doped graphitic carbon materials. Advanced Energy Materials, 11(3):2002459, 2021.

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NANOSTRUCTURES / 373

SERS PLATFORMS COUPLED TO PORTABLE SEPARATION MECHANISMS FOR THE DETERMINATION OF PESTICIDES

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In recent decades, the excessive use of synthetic pesticides in crop systems has increased, resulting in ecosystem degradation and severe damage to human health. Currently, the mostcommonly used methods to determine pesticide concentration are either complex or limited in accessibility, which would make existing detection methods unsuitable for large-scale applications. Therefore, it is necessary to incorporate simple and portable strategies for separating and preconcentrating the analyte from complex matrices.
Surface-enhanced Raman scattering (SERS) is a powerful analytical technique that can be used to detect and analyze molecules at trace levels. SERS is based on the enhancement of Raman scattering signals that occur when a molecule is in close proximity to certain types of nanostructures, typically metallic nanoparticles. In complex media, such as environmental samples, food matrices, and biological fluids, the detection of trace levels of target analytes using analytical methods can be challenging due to the interference of matrixcomponents. SERS can overcome these limitations by enhancing the Raman signal of the analyte, making it possible to detect low concentrations of the target analyte even in complexmedia. To perform SERS analysis in complexmedia, the target analyte must be separated and preconcentrated to increase the signal-to-noise ratio of the measurement. Several techniques have been developed to achieve this, including solid-phase extraction, liquid- liquid extraction, and membrane filtration. Once the analyte is separated and preconcentrated, it can be analyzed using SERS. As pre-conditioning techniques can be complicated, this work aims to develop SERS substrates integrated with portable strategies for separating analytes from complex media, such as thin layer chromatography and porous or reticulated systems. Gold nanospheres and nanostars were synthesized using modified Turkevich methods and characterized via STEM and UV-Vis. The characteristic fingerprint of organophosphate pesticides was determined using substratescontaining these materials, resulting in enhancement factors of several orders of magnitude.

Keywords:

SERS, Organophosphate pesticides, thin-layer chromatography, Gold Nanostars, quantification of contaminants

Reference:

Vargas-Zamarripa, M., Rivera, A. A., Sierra, U., Salas, P., Serafín-Muñoz, A. H., & Ramírez-García, G. (2023). Improved charge-transfer resonance in graphene oxide/ZrO2 substrates for plasmonic-free SERS determination of methyl parathion. Chemosphere, 320, 138081.

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NANOSTRUCTURES / 316

SYNTHESIS OF POROUS SiO2 SPHERES AND ITS CHARACTERIZATION AFTER A LOW TEMPERATURE HEAT POST-TREATMENT

Author: Enrique Sánchez Mora[1]

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Silica spheres are widely used as catalysts, adsorbents, templates and substrates due to their large specific area and uniformity. In this work, we demonstrate that after low-temperature (≤400℃) heat treatments of the spheres, their optical response is modified without sintering effects or changes in their morphology. Initially, colloids of SiO_2 spheres were synthesized by the Stöber method [1]. Several samples with average diameters ranging from 200 to 450 nm were obtained. Each sample was characterized by X-ray diffraction, and an increase in the crystallite size was observed in some of them. The reflectance of the spheres was also affected by the heat treatment, with a consequent effect on the band gap. For example, the sample with 200 nm spheres had a band gap of 5.5 eV before the treatment and 6 eV after the treatment, presumably due to changes in the porosity composition. We conclude that the use of low-temperature heat treatment allows the optical band gap to be tuned without changing the morphology.

Keywords:

SiO2, porosity, heat treatment, XRD, band gap

Reference:

W. Stöber, A. Fink and E. Bohn, Controlled growth of monodisperse silica spheres in the micron size range, J. Colloid Interface Sci. 26 (1968) 62-69. https://doi.org/10.1016/0021-9797(68)90272-5

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NANOSTRUCTURES / 299

SERS DETECTION OF ADDITIVES IN FOOD PRODUCTS

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In recent years, the use of colorants has increased in the food industry around the world, unfortunately, some illegal additives were detected. In particular, Rhodamine B and Rhodamine 6G have been detected in chili products, that is a disturbing situation because these products are part of the Mexicans daily life and could have negative effects on health. An ideal technique to detect these additives is the surface-enhanced Raman scattering (SERS) because it is nondestructive, highly sensitive and easy to reproduce. In this study we analyze a chili powder product, which was purchased in Mexico. We developed two SERS substrate based on Ag nanoparticles (diameter of approximately 40 nm) deposited on a Si wafer by two diferent methods, the first one by Spin Coating and the second one by a a Teflon ring device. Scanning electron microscopy (SEM) demonstrated that Spin Coating allowed to have a homogeneous nanoparticles distribution throughout the silicon wafer surface. The Teflon ring device is a novel device that allowed clusters of Ag nanoparticles to be formed.

Energy-dispersive X-ray spectroscopy (EDS) helped us to verify the information about the SERS substrates composition. We detected Rhodamine B and Rhodamine 6G in the chili powder product by both SERS substrates. 1225, 1358 and 1479 cm^{-1} were some of the main signals of Rhodamine B and Rhodamine 6G that were identified by both SERS substrates. The results showed that the SERS substrate based on Ag nanoparticles deposited by the Teflon ring device, got a higher and defined spectrum than the other SERS substrate. This is due to the nanoparticles distribution, clusters allows a greater generation of hot spots than the homogeneous layer of nanoparticles dispersed by Spin Coating.

Keywords:

SERS, chili products, illegal additives.

Reference:

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NANOSTRUCTURES / 242

SYNTHESIS OF IRON (III) OXIDE AND AU NANOPARTICLES VIA LASER ABLATION OF SOLIDS IN LIQUIDS

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This work presents the results obtained from the synthesis of metallic Au and iron oxide nanoparticles through the laser ablation of a target immersed in different liquid media. Eight samples were synthesized using an Fe2O3 target, four different liquid media (acetone, bidistilled water, isopropanol, and ethanol), and two different laser intensities (475 and 640 mJ). Additionally, eight samples were obtained using a gold target and the same liquid media and laser intensities 475 and 710 mJ.
The results obtained from UV-vis spectroscopy Au samples synthesized in water and acetone media show an absorption maximum (520-550 nm), associated to the plasmonic resonance of this material, characteristic of small-sized nanoparticles.
TEM micrographs of both materials confirmed the synthesis of spherical nanoparticles. The Fe2O3 samples synthesized in water and ethanol exhibited greater size homogeneity, with a size of ~50 nm. On the other hand, the micrographs of the gold samples, in accordance with UV-vis, confirmed that the nanoparticles synthesized in acetone and water had a narrow size distribution and a small particle size of ~30 nm.
XPS confirmed the exclusive presence of iron species formed by Fe3+ ions in all samples, thus ruling out the presence of iron oxides other than Fe2O3. Concentration analysis showed that, besides Fe2O3, the samples contained species with Fe-OH bonds, with the H2O-60 and isopropanol-synthesized samples having the highest Fe2O3 rate.

It was possible to synthesize spherical Fe2O3 and Au nanoparticles using the laser ablation of solids in liquids technique. For Au, the liquid medium appears to have a significant influence on the size distribution of the synthesized samples, with acetone and water yielding the best results. Conversely, the iron oxide samples with the most homogeneous size distribution were those synthesized in ethanol and water, with the H2O-60 Fe2O3 sample demonstrating the best synthesis yield for this oxide.

Keywords:

PLAL, nanoparticle, iron oxide, gold

Reference:

N/A

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NANOSTRUCTURES / 314

NUMERICAL CALCULATIONS OF OPTICAL EFFICIENCIES, LOCAL ELECTRIC FIELD AND RADIATION PRESSURE OF POROUS DIELECTRIC SPHERES

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Dielectric spheres made of polymethylmethacrylate, polystyrene or silicon dioxide, with diameters ranging from a few to several hundred nanometers, are commonly used as building-blocks of artificial opals or as templates for inverse opals. In particular, porous silica spheres have also been proposed as substrates for metal nanoparticles for SERS applications [1] . In this work, we have explored the effect of size and pore distribution on the optical response of the spheres. We used the discrete dipole approximation model to study a sphere with cylindrical mesopores. The diameter of the spheres was varied from 200 nm to 500 nm. A wavelength-independent refractive index of 1.46 was employed. The simulated optical response was compared with that obtained using effective medium theories. The radiation pressure on the spheres with different porosities is shown. The behavior of the electric field inside the pores when the latter are occupied by air or water is also shown. The results are of great importance for the applications of the dielectric spheres as gas sensors, molecular sensors or carriers.

Keywords:

porous SiO2, DDA, near electric field, extinction, radiation pressure

Reference:

[1] P. de León Portilla, E. Sánchez-Mora and A. L. González, Influence on SERS enhancement factor of the components of an artificial opal loaded with metal NPs: A systematic study, Curr. Appl. Phys. 39

(2022) 248-257. https://doi.org/10.1016/j.cap.2022.05.003

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NANOSTRUCTURES / 285

STRUCTURAL PROPERTIES OF INAS NANOWIRES GROWN BY MBE ON GRAPHENE-COATED SUBSTRATES

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Nanoscale semiconductor materials are among the most promising technologies for developing novel optoelectronic devices. This potential is especially significant when using well-known, highly remarkable semiconductor materials like those from the III-V family, with indium arsenide (InAs) being a notable example. InAs, with its direct band gap and high electron mobility at room temperature, is particularly suitable for integration into nanowire manufacturing for optoelectronic applications in the near to mid-infrared range. In this study, we present a novel approach to fabricating InAs nanowires using molecular beam epitaxy (MBE) on Si (111) substrates coated with a monolayer of graphene. This innovative substrate configuration promotes more uniform nanowire growth, enhancing the performance and reliability of the resulting optoelectronic devices. InAs nanowires were grown by MBE on Si (111) substrates coated with graphene at various temperatures, as well as on Si substrates without graphene. Structural and microscopic studies were conducted to observe the presence and distribution of the nanowires on the substrates. High-resolution X-ray diffraction (HR-XRD) analysis confirmed the presence of crystalline InAs on the surface of the Si (111) substrates, with reflections corresponding to the 111, 022, and 222. Scanning electron microscopy (SEM) micrographs provided insights into the morphology and overall distribution of the nanowires. These studies offer evidence supporting the formation of the proposed nanostructures. Overall, the growth of InAs nanowires on Si (111) substrates, particularly those coated with graphene, demonstrates promising structural characteristics and distribution, affirming their feasibility for integration into optoelectronic devices.

Keywords:

InAs nanowires, Molecular Beam Epitaxy (MBE), Graphene-coated substrates, III-V semiconductors

Reference:

1. Liu, Junting, et al., J. Phys. Chem. Lett. 10, (2019).
2. Paladugu, Mohanchand, et al., Small 3.11 (2007).

3. Sumikura, Hisashi, et al, Nano Letters 19.11 (2019).

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NANOSTRUCTURES / 263

IN-SITU SYNTHESIZED SIO2 NANOPARTICLES AS SILICON POLYMERIC COMPOSITE MODIFIERS FOR IMPROVED MECHANICAL RESPONSE

Author: Aldo Córdoba Guerrero[1]

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The increasing demand for polymeric materials in various industries, including packaging, automotive, and electronics, has driven the need for improved mechanical properties in these materials. In the electrical industry, mechanical fatigue in insulating polymer coatings is a significant concern, leading to reduced electrical resistivity and potential safety hazards. This research focuses on enhancing the mechanical response of polydimethylsiloxane (PDMS) coatings, commonly used as electrical insulators, by incorporating SiO2 nanoparticles synthesized in-situ through the sol-gel method. The investigation seeks to improve the interaction between polymer chains and nanostructures, thereby enhancing mechanical properties without compromising hydrophobicity properties. SiO2 nanoparticles were synthesized in both acidic and alkaline media, and PDMS-SiO2 nanocomposites were prepared using an in-situ sol-gel method. Characterization techniques such as Raman, FT-IR, and XPS were employed to analyze the physicochemical properties of the nanoparticles and nanocomposites. The results revealed distinct morphological and chemical differences between nanoparticles synthesized in acidic and alkaline media. Preliminary mechanical tests on the nanocomposites demonstrated a significant improvement in tensile strength, particularly in the composite with the highest SiO2 concentration (PDMS 5-15b). This research contributes to the development of advanced polymer nanocomposites with enhanced mechanical properties for electrical insulation applications, addressing the industry's need for more durable and reliable insulating materials.

Keywords:

silicon polymers, nanocomposites, in-situ, SiO2, sol-gel

Reference:

: A. Córdoba, J. V. Cauich-Rodríguez, R. F. Vargas-Coronado, R. Velázquez-Castillo, and K. Esquivel. A Novel In Situ Sol-Gel Synthesis Method for PDMS Composites Reinforced with Silica Nanoparticles. Polymers (Basel) 16 (8) (1125) (2024). https://doi.org/10.3390/polym16081125.

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NANOSTRUCTURES / 276

NANOSTRUCTURED TiO2 LAYERS PREPARED BY ANODIZATION: INFLUENCE ON THE EFFICIENCY OF PEROVSKITE SOLAR CELLS AND OSTEOBLAST CELLS GROWTH

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TiO2 layers have been widely used in diverse applications. Some of them can be improved with the used of nanostructures. For example, in perovskite solar cells, the efficiency is increased if the TiO2 electron transport layer is nanostructured. In Ti medical inserts, in another hand, the TiO2 layer on top, responsible of the biocompatibility, can also promote osteoblasts proliferation when nanostructures are present. In both cases, the performance improvement was achieved after the optimization of the synthesis process and nanostructures characteristics, as will be shown in this work.

The TiO2 nanostructures were prepared by anodization. For the perovskite solar cells, Ti/FTO/glass films were placed in the anode and the electrolyte was based on NH4F (1.2 wt %). 30V were applied during lapses ranging from 3 to 14 min to obtain porous, then sponges and finally nanotubes (TNT). After annealing at 450℃/4 h, the samples exhibited a TiO2 anatase phase, pore diameters between 27 to 47nm, lengths from 330 to 700nm, a transmittance above 70% and a band gap of 3.30eV. A perovskite (CH3NH3PbI3) layer and then top Au electrodes were grown to conform the entire solar cell (Au/perovskite/TiO2/FTO/glass). The efficiency was successfully increased to 11.2 % for sponges and 12.8% for nanotubes, in comparison to a continuous (3.6%) or porous (8.6 %) TiO2 layer.

For the osteoblast proliferation, Ti/glass films were anodized with different voltages (25 to 45V), times (1 to 15min) and electrolyte concentrations (3 to 6 wt% NH4F). The samples were annealed at 450℃/4 h. The osteoblast proliferation was effectively increased in more than 50%, when nanostructured TiO2 layers, in comparison with the normal continuous layer, were used.

Keywords:

TiO2, nanostructures, TNT, perovskite solar cells, cell proliferation

Reference:

Marcos Luna-Cervantes, Duilio Valdespino-Padilla, Jesús M. Siqueiros Beltrones, Luis Zamora Peredo, Julián Hernández Torres, Ma. de la Paz Cruz-Jáuregui, Nanostructured Thin Films of TiO2 Tailored by Anodization, Mater. Res. Express. 11 (2024) 025007. https://doi.org/10.1088/2053-1591/ad2a89.

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NANOSTRUCTURES / 335

EFFECT OF NANOTUBULAR MORPHOLOGY AND SILVER DOPING ON THE CHARGE TRANSFER RESISTANCE OF A TiO2 NANOTUBE NANOSENSOR APPLIED IN ASCORBIC ACID DETECTION

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Titanium oxide (TiO2) is a highly relevant multifunctional material due to its catalytic and semiconducting properties, low toxicity, and excellent chemical and mechanical stability. In a tubular nanostructured form, TiO_2 plays an important role in the development of nanosensors. This morphology is crucial for the sensitivity of detection, increasing the surface area, which has an effect on the charge transfer resistance (Rct). Another strategy to optimize charge transport in TiO_2 is to reduce electron-hole recombination by doping1. This study investigates the effect of nanotubular morphology and silver (Ag) doping on the charge transfer resistance of a TiO_2 nanotube nanosensor (TiO_2NTs) designed to detect ascorbic acid. The fabrication of TiO2NTs electrodes involved a simultaneous synthesis and doping process, whereby a titanium (Ti) foil was subjected to electrochemical anodization, followed by heat treatment. Morphological, compositional and elemental distribution characterizations were performed by scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS). The electrochemical properties were evaluated by electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV). The results demonstrated the formation of a highly ordered matrix of TiO2NTs, with the presence of Ag distributed uniformly. The EIS results were approximated to an equivalent circuit [Rs(RiCPEi(RctCPEdl(Wpb)))], resulting in Rct values of 909, 890, and 500 Ω for the Ti, TiO2NTs/Ti and Ag-TiO2NTs/Ti electrodes, respectively. In the voltammograms, a null response to ascorbic acid was observed in Ti electrode. In contrast, the TiO2NTs/Ti and Ag-TiO2NTs/Ti electrodes registered an oxidation peak, which was of higher intensity in the Ag-TiO2NTs/Ti electrode, this was attributed to higher sensitivity. Both tubular morphology and Ag doping have a favorable effect on sensitivity enhancement in TiO2 nanosensors

Keywords:

TiO2-NTs impedance, Ag-doped TiO2, Electrosensing, ascorbic acid nanosensor, quality control

Reference:

[1] S, Sharma, S.K. Ganeshan, S. Kundu and N. Chappanda. Effect of doping on TiO2 nanotubes based electrochemical sensors: Glucose sensing as a case study. IEEE Transactions on nanotechnology. 20 (2021) . Doi:10.1109/TNANO.2021.3060786

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NANOSTRUCTURES / 384

INVESTIGATING QUANTUM COHERENCE IN 3D SEMICONDUCTOR NANOWIRE ARRAYS FOR ADVANCED QUANTUM TECHNOLOGIES

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The investigation of quantum coherence in nanostructures is a vital area of research with significant implications for the development of quantum information, communication, and sensing technologies. Traditionally, studies have focused on coherent tunneling phenomena within a limited set of quantum nanostructures, such as quantum dots or rings, resulting in the formation of delocalized molecular states with strong electron and hole coupling. These interconnected quantum dots and rings, acting like artificial molecules, show promise for the creation of quantum gates through coherent coupling, thereby forming the basis for essential components in quantum technologies.

In this presentation, we will discuss our latest theoretical advancements in nanowire coupling. Specifically, we focus on the coherent transverse coupling within three-dimensional arrays of closely packed, vertically aligned nanowires. These nanowires exhibit a discontinuous charge distribution along their axial direction, which has allowed us to observe significant redistribution of carrier populations across various excited states within the array.

In addition to our theoretical work, we are actively involved in developing actual prototypes using cutting-edge epitaxial growth and nanowire self-assembly techniques. While the fabrication of these prototypes is still underway, this effort is a crucial step toward validating our theoretical predictions in practical settings. Successfully creating these prototypes will not only deepen our understanding of quantum coherence in nanostructures but also pave the way for advancements in quantum computing and sensing technologies.

Keywords:

Coherence, Nanowires, Devices

Reference:

R. Méndez-Camacho and E. Cruz-Hernández, Tunneling between Parallel One-Dimensional Wigner Crystals, Sci Rep. 12, 4470 (2022).

This work was supported by:

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NANOSTRUCTURES / 35

Structural and Spectroscopic Characterization of N, B Bi-Doped and Difunctionalized Carbon Quantum Dots

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Carbon quantum dots are a type of 0D spherical nanomaterials with different types of properties such as chemical stability, biocompatibility, low toxicity, modulable band gap, photoluminescence, electrochemical, and heteroatomic doping. These properties have allowed these nanomaterials to be used in different kinds of applications such as in vitro and in vivo cellular imaging, fluorescent sensors to different analytes, drug delivery, anticancer therapy, and solar cell technology. In this work, we employed a novel microwave-assisted synthesis method to produce nitrogen and boron co-doped carbon dots. To achieve optimal synthesis, we conducted a parameter modulation, combining synthesis temperatures, times, and precursor concentrations, while keeping the power constant at 150 W and pH 5, where 120 °C, 3 min, and a precursor concentration of 1 mg/mL were found as optimal. Characterization with FE-SEM revealed these CDs to have a spherical morphology with an average size of 10.9 ± 3.38 nm. Further HR-TEM showed an interplanar distance of 0.23 nm, which is in line with prior findings of CDs that present a 0.21 nm distance corresponding to the (100) plane of graphite. UV–vis absorption showed distinct π–π*and* n–π transitions. Fluorescence spectroscopy highlighted an emission peak at 375 nm when excited at 295 nm, achieving a quantum yield of 56.7%. FTIR and Raman spectroscopy analyses confirmed the boronic acid and amine groups'presence, underscoring the graphitic nature of the core and the co-doping of boron and nitrogen. These empirical observations were compared with theoretical investigations through simulated Raman spectra, proposing a potential structure for the CDs. XPS further endorsed the co-doping of nitrogen and boron, along with the detection of the specified functional groups. All these characteristics could lend this nanomaterial to different types of applications such as fluorescent probes for a broad range of analytes and fluorescent cell imaging.

Keywords:

carbon dots; co-doped carbon dots; difunctionalized carbon dots

Reference:

Nanomaterials 2023, 13(20), 2753; https://doi.org/10.3390/nano13202753

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NANOSTRUCTURES / 387

STUDY OF MBE GROWTH ON HIGH INDEX GaAs (811) SURFACES

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High-index substrates have long been of interest due to their surface physical properties. For example, GaAs (n11) surfaces with n = 1, 2, 3, ⋯have provided promising results in solar cells demonstrating higher efficiency, terahertz devices, and have been employed in heteroepitaxial growth on GaN.
In this work, we focused on the investigation of growing AlGaAs/GaAs heterostructures on GaAs (811) substrates. The (811) surface can be seen as composed of narrow terraces of the crystal plane (100) with a width of 1.6 nm. Reflection high-energy electron diffraction (RHEED) patterns exhibit split streaks with the characteristic symmetry of the (100) surface, misoriented by an angle of 10° with respect to the [100] direction.
Heterostructures growth was performed using an MBE Riber C21 system. By varying the temperature range and V/III flux ratio, we explored changes in the characteristics of the epitaxial layers.
Atomic force microscopy (AFM) showed that during the growth of GaAs on (811) substrates, surface morphology can vary significantly depending on specific growth parameters, yielding either flat surfaces or surfaces that exhibit macroscopic faceting. After the homoepitaxy process, AlGaAs/GaAs quantum well (QW) structures were grown at a very high substrate temperature (Tg = 680℃).
AFM images showed the formation of facets up to 10 μm in length. The photoreflectance spectrum of the QW structure was dominated by optical interference. By performing FFT filtering, a better spectrum was obtained, allowing us to clearly observe electronic transitions in the QWs. Further results on the characterization of these structures will be shown and discussed.

Keywords:

GaAs, AlGaAs, RHEED, QW

Reference:

Control of the formation of self-assembled nano-voids at the GaN/GaAs interface.
Briseida G. Pérez-Hernández, Mario A. Zambrano-Serrano, Salvador Gallardo-Hernández, Yenny L. Casallas-Moreno, Ángel Guillén-Cervantes and Máximo López-López, Applied Physics Express 2021 14 (8), 085507.

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NANOSTRUCTURES / 399

Study of AlGaAs/GaAs quantum Wells grown on GaAs (118) by MBE

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In this work, we have grown AlGaAs/GaAs quantum wells using Molecular Beam Epitaxy (MBE) on high-index GaAs substrates. We performed a comprehensive study of the structures employing a variety of characterization techniques. AlGaAs layers, serving as barrier materials, are crucial for confining electrons within the GaAs quantum well region. This confinement is essential for the functionality of GaAs-based heterostructure devices, including Quantum Well Infrared Photodetectors (QWIPs) and double-heterostructure laser diodes, which operate in the red to near-infrared spectrum (700–1100 nm).
To understand the electronic structure and energy levels of the quantum wells, we solved the Schrödinger equation, providing insights into the quantum states and their respective energy levels.
For optical characterization, we employed photoluminescence (PL) and photoreflectance (PR) spectroscopy. PL measurements allowed us to probe the emission properties and confirm the quantum well's energy levels, while PR spectroscopy provided information on the electronic transitions and optical properties of the quantum wells.
Raman spectroscopy was used to analyze the vibrational modes within the quantum wells, offering valuable data on phonon interactions and Al composition. Additionally, atomic force microscopy (AFM) was utilized to assess the surface morphology and measure the root mean square (RMS) roughness of the quantum wells, which is critical for understanding the surface quality and its impact on device performance.

Keywords:

Quantum Wells, energy levels, photoluminescence.

Reference:

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PLASMA AND VACUUM / 27

Fitting Strategies for Metallic and Partially Oxidized Al 2p Spectra Containing Suboxides.

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Aluminum, a reactive metal, rapidly reacts with oxygen to form a protective aluminum oxide layer. It has three electrons in its valence shell, allowing it to form oxidation states of Al+1 and Al+2, with Al+3 being the most stable oxidation state.

Film deposition of metallic aluminum (99.99% pure aluminum pellets from Sigma Aldrich) through thermal sublimation under ultra-high vacuum conditions was done on silicon substrates (100). The background pressure in the processing chamber was 1.5×10-7 Torr and the pressure during sublimation was 6.5×10 6 Torr. The initial oxidation stages were achieved by exposing the surface to a precisely controlled ultra-pure oxygen atmosphere with varying gas dosages from 1 ×103 L to 1×107 L (1 L ≡ 1×10 6 [Torr][s]). The metallic and oxidized film was characterized using an X-ray photoelectron spectroscopy (XPS) instrument with a monochromatic source (1487.6 eV, XR5 from ThermoFisher) and a 7-channeltron hemispherical spectrometer (Alpha110, from ThermoFisher) assembled by Intercovamex.

Robust analysis techniques for peak fitting ARXPS data from Al 2p and O 1s, including the block approach and simultaneous fitting, as well as background modeling with the active approach, Shirley-Vegh-Salvi-Castle (SVSC), and the Two-Parameter Tougaard background 1, were employed to determine the chemical composition and surface structure during the initial stages of oxidation of pure metallic aluminum samples. It was observed that the layer oxide growth model incompletely replicates the behavior seen in ARXPS spectra, whereas the growth behavior of oxides through protrusions with aluminum sub-oxides does. The oxidation of metallic aluminum involves the formation of an Al+3 oxide layer along with deep protrusions and an Al+1 and Al+2 interface layer between the metallic aluminum and the protrusions.

Keywords:

Photoemission Spectra, Chemical Composition, Peak Fitting

Reference:

1 A. Herrera-Gomez, M. Bravo-Sanchez, O. Ceballos-Sanchez, M.O. Vazquez-Lepe, Practical methods for background subtraction in photoemission spectra, Surf. Interface Anal. 46 (2014) 897–905.

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PLASMA AND VACUUM / 23

THE ASYMMETRIC SHAPE IN PHOTOEMISSION SPECTRA: THE EXPERIMENTAL POINT OF VIEW

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The main peak of most of the *p*, *d*, and *f* X-ray photoemission spectra from transition metals exhibit an asymmetry that extends towards the high binding energy side. This asymmetry is observed also in some oxides. The asymmetry in peaks of photoemission spectra arises from a non-symmetric distribution of the final states of the core hole. These states can be related to multiplet components or to transitions of Fermi-level electrons.
We analyzed the 3*d* photoemission spectra of the 5th -period elements (from Rb to In), modeling the asymmetries with a Double-Lorentzian (DL) line shape. The DL line shape closely reproduces the asymmetries, and the asymmetry parameter exhibits a clear trend across the 5th period elements. For instance, there is a significant difference in the DL parameter between the two 3d branches for elements with an empty 4d band (Rb and Sr). In contrast, for elements with a partially or completely filled 4d band, this difference is smaller. Additionally, the DL parameter is lower for elements with a half-filled (Mo [Kr]5s1 4d5), almost filled (Ru [Kr]5s1 4d7 and Rh [Kr]5s1 4d8) or completely filled 4d band (Ag [Kr]5s1 4d10, Cd [Kr]5s2 4d10, and In [Kr]5s1 5p1) compared to those with an empty (Rb [Kr]5s1 and Sr [Kr]5s2), less than half-filled (from Y [Kr]5s2 4d1, Zr [Kr]5s2 4d2, and Nb [Kr]5s1 4d4), or completely filled 4d band (Pd [Kr]4d10). These results also suggest a possible relation between the d valence electrons and the physical origin of the asymmetric shape.

Keywords:

asymmetry, 3d photoemission spectra, metals, valence electrons

Reference:

A. Herrera-Gomez, et al., Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy, J. Vac. Sci. Technol. A 41 (2023). https://doi.org/10.1116/6.0002602.

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PLASMA AND VACUUM / 24

Basic aspects of the asymmetry of lineshapes in photoemission spectra caused by a cascade of excitations of Fermi-level electrons

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The effect of cascade excitations of Fermi-level electrons on the lineshape of photoemission spectra was treated by Doniach and Sunjic (DS) in 1970.1 Their derived lineshape has many issues such as its lack of integrability and failure to closely reproduce experimental data.2 We analyze this problem using a formalism rooted only in the basic quantum mechanics of resonances with a minimalist diagrammatic veneer to categorize the many-body of processes (Tougaard losses, plasmons/hole-shielding, multiplet structure, and perhaps the Shirley background). The accounting for these processes can be done with varying levels of rigor, from simple consideration of energy scales, oscillator strengths, and couplings, through to ab initio calculations of matrix elements. A density-matrix formulation in the many-body space can be applied to remove spurious interferences of states that have ill-defined/incoherent relative phases (differ from shot to shot, due to pulse noise, sample inhomogeneities, temperature, etc.). In our work, we will apply the simplest level of semi-quantitative analysis to propose possible alternatives to the problematic DS lineshape. For example, an incoherent superposition of exponential decays in time yields a lineshape that is asymmetric but integrable.

1 S. Doniach and M. Šunjic, "Many-electron singularity in X-ray photoemission and X-ray line spectra from metals,"Journal of Physics C: Solid State Physics 3, 285–291 (1970).

2 A. Herrera-Gomez, D.M. Guzman-Bucio, A.J. Carmona-Carmona, O. Cortazar-Martinez, M. Mayorga-Garay, D. Cabrera-German, C.A. Ospina-Ocampo, B.V. Crist, and J. Raboño-Borbolla, "Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy,"Journal of Vacuum Science & Technology A 41(4), (2023).

3 A. Herrera-Gomez, D. Cabrera-German, A. D. Dutoi, M. Vazquez-Lepe, S. Aguirre-Tostado, P. Pianetta, D. Nordlund, O. Cortazar-Martinez, A. Torres-Ochoa, O. Ceballos-Sanchez, and L. Gomez-Muñoz, "Intensity modulation of the Shirley background of the Cr 3p spectra with photon energies around the Cr 2p edge,"Surface and Interface Analysis 50, 246–252 (2018).

Keywords:

Doniach-Sunjic lineshape, final state effects, multiplets, double-Lorentzian, AAnalyzer

Reference:

Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy."Alberto Herrera-Gomez, et. al. Journal of Vacuum Science and Technology A 41, 043208 (2023); doi: 10.1116/6.0002602. ISSN 0734-2101.

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PLASMA AND VACUUM / 26

MULTILAYER MODEL SOFTWARE FOR CHEMICAL COMPOSITION ANALYSIS FROM XPS DATA

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X-ray Photoelectron Spectroscopy (XPS) is renowned for its acute sensitivity to surface characteristics, which enables detailed quantitative analysis of the elemental and chemical state of surface layers up to approximately 10 nanometers deep. XPS is extensively employed across various industrial and academic settings due to the widespread availability of commercial systems that facilitate comprehensive quantitative studies.

The precision of quantitative XPS analyses hinges on the meticulous fitting of emission peaks and the accurate extraction of their intensities from spectral data, which are critical for correctly determining the sample's chemical makeup. However, this process is complicated by the lack of a unified method within the XPS community for calculating surface compositions, with prevalent studies often misestimating the areas under the emission peaks. The misinterpretations of the data are exacerbated by the extended use of flawed modeling approaches and merely qualitative quantification methods like sensitivity factors and maximum entropy models.

In this study, we present a computational tool that implements the multilayer method (MLM). It is based on databases containing key physical parameters, including photoelectron cross sections, effective electron attenuation lengths, and take-off angles. The analysis is tailored to each elemental species, which significantly refines the precision of structural parameter uncertainties.

We demonstrate the effectiveness of this method by accurately replicating the chemical compositions of several first-row transition metal oxides, such as ferric oxide 〖Fe〗*(2.00±0.05) O_3 1, cobalt in cobalt spinel* 〖*Co*〗 *_3 O*(4.0±0.25) [2] and zinc oxide 〖ZnO〗 _(1.00±0.10) [3]. These examples highlight the usefulness of the software and its potential to advance research in materials science.

1 Bravo Sanchez, M., Huerta-Ruelas J.A., Cabrera-German D., Herrera-Gomez A. Composition assessment of ferric oxide by accurate peak fitting of the Fe 2p photoemission spectrum. Surf Interface Anal. 2016;49:253-260. https://doi.org/10.1002/sia.6124

Keywords:

Photoemission spectra, Chemical Quantification, MultiLayer Model

Reference:

Cabrera-German, D., Gomez-Sosa, G., Herrera-Gomez, A. Accurate peak fitting and subsequent quantitative composition analysis of the spectrum of Co 2p obtained with Al Kα radiation: I: cobalt spinel. Surf. Interface Anal. 2016, 48, 252–256. https://doi.org/10.1002/sia.5933

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PLASMA AND VACUUM / 29

Keeping a 20-year-old XPS equipment providing good data

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The XPS equipment at the Laboratorio de Procesamiento y Caracterización de Nanopelículas (LPCN) at Cinvestav-Querétaro, is one of the oldest XPS pieces of equipment that still provides high-quality data. Besides basic issues such as keeping it clean and employing a low base pressure (in the 10-10 Torr range), two of the reasons that have kept this equipment competitive are the following:
1) Alignment. The equipment is carefully aligned to coincide the waist of the (monochromatized) X-ray beam with the waist of the spectrometer analysis volume 1. The method for the alignment is discussed in this paper.
2) Spectrometer mode. Instead of the ARXPS mode of the spectrometer, which has a small angular acceptance, we employ a wide angular acceptance mode even for angle-resolved studies. The reason why this does not affect the angular resolution is discussed in this paper. The wide angular acceptance mode results in two orders of magnitude more counts, providing enough statistics.

Keywords:

Vacuum, XPS, X-ray

Reference:

A. Herrera-Gomez, F.S.S. Aguirre-Tostado, P.G.G. Mani-Gonzalez, M. Vazquez-Lepe, A. Sanchez-Martinez, O. Ceballos-Sanchez, R.M.M. Wallace, G. Conti, Y. Uritsky, Instrument-related geometrical factors affecting the intensity in XPS and ARXPS experiments, J Electron Spectros Relat Phenomena 184 (2011) 487–500. https://doi.org/10.1016/j.elspec.2011.08.002.

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PLASMA AND VACUUM / 34

Fit and background parameters of the 4f core level of the sixth-row elements using the double Lorentzian line shape.

Authors: Abraham Jorge Carmona Carmona[1]; Alberto Herrera Gómez[2]; B. Vincent Crist[3]; Carlos Alberto Ospina Ocampo[4]; Dulce María Guzmán Bucio[5]; Orlando Cortazar Martinez[6]

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In this work we will show the fit of some of the transition metals of the sixth period, using the Double Lorentzian line shape, specifically the 4f orbitals with their two branches 7/2 and 5/2 and the background used will be the Shirley-type background (SVSC). The fits were performed with the AAnalyzer© software and shared on the web at the https://xpsoasis.org/ platform. The use of the DL line shape has allowed us to perform high-quality fits in addition to reducing the number of peaks used for each fit, simplifying the analysis process. The DL line shape very accurately models the main peak in all fits, but it was observed that it is always necessary to supplement it with an additional component. The DL line shape is a great alternative for fitting asymmetric spectra compared to the Doniach-Šunjić and Mahan profile which usually do not capture the line shape as well when using an energy range higher than 3 eV, such as when fitting both spin-orbit splitting peaks for p, d and f orbitals, as well as not being integrable. The use of AAnalyzer© software in combination with the DL line shape allowed the resolving overlapping peaks that are not obvious to the naked eye as in the case of Os 4f where the satellites overlap with the 5p component. this phenomenon is also present in the spectra of W4f and Re 4f.

Keywords:

Double Lorentzian line shape, XPS, AAnalyzer, SVSC, 4f core level

Reference:

A. Herrera-Gomez et al., "Double Lorentzian lineshape for asymmetric peaks in photoelectron spectroscopy,"Journal of Vacuum Science & Technology A, vol. 41, no. 4, pp. 1–9, 2023, doi: 10.1116/6.0002602.

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PLASMA AND VACUUM / 49

Evaluation of carbon ultrathin films as protective layers to prevent oxidation of titanium

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Co-authors: Orlando Cortazar Martinez [2]; Marisol Mayorga Garay [3]; Joaquin Gerardo Raboño Borbolla [4]; Dulce María Guzmán Bucio [5]; Carlos Alberto Ospina Ocampo [6]; Alberto Herrera Gómez [7]

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Carbon layers of different thicknesses were evaluated as protective layers on titanium to prevent metal oxidation. Titanium films (99.95% purity) 100 nm thick were deposited on Si (100) in a high-vacuum magnetron sputtering system with a working pressure of 5 mTorr. A Pinnacle source with 150 Watts and 20 kHz was used. The target contained surface oxide which was deposited on the substrate. With each deposition, the surface of the target became increasingly metallic, eventually enabling the formation of ultra-thin films of pure Ti. Carbon layers were deposited with a secondary sputtering magnetron with a 99.99% pure carbon target. All the samples were studied by X-ray photoelectronic spectroscopy (XPS). The XPS instrument has a 1486.7 eV Al K monochromatic source, and a 7 channeltron hemispherical spectrometer (Alpha110). The objective of the study is to find the thinnest carbon film that completely prevents the oxidation of titanium when exposed to atmospheric conditions for one month. These samples are required for synchrotron studies of the Shirley background of photoemission spectra of titanium core levels.

Keywords:

photoemission spectra, XPS, carbon ultra thin films, synchrotron

Reference:

A. Herrera-Gomez, M. Bravo-Sanchez, F.-S. Aguirre-Tostado, M.-O. Vazquez-Lepe, The slope-background for the near-peak regimen of photoemission spectra, J. Electron Spectros. Relat. Phenomena. 189 (2013) 76–80.

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PLASMA AND VACUUM / 278

AUTOMATION OF A DROPWISE CONDENSATION COLLECTION WATER SYSTEM WITH ARDUINO.

Authors: Veronica Cristel Vázquez De la Cruz[1]; Stephen Muhl[2]; Julio Cruz[2]; Ivan Camps[3]; Marco Antonio Martinez Fuentes[2]

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An automation system was designed and implemented, using ARDUINO, that allows us to continuously measure the environmental conditions and know the corresponding dew point at which we will obtain condensed water in the collection system. Specifically, this system uses a copper plate in good thermal contact with a Peltier cell. From the temperature and humidity obtained with a DHT11 sensor, and using a calibration curve that related the voltage and temperature of the surface of the Cu plate, the ARDUINO program determined the voltage needed to adjust the temperature to the dew point. The system is intended to regularly send to the power supply, or temperature controller, a signal to adjust the voltage on the cell and thus, managing to maintain the optimal conditions to constantly condense the water under any external conditions. In this regard the project aims to propose an alternative to facilitate the adjustment of parameters that may be constantly changing

when there is no isolated or controlled system and is required a continue adaptation to get favourable results, in this case, improve the quantity of water collected in a specific time.

Keywords:

ARDUINO, dropwise condensation, automation, Peltier cell.

Reference:

Thanh X. Nguyen, et al., J. Phys. Chem. C 2011, 115

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PLASMA AND VACUUM / 56

Analysis of Sputtering Yield Amplification (SYA) using Optical Emission Spectroscopy (OES), employing materials Cu, Ti, Mo, Ta, C, and Si

Author: Marco Antonio Martinez Fuentes[1]

Co-authors: Julio Cesar Cruz Cardenas [1]; Stephen Muhl [1]; Carlos David Ramos-Vilchis [1]

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Sputtering Yield Amplification (SYA) is a phenomenon involving the modification of collision cascades induced by momentum transfer on a target's surface through the addition of heavy dopant atoms. This process enhances the emission of target atoms, typically lighter than the dopants. In our study, we employed small pieces of three doping materials (Ta, Mo, and Cu) to generate individual film deposits, from which atoms are expelled and returned to the surface of the Si target. Using Optical Emission Spectroscopy (OES), we analyzed the intensity of emission lines from both neutral and ionized species within the sputtering plasma in situ. This data provided real-time insights into the behavior of the SYA phenomenon. Furthermore, we compared these results with an SYA experiment using five small pieces of different doping materials (Cu, Ti, Mo, Ta and C) simultaneously, employing the OES technique.

Keywords:

SYA, OES, Mo, Ta, Cu, C, Ti

Reference:

J Cruz et al, "Si sputtering yield amplification: a study of the collisions cascade and species in the sputtering plasma", J. Phys. D: Appl. Phys. 54 (2021) 375201, https://doi.org/10.1088/1361-6463/ac0c4e

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PLASMA AND VACUUM / 220

During DC magnetron sputtering what is the surface temperature of the water-cooled target?

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The surface temperature of a 2”diameter water-cooled titanium target was measured, using an electrically floating fine, 0.005”wire, type K chromel-alumel thermocouple, during sputtering as a function of the DC plasma power (power densities of 1.0, 2.2 and 4.1 W/cm2) and gas pressures of 10 to 60 sccm. The temperature difference between the centre of the target and inside the racetrack was more than 200 oC, the racetrack temperature increased almost linearly with the applied power to a maximum value of ⊠850 oC.
The target temperature measurements were also carried out as a function of the N2 gas concentration in the Ar gas mixture (1 to 20%), and these measurements were complemented with the analysis of the elemental composition of the deposits prepared under the different conditions.

Keywords:

magnetron sputtering, target, reactive sputtering

Reference:

J. Vac. Sci. Technol. A 42, 033002 (2024)

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PLASMA AND VACUUM / 282

ANALYSIS OF THE INTENSITY OF SPECTRAL LINES FROM EXCITED STATES OF TA AND GE USED FOR SPUTTERING YIELD AMPLIFICATION OF SI

Authors: Rebecca Giffard Mendoza[1]; Julio Cesar Cruz Cardenas[2]; Marco Antonio Martinez Fuentes[2]; stephen Muhl[3]; Luis Fernando Benítez Rodríguez[4]; Veronica Cristel Vazquez De la Cruz[4]

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The Sputtering Yield Amplification, SYA, phenomenon discovered by S. Berg in 1996. Consists of increasing the sputtering yield value by doping the target surface with generally heavier elements; modifying the collision cascade, promoting the increase in the number of deposited atoms on the substrate. However, there are cases in which certain combinations of elements do not produce SYA, in the case of Si, there is an increase of deposition with Ta and, not a change with Ge. In DC magnetron sputtering, after the expulsion of atoms from the target, they undergo potential elastic collisions with neutral gas atoms and, even fewer inelastic collisions with energetic electrons when traveling through the gaseous phase. If the energy transferred from the collision with the particle is sufficient, it will change its state into an excited one, resulting in the emission of radiation. Study of these spectra can be achieved by Optical Emission Spectroscopy, OES. The decrease or increase of the line intensity gives an approximation of the presence of atoms deposited on the substrate, suggesting insights into the interaction between the sputter atoms inside the plasma in function to the chamber' s pressure. Given the above, the following work compares with OES the intensity of the spectral lines from excited species of Ar, Ge, Si, and Ta, during the process of DC magnetron sputtering when performing SYA of Si using Ta and Ge as doping elements. The results showed an increase in the intensity of the spectral line of Si on the racetrack when using Ta, contrary to Ge where the Si intensity didn't change significantly. Simulations using the binary collision by Monte Carlo software, SIMTRA, were performed for the analysis of the spatial distribution of the redeposited atoms on the target to contrast the intensity increase results with the theoretical redeposition.

Keywords:

Sputtering Yield Amplification, Si-doped, Tantalum, Germanium, Optical Emission Spectroscopy.

Reference:

J. Cruz et al. " Si sputtering yield amplification: a study of the collisions cascade and species in the sputtering plasma", Journal of Physics D: Applied Physics, Vol. 54, No. 37, 2021, DOI: 10.1088/1361-6463/ac0c4e.

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PLASMA AND VACUUM / 268

NEODYMIUM OXIDE THIN FILMS DEPOSITED BY PLD: OPTICAL AND STRUCTURAL EVOLUTION ANALYSIS

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Neodymium oxide is a material highly used in different applications fields, such as, optoelectronics and biomedical.
Pulsed laser deposition (PLD) was used as a synthesis method to grow thin films at different pressures, going from $2x10^{-5}$ Torr to $1x10^{-2}$ Torr. For the experiments, a 2 inches neodymium disk was used as target. It was ablated with a pulsed Nd:YAG laser emitting at 1064 nm with an energy per pulse of 190 mJ. Experiments were carried out in vacuum and in oxygen/argon background gas. To control the plasma parameters a Langmiür planar probe was used.
The obtained neodymium oxide thin films were analized optically and structurally to evaluate the pressure effect in the chemical grow mechanism.

Keywords:

NEODIMIUM OXIDE, PLD, THIN FILMS, OPTICAL PROPERTIES, STRUCTURAL PROPERTIES

Reference:

No reference

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PLASMA AND VACUUM / 53

OPTICAL AND ELECTRICAL BEHAVIOR OF THIN ZnO:Al FILMS WHEN CONFRONTING OTHER TRANSPARENT CONDUCTING OXIDES

Authors: Dagoberto Cardona Ramírez[1]; Enrique Camps Carvajal[2]; Jonathan Vera Montes[1]; José Guadalupe Quiñones Galvan[3]; Pablo Agustín Calderón Franco[1]

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Semiconductor materials by nature have high optical transparency and are good electrical insulators, but we can improve their properties through some impurification or also called doping, obtaining materials with high optical and electrical transparency. Transparent conductive oxides or also called TCO's are electrically conductive materials with high optical transparency. They are used in a variety of applications, particularly for flat screens, solar cells, etc.⋯The most used TCO is ITO or also called indium-doped tin oxide, however, indium is a rare element on Earth. For this reason, in this work we took on the task of studying the optical and electrical properties of zinc oxide doped with aluminum or AZO in order to obtain properties similar to ITO and thus propose it for these applications. 5 samples were synthesized, using the laser ablation or PLD technique, ablating two targets simultaneously under an oxygen atmosphere, keeping the Zn plasma constant and varying the Al plasma with the support of a Plasma diagnostic technique such as the Langmuir probe and commercial conductive FTO and ITO glasses were used for this study. This work presents a study on the optical and electrical properties of aluminum-doped zinc oxide thin films in contrast to other popular transparent conductive oxides such as FTO and ITO. The films were analyzed by UV-Vis

spectroscopy and subsequently the electrical resistance of the films was measured using the four-point technique to calculate their resistivity, subsequently the film with the best properties was chosen and contrasted with those of the FTO and the ITO. The results showed that AZO presents the best optical and electrical properties compared to the other two oxides with a transparency of 93% and a resistivity of 1.6x10-6 Ωm. With this we can say that AZO can be considered for the manufacture of different electronic devices.

Keywords:

semiconductors, plasma parameters, conductive oxides, laser ablation, thin films.

Reference:

J. A. Guerrero de León et al., "Influence of the Zn plasma kinetics on the structural and optical properties of ZnO thin films grown by PLD,"SN Appl Sci, vol. 1, no. 5, May 2019, doi: 10.1007/s42452-019-0497-1.

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PLASMA AND VACUUM / 267

Pulsed laser deposition of thin films from the ablation of $BaTiS_3$ perovskites at different fluences

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Thin films were deposited from the ablation in vacuum of a bulk $BaTiS_3$ perovskite target with a Nd:YAG laser emitting at 1064 nm with 10 Hz repetition rate and 6 ns pulse duration. The output energy per pulse of the laser is 750 mJ. However, for the present experiments, the energy was attenuated by the use of a polarizing beam attenuator in order to change the energy density (fluence) incident on the target.
Thin films were deposited on glass substrates at 4 different fluences: 15.2, 8.1, 4.1 and 2.7 J/cm^2. The laser produced plasmas were diagnosed by means the of time of flight curves obtained from planar Langmuir probe measurements in order to estimate the ion mean kinetic energy and density. It was found that ion density remained constant for increasing fluence. The mean kinetic ion energy was calculated considering both Ba and Ti positive ions and it was found that the energy increases with fluence.
The obtained films were structurally characterized by XRD where an amorphous structure was revealed regardless the fluence. Optical characterization was carried out by means of UV-Vis spectroscopy. The films showed transmittance values in the range of 60-80 % for 600-1100 nm without a clear dependence on fluence, however, the estimated band gap from Tauc plots, shows a trend to increase with increasing fluence, having values between 2.76-2.98 eV. Finally, the chemical composition and oxidation states were studied by means of XPS.

Keywords:

Perovskite, PLD, plasma diagnosis, Langmuir probe, Thin films

Reference:

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PLASMA AND VACUUM / 22

XPS ANALYSIS OF THE INTERFACE LAYER IN NITRIDED HfO2/Si NANOFILMS

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Co-authors: Diamanta Perle Silvas-Cabrales [2]; Felipe Corona-Davila [2]; Jorge Alejandro Torres-Ochoa [3]; Orlando Cortazar-Martinez [2]; Alberto Herrera-Gomez [2]

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Hafnium-based materials have been crucial in electronic devices in the last few years. Current challenges are species migration and the growth of an interfacial layer (mainly after annealing), both hindering device performance. Nitridation is a possible solution. ARXPS provides non-destructive depth profiling information, offering valuable insights to understand the nitridation mechanism.
Using angle-resolved X-ray photoelectron spectroscopy, we characterized and explored the interface layer in HfO2/Si nanofilms before and after nitridation achieved through remote plasma. Hf 4f, Si 2p, O 1s, C 1s, and N 1s spectra were acquired at various plasma power levels (500 W-2500 W). We identified the peak components using advanced tools for spectral analysis, such as the Active Background and Simultaneous Fitting Approaches, both encompassed in the AAnalyzer®. By using the MultiLayer Method it was possible to assess the structure and composition, including undertainties, of the multilayered nanofilms.1
The growth of hafnia on silicon causes the formation of a high hafnium content silicate interfacial layer with a thickness of ~5 Å. Nitridation causes changes in composition in both the hafnium and silicate layers. HfO2 and HfO2-xNx coexist with the thickness remaining without significant changes. Hf1-wSiwO2 and Hf1-vSivO2-zNz coexist in augmented layer; this increment is due to residual oxygen in the plasma and exhibits a saturation behavior. The generation of a monolayer (~3 Å) of Si2+-N at the interface was observed; the electrical dipole of this structure causes a shift of ~0.2 eV to lower binding energies in the Hf 4f, O 1s, and C 1s spectra.

Keywords:

XPS, Nitridation, interface, HfO2/Si

Reference:

1 A. Herrera-Gomez, D.M. Guzman-Bucio, M. Mayorga-Garay, O. Cortazar-Martinez, Angle resolved x-ray photoelectron spectroscopy assessment of the structure and composition of nanofilms—including

uncertainties—through the multilayer model, Journal of Vacuum Science & Technology A 41 (2023).

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PLASMA AND VACUUM / 394

Exploring the synthesis of a C-Cu-Mo-Ti-Ta Multi-Elemental Alloy/High-Entropy Alloy, through DC magnetron sputtering

Author: Julio Cesar Cruz Cardenas[1]

Co-authors: Fernando Benítez [2]; Cecilia Molina [2]; Stephen Muhl [1]; Marco Martínez [1]; Verónica Vázquez [2]; Juan Muro [2]; Natalia Rivera [2]

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High Entropy Alloys, HEA, since their introduction in 2004 by Yeh and Cantor have been seen to have superior properties to conventional metallic alloys. In recent years efforts have been made to develop HEAs with beneficial properties for the industry. For example, increased hardness, wear, and temperature resistance. In the present work, we studied the synthesis of a Multi-Elemental Alloy, MEA/High Entropy Alloy, HEA, of CCuMoTiTa deposited using the DC magnetron sputtering technique. A HEA with these materials has not been reported in the literature, therefore, it is expected that it might have new and different properties. The synthesis was carried out by adding small pieces of the different elements onto the racetrack of a 4"Ti target. After deposition, the films were annealed for one hour at 800℃ using an Annealsys Rapid Thermal Processing (RTP) system. The samples were characterized by RAMAN spectroscopy, Rutherford Backscattering Spectrometry (RBS), X-ray photoelectron spectroscopy (XPS), Scratch testing, and X-ray diffraction (XRD). The XRD and RAMAN measurements showed that the films had a crystalline structure, before and after annealing. In addition, they contained a mixture of oxides, mostly rutile. With XPS, the bonding of most elements with oxygen atoms was observed. The composition was studied using the RBS technique with a 1.5 MeV protons beam. Finally, with the Scratch testing, the critical loads, Lc1 and Lc2, of the deposited films before annealing were determined.

Keywords:

Multi-Elemental Alloy, HEA, Sputtering deposition, HEA XPS

Reference:

Yeh et al. Nanostructured High-Entropy Alloys with Multiple Principal Elements: Novel Alloy Design Concepts and Outcomes. Advanced Engineering Materials. 2004. https://doi.org/10.1002/adem.200300567

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PLASMA AND VACUUM / 388

PLASMA CHARACTERIZATION IN THE PRODUCTION OF ZrO2-Ni COATINGS BY CO-SPUTTERING

Author: Roger Mauricio Pérez Cruz[1]

Co-authors: Jhon Jairo Olaya Florez [2]; José Edgar Alfonso Orjuela [2]; Catalina Melo Piraquive [2]; Oscar Edwin Piamba Tulcán [2]

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In this experimental study, the focus was on characterizing the plasma generated during the production of ZrO_2-Ni films using a Co-Sputtering system. The primary objective is to analyze the plasma through optical emission spectroscopy (OES) to identify the density of emitted species (ions and electrons), the electron temperature, and to correlate these characteristics with the structure and chemical composition of the resulting coatings. The ZrO_2-Ni coatings were deposited using a pulsed RF-DC Co-Sputtering system, with variations in the working pressure and discharge power of the two sources (RF and DC). Argon was employed as the gas to generate the discharge once the working pressure of 10^{-3} mbar was achieved. Optical characterization was performed using a spectrometer equipped with a 400 lines/mm diffraction grating. The structure of the coatings was analyzed using X-ray diffraction (XRD), and the chemical composition was determined via energy-dispersive X-ray spectroscopy (EDX). This analysis aids in improving the synthesis process of ZrO_2-Ni films for solid oxide fuel cell applications, offering a deeper understanding of the relationship between plasma characteristics and the quality of the deposits.

Keywords:

Optical, ZrO_2-Ni, Sputtering, Plasma

Reference:

1 R. M. Andrii Rednyk, Liquid plasma spraying of NiO-YSZ anode layers applicable for SOFC., Materials Today Communications, Volume 38., 2024.

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PLASMA AND VACUUM / 389

Study of the effect of Nitrogen flow on the structure, chemical

composition and plasma generated in the synthesis of TiAlTaNbZrN coatings using the HiPIMS system

Author: Sara Mendoza Castañeda[1]

Co-authors: Ingrid Johana González Ávila [2]; Jhon Jairo Olaya Florez [2]; Juan Pablo González Lozano [2]; Óscar Edwin Piamba Tulcán [2]

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The aim of research is to evaluate how the nitrogen flow in a HiPIMS system affected plasma and microstructural characterization during the deposition of TiAlTaNbZrN. First, the synthesis conditions for producing the TiAlTaNbZr metallic coatings were optimized by varying the pressure and substrate bias in orden to identify the best conditions in terms of FCC structure (using X-Ray Diffraction (XRD)) and adhesion (using Scratch Test). Subsequently, TiAlTaNbZrN coatings were deposited varying nitrogen flows, and simultaneously the plasma parameters were studied using Optical Emission Spectroscopy (OES). Lastly, the results of plasma characterization were correlated with the microstructure and chemical composition of the films deposited, using XRD for determining crystalline structure and Energy Dispersive Spectroscopy (EDS) for determining the elemental concentration.

Keywords:

Sputtering, HiPIMS, TiAlTaNbZrN, Optical, Plasma

Reference:

L. Wang, J. Jin, C. Zhu, G. Li, X. Kuang, y K. Huang, "Effects of HiPIMS pulse-length on plasma discharge and on the properties of WC-DLC coatings", Appl Surf Sci, vol. 487, pp. 526–538, sep. 2019, doi: 10.1016/J.APSUSC.2019.05.046.

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PLASMA AND VACUUM / 260

Plasmon resonance absorption of Ag nanoparticles deposited at different fluence by PLD

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Silver nanoparticles were deposited on glass substrates by means of PLD. Two fluence values were used for the experiments, 2.5 and 8.3 J/cm2. Four films were grown for each fluence changing the number of pulses (300, 600, 900 and 1200 pulses). The laser produced plasmas were diagnosed by means of Langmuir probe measurements, from which time of flight curves (TOF) were obtained. Mean kinetic ion energy and density were calculated form TOF curves. The ion density was fixed at 6 x1013 cm-3 while the mean kinetic ion energy changed from 162 eV for 2.5 J/cm2 to 254 eV for 8.3 J/cm2.

The nanostructured thin films were optically characterized by UV-Vis spectroscopy, from which the well known signal of surface plasmon resonance absorption near 400 nm was observed for all the samples. The analysis of the absorption band, revealed that signals corresponding to samples grown at 8.3 J/cm2 are narrower than those of the samples grown at 2.5 J/cm2, indicating a lower size dispersion when using higher fluence, however the absorption maximum is much higher for samples grown with low fluence, which is related to particle density, which means that lower fluence allows deposition of a higher number of nanoparticles. On the other hand, the peak position shifts to higher wavelengths as fluence decreased, which indicates that nanoparticles deposited with higher fluence are smaller. Regarding number of pulses, for both fluence values, an increase of the absorbance maximum with the number of pulses was observed, revealing the increase of nanoparticles density deposited in the glass substrates. Finally, representative samples were measured by AFM, which corroborated the results from UV-Vis.

Keywords:

Pulsed Laser Deposition, Ag nanoparticles, Fluence, surface plasmon resonance absorption

Reference:

Does not apply

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RENEWABLE ENERGY / 247

Ciprofloxacin degradation using BiVO4 chemically modified with low amounts (0.1-1wt) of Rubidium

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Nowadays safe water access is decreasing due to many factors as demographic explosion and water pollution. Among the principal water pollutants, there is the pharmaceutical compounds, e.i. ciprofloxacin, which after human consume, it is integrates to water as contaminant agent. This research is a contribution toward materials development for chemical compounds remotion. In

this work, BiVO4 chemically modified with Rubidium at different concentrations (0.1-1%) were synthetized by hydrothermal synthesis method. The present work explores the influence of Rubidium in BiVO4 lattice and their photocatalytic activity. Catalysts powders were obtained in one-pot hydrothermal method, and characterized via X-Ray diffraction, Fourier-Transform Infrared spectroscopy, N2 adsorption-desorption test, UV-Vis-NIR spectroscopy and X-Ray photoelectron spectroscopy. As results, for concentrations of 0.1 and 0.5% Rb on BiVO4, the photo-degradation of ciprofloxacin evaluated via UV-Vis spectroscopy reach to be more than 58% in 4 hours with rubidium implementation samples, compared with 48% of CIP degradation in 4 hours with pure BiVO4. The influence of synthesis parameters in the physical and chemical properties is discussed.

Keywords:

Hydrothermal, Ciprofloxacin, BiVO4

Reference:

L. Lin,Frontiers in Environmental Science, vol. 10., 2022. 880246.
P. Pookmanee, Ferroelectrics, vol. 456, no. 1, pp. 45–54, Jan. 2013

This work was supported by:

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RENEWABLE ENERGY / 261

PHYSICAL PROPERTIES OF CdS ULTRA-THIN FILMS INFLUENCED BY ON-OFF AND THERMOSTATIC CHEMICAL BATH DEPOSITION TECHNIQUE FOR SOLAR CELLS APPLICATIONS

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CdS is an n-type semiconductor typically used in CdS/CdTe solar cells as window material due to high optical transparency, wide band gap (2.28-2.50 eV), manipulable thickness less than 100 nm, low temperature deposition process (< 75 °C) and compatibility with several kind of substrates. Usually, CdS is deposited by chemical bath deposition (CBD) technique, which is a simple and inexpensive solution-based process1. The chemical reactions are influenced by thermal transfer, in consequence, parameters as deposition time and growth ramp, as well as CdS ultra-thin film physical properties are modified on dependance of temperature indicator controller. An On-Off temperature indicator controller provides a ± 2℃ temperature variation range, with lesser water volume glass-container; while thermostatic temperature indicator controller provides a ± 0.1℃ temperature variation range, with bigger water volume polymer-container. Optimal growth parameters were obtained to control

the thickness value in a range from 30 nm to 120 nm on dependance of several applications, including deposition of CdS ultra-thin films window material applied to CdTe solar cells. Moreover, the ability of doping during CdS in-situ CBD process could lead to a potential optimization in device performance and will allow the development of other novel structures, including some ternary compounds. CdS thin films was grown by On-Off and thermostatic chemical bath deposition technique (CBD) on FTO (SnO2:F) substrate at 75℃ with different deposition time. The CdS by in-situ CBD process uses CdCl2 (0.1 M), SC(NH2)2 (0.3 M) as precursor solutions, and NH4Cl (0.2 M), NH4OH (2 M) were used to promote the formation of complex compounds. Comparison of some physical properties was studied, including optical, morphological, and structural properties.

Keywords:

CdS, CBD, CdTe solar cells, CdO, thermostatic

Reference:

1 J.M. Flores-Marquez, M.L. Albor-Aguilera, et al, Improving CdS/CdTe thin film solar cell efficiency by optimizing the physical properties of CdS with the application of thermal and chemical treatments, Thin Solid Films 582 (2015) 124-127. http://dx.doi.org/10.1016/j.tsf.2014.10.070

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RENEWABLE ENERGY / 270

The Influence of Argon Deposition Pressure on LiMn2O4 Thin Film Electrochemistry for Li-Ion Batteries

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Advances in battery technology can lead to longer-lasting devices, cleaner energy storage, and more efficient transportation systems. LiMn2O4 is a suitable cathode material for high-capacity Li-ion batteries. Hence, it is crucial to comprehend the impact of sputtering deposition conditions on the quality and performance of LiMn2O4 to optimize battery efficiency. This research investigates the influence of argon deposition pressure on the stoichiometry characteristics and electrochemical performance of LiMn2O4. The physicochemical and electrochemical results reveal that varying argon deposition pressures, ranging from low (5 mTorr) to high (30 mTorr), result in the formation of distinct coating stoichiometries. An argon deposition pressure of 10 mTorr led to the formation of group I, which included stoichiometric LiMn2O4 cathode coatings with the highest discharge capacity (105 mAh/g). On the other hand, using small (5 mTorr) and high (20-30 mTorr) argon deposition pressures led to the formation of group II, which included non-stoichiometric LiMn2O4 with Lithium

deficiency. This group showed an attenuated electrochemical behavior, reaching a discharge capacity of 70 mAh/g (5 mTorr). Medium argon deposition pressure (15 mTorr) led to the formation of non-stoichiometric LiMn2O4 with Manganese deficiency (group III). The absence of Manganese resulted in a severe reduction of electrochemical performance, due to high surface charge transfer (R2= 22,982 Ω), resulting in a low discharge capacity of 7 mAh/g.

Keywords:

Lithium-ion battery, LiMn2O4 cathode materials, Sputtering deposition, storage energy.

Reference:

A. Rambabu et al. Proc Indian Natn Sci Acad. 85 (2019) 121-142
Y. Yu et al. Next Nanotechnology. 3-4 (2023) 100028
Y. Zhou et al. J. Power Sources. 234 (2013) 310-332

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Author approval:

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RENEWABLE ENERGY / 30

Solvent and pH implication on the synthesis of CuBi2O4 as photocatalyst for various applications

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Climate change, water scarcity, energy shortages and hard-to-remove pollutants are now the vanguard of menacing risks not just for human kind but, other lifeforms, ecosystems and the planet itself. In response, the human race has devoted an uncountable number of efforts to diminish the effect of these harmful phenomena, including novel water purifying technologies, advanced oxidation processes to eliminate pollutants, health care products environmentally compatible and alternative energy production methods. Another exceptional alternative is photocatalysis which has a wide range of application in environment remediation. Low studied catalyst such as CuBi2O4 is regarded as propitious one due its narrow band gap (1.2 –1.6 eV) suitable conduction and valence band edges, low recombination rate, high photo and chemical stability and economic viability. In this work, it was studied the relationship between solvent and pH modulation and pure phase obtention in the synthesis process. CuBi2O4 was synthesized by a standard solvothermal reaction (180 ℃, 10 h) using bismuth nitrate (Bi(NO3)3) and copper nitrate (Cu(NO3)2) as Bi and Cu sources, respectively. The solvent used in the reaction was varied, water (H2O), Ethanol (ET), Ethylene Glycol (EG) and Glycerol (GLY), and pH values, acidic (2), neutral (8) and basic (14). The characterization techniques employed were X-Ray Diffraction (XRD), Diffuse Reflectance Spectroscopy (DRS) and Fourier Transform Infra-Red (FTIR). Pure phases were obtained with almost all solvents, being the ones with water, the most crystalline. Samples synthesized with non-basic pH values did not show a single-phase diffraction pattern, indicating the presence of reagents. FTIR spectra corroborated XRD results. The bandgap of the samples was estimated by DRS and the Kubelka-Munk theory, values were found in the 1.2 – 1.6 eV range.

Keywords:

copper bismuthate, photocatalysis, solvothermal, pH moduletion

Reference:

S. Yuvaraj, K. Karthikeyan, D. Kalpana, Y. S. Lee, and R. K. Selvan, Surfactant-free hydrothermal synthesis of hierarchically structured spherical CuBi2O4 as negative electrodes for Li-ion hybrid capacitors, Journal of Colloid and Interface Science.469, (2016)47–56 https://doi.org/10.1016/j.jcis.2016.01.060.

This work was supported by:

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RENEWABLE ENERGY / 286

ANALISIS OF THE CONVERSION EFFICIENCY OF A SOLAR TREE STRUCTURE

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It is common to find conventional solar panels in the city supplying energy to homes, parks or schools; unfortunately, these systems disturb the image of the environment generating visual pollution and affecting people's mental health. In recent works, structures have been developed that maintain a balance between energy efficiency and design, focused on using conventional solar cell technology resulting in tree designs that look far from the real ones. The objective of this work is to model a tree-shaped structure assuming possible technologies that allow having solar cells with shape and curvature similar to that of a real leaf in order to design a structure according to the essence of the environment in which it is installed. For this purpose, the three-dimensional model of a tree defined from parametric equations that generate the trajectories in space for the shape of the trunk and branches by varying a scalar parameter is used; likewise, paraboloids are used to create the geometric locations of the leaves and shape them by manipulating concavity, curvature and rotation parameters. As part of the analysis of this model, an algorithm was created in Python, which replaces the paraboloid structure with the shape of a tree leaf where the distribution of solar energy on the surface is studied as a function of its curvature and the angle of incidence of the light rays; in this way, a graphic approximation of the energy efficiency of the structure was obtained, as a function of the curvature of the leaves, to seek a balance between maximum energy conversion and a design in harmony with the environment.

Keywords:

Photovoltaic structure, parametric equations, visual pollution, energy analysis

Reference:

S. Dey y B. Pesala, ((Solar tree design framework for maximized power generation with minimized structural cost,)) Renewable Energy, vol. 162, p´ags. 1747-1762, 2020, ISSN: 0960-1481. DOI: https://doi.org/10.1016/j.renene.2020.07.035.

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RENEWABLE ENERGY / 31

NaBiO3 Photocatalysis for Environmental Remediation, dye and drugs remotion.

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The raising of emergent contaminants is characterized by a detrimental effect on the quality of water, soil and air, affecting the wellbeing of many types of organisms and the difficulty of their degradation by conventional methods. Research about the harmful effects of these substances show that although they cannot be acutely toxic in the early term, there are potential risk against reproductive processes of aquatic lifeforms, cytotoxic and genotoxic effects, high oxidative cell stress, and adverse effects on growth rate. Furthermore, the problem aggravates by the low regulation in both, consumption and residual treatment, and the poor removal efficiency of wastewater treatment plants. One way to make a stand against this alarming situation is the use of an Advanced Oxidation Process (AOP), such as photocatalysis. NaBiO3, a semiconductor catalyst, has been regarded as an 'excellent'catalyst for this kind of application in recent years as a result of its outstanding properties including fast charge carrier separation, visible-light absorption and chemical stability. In this research it is presented the photocatalytic performance of NaBiO3 in the remotion of emergent contaminants (Rhodamine B, Ciprofloxacin and Ibuprofen). The synthesis was carried out by a conventional coprecipitation technique using bismuth nitrate (Bi(NO3)3) and sodium hydroxide (NaOH) as Bi and Na sources. X-Ray Diffraction (XRD) and Diffuse Reflectance Spectroscopy (DRS) were performed to characterize the sample. Photocatalysis experiments measured the loss on intensity of the characteristic peaks of the contaminant. Total RhB decolorization was achieved in 90 minutes, meanwhile the ciprofloxacin solution was removed about 50 % in 150 minutes, in contrast, ibuprofen was not degraded due to the oxidation and reduction potentials of NaBiO3.

Keywords:

sodium bismuthate, emergent contaminants, photocatalysis, environmental remediation

Reference:

W. Wu and & H. Zhou. One-pot preparation of NaBiO3/PNMA composite: surface properties and photo-catalytic performance. Applied Surface Science 544 (2021) , 148910 https://doi.org/10.1016/j.apsusc.2020.148910.

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RENEWABLE ENERGY / 305

PHOTODEGRADATION DEPTH PROFILES OF NON-FULLERENE ACCEPTOR ORGANIC SOLAR CELLS

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Non-fullerene acceptor (NFA)-based organic solar cells have garnered attention in the photovoltaic field owing to their low manufacturing costs, flexibility and power conversion efficiency enhancement. However, these devices have short lifetimes owing to the nature of organic semiconductors, which can be altered by external stresses, such as photon illumination, electronic and optoelectronic properties. These factors have made it necessary to investigate new materials used in structural configuration layers to improve the efficiency and stability of devices. In this work, we present an analysis of the chemical characterizations made by SIMS and XPS of bulk heterojunction inverted organic solar cells (iOSC) fabricated using a small molecule as the acceptor material. The materials used for the fabrication of the active layer of the cell were the donor PM6 (polymer) and acceptor Y7 (small molecule, non-fullerene acceptor) 1, and PDINO (polymer) was used as the electron transport layer (ETL). Chemical characterizations were carried out on non-encapsulated organic solar cells with prior electrical characterization (*I-V* characteristic curve) considering the ISOS-D1 protocols.

Keywords:

organic solar cell, PM6:Y7 blend, SIMS, XPS, non-fullerene acceptor

Reference:

Sacramento, A., Abad, J. L., Ramírez-Como, M., Balderrama, V. S., & Estrada, M. (2024). Degradation analysis of inverted PM6 (PBDB-T-2F): Y7 (BTP-4CI) solar cells with PDINO and MoO 3 as the ETL/HTL. Sustainable Energy & Fuels, 8(1), 103-112.

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RENEWABLE ENERGY / 306

HYDROGEN GENERATION FROM Co Ni-BASED CATHODES DEVELOPED FROM WASTED NiMH BATTERIES.

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Currently, there is a significant dependence on fossil fuels, which are non-renewable. When these fuels are used in combustion processes, they generate greenhouse gases that contribute to climate change. Accordingly, it is crucial to develop more environmentally friendly energy sources enabling to underpin futures demands. In this context, hydrogen stands out as an attractive alternative due to its high energy density (140 MJ/kg) and its clean byproducts, producing only water and energy when burned 1. There are various methods to produce hydrogen, with water electrolysis being one of the most notable, as it can be powered by renewable sources such as solar and wind energy. Co Ni-based electrodes are a promising option for the hydrogen evolution reaction (HER) due to their low overpotential, stability in alkaline media, and good electrical conductivity. Utilizing discarded NiMH batteries is an interesting approach, as one of their main components is nickel, adding value and preventing them from becoming pollutants. In this research, Co-Ni-based electrodes were obtained from leachates of discarded NiMH batteries, which were subsequently used to catalyze the HER. For this purpose, the leaching liquors from the batteries were recovered, and deposits were generated using the pulsed current technique (PP). This was done on carbon steel supports, employing current densities of -100 mAcm-2 and -55 mAcm-2, with charges of 6 C and 11 C, and a 50% duty cycle. The electrodes were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) to determine their morphology and elemental composition. The performance of the electrodes was electrochemically evaluated using techniques such as linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS), employing KOH as the electrolyte. The results indicated that Co-Ni-based deposits with different characteristics can be successfully applied to develop macroscopic applications of green hydrogen production.

Keywords:

Hydrogen production, Nickel, Water electrolysis, Electrodeposited nickel electrode, Electrocatalysis

Reference:

1 Chi, Jun, and Hongmei Yu. “Water electrolysis based on renewable energy for hydrogen production.” Chinese Journal of Catalysis 39.3 (2018): 390-394, https://doi.org/10.1016/S1872-2067(17)62949-8.

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RENEWABLE ENERGY / 310

GROWTH OF ZINC OXIDE NANOSTRUCTURES BY THE VAPOR-LIQUID-SOLID TECHNIQUE: EFFECT OF THERMAL TREATMENT

ON THE SEED LAYER AND CATALYST

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In this work, zinc oxide nanostructures were grown using the Vapor-Liquid-Solid (VLS) growth technique. To promote the growth of the nanostructures, a seed layer of aluminum-doped zinc oxide (AZO) and gold as a catalyst was used. This study investigates the effect of thermal treatment on the seed layer and the catalyst before to VLS growth, aiming to ensure that the seed layer and the catalyst undergo minimal changes during the initial stages of growth. As a result of the thermal treatment, changes in the morphology of both the seed layer and the catalyst were observed. If these changes occur during the initial stages of growth, they would affect the growth of the nanostructures and prevent them from growing in the same direction as the grains in the seed layer. The growth direction is crucial as it defines the morphology and the crystal planes on the surface. Additionally, displacement and fragmentation of the catalyst were observed, generating branches, except for the nanostructures where the catalyst is located on the polar planes (0002), indicating that the Au/Zn mixture has lower solubility on the polar planes (0002)

Keywords:

zinc oxide, nanostructures, crystal planes, seed laye

Reference:

Functionalization of 3-aminopropyltrimethoxysilane Self-Assembled Monolayers on ZnO/Au nanowires: Role of the Seed layer. DOI:10.1016/j.matlet.2021.129452

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RENEWABLE ENERGY / 313

Effect of WS2 Monolayer as complementary ETL in a FAPbI3-based Heterostructure

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In this work the incorporation of a monolayer of WS2 in a FAPbI3 perovskite based heterostructure is presented. FAPbI3/WS2/TiO2/ITO and FAPbI3/TiO2/ITO heterostructures were analyzed by UV-Vis spectroscopy, X-ray diffraction, scanning electron microscopy and Kelvin probe force microscopy (KPFM). The configuration with WS2 interlayer presents higher absorption in the visible region with a bandgap of ~1.44 eV. WS2 also enhances the deposition process of FAPbI3, resulting in the formation of pure photoactive α-phase. The smooth surface of WS2 favors a homogeneous morphology and an increase of the grain size to ~4.5 μm, the largest reported for similar structures. An energy band alignment between FAPbI3, WS2, and ITO is proposed based on the work function obtained by KPFM. These findings strongly suggest that the interfacial coupling of FAPbI3/WS2 could be a promising candidate in photovoltaic applications.

Keywords:

FAPbI3, WS2, perovskite solar cells

Reference:

no reference

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RENEWABLE ENERGY / 315

Bi-metallic MXenes Mo2V2C3T2 (T = O, F, OH) for energy storage devices. Atomisitics insigts on ion-adsorption process

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MXenes materials have shown good electrochemical properties for energy storage such as metallic behavior, high electrical conductivity and low energy barriers for ions diffusion. Recent studies have shown that bi-metallic MXenes, such as $Ti_2Ta_2C_3$, exhibit superior electrochemical behavior compared to monometallic counterparts, offering potential for extended lifespan in energy storage systems, as Maldonado-Lopez reports in 2022 1. This study reports the functionalization of bi-metallic MXene Mo_2V_2C_3 with O, F, and OH. Moreover, highlights the significance of bi-metallic MXenes and surface functionalization in advancing energy storage technologies, suggesting avenues for improving cycling stability and energy efficiency in next-generation energy storage devices. Our results suggest that the oxidized phase grants a better performance as anode in batteries, and the Li-ion offers a higher gravimetric capacity.

Keywords:

MXenes Materials

Reference:

Maldonado-Lopez, Daniel; et al., Atomic-Scale Understanding of Li Storage Processes in the Ti4C3 and Chemically Ordered Ti2Ta2C3 MXenes: A Theoretical and Experimental Assessment ACS Appl. Energy Mater. 2022, 5, 2, 1801−1809

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RENEWABLE ENERGY / 324

TEXTURED Al-DOPED ZnO (AZO) TCO OBTAINED VIA MAGNETRON SPUTTERING UNDER A NOVEL SOFT-DEPOSITION METHODOLOGY

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Transparent conducting oxides (TCOs) like Al-doped Zinc Oxide (AZO) are highly sought after for their unique electrical conductivity and optical transparency combination. AZO offers advantages over ITO and FTO, including processing costs, environmental and health considerations, stability, ease of processing, and versatile fabrication techniques. This work explores the viability of obtaining AZO films under soft deposition conditions via the magnetron sputtering technique. Aside from their exceptional electrical and optical properties, this research reports the obtention of textured AZO using a novel one-step sputtering method. The impact of adjusting the target-to-substrate distance (dTS), argon gas flow (FAr), and sputtering power (PW) was investigated on the ultimate characteristics of AZO films through X-ray diffraction, scanning electron microscopy, UV-vis spectrophotometry, and Hall-effect measurements. Films displaying the most favorable electrical properties (3.2x10-4 Ω*cm, 21.3 cm2 V-1 s-1, and 9.2x1020 cm-3) were produced at a FAr of 5 sccm, a PW of 45 W, and room temperature. Furthermore, AZO thin films deposited within the high-density zone (HDZ, dTS < 6 cm) of the plasma sputtering exhibited a textured surface with crater-like features, which were more pronounced in films deposited at reduced FAr (5 sccm) and low PW (45 W) values. The obtention of a textured TCO film at soft deposition parameters offers several advantages in film technology by enhancing light management (trapping and scattering), improving film mechanical and chemical stability, increasing surface area, and providing enhanced performance, which could be highly beneficial for the cost-effective production of AZO for its implementation cutting-edge optoelectronic applications such as flexible solar cells and electroluminescent devices.

Keywords:

Textured TCO, Al:ZnO, soft-deposition, sputtering,

Reference:

K. Portillo-Cortez, S.R. Islas, A. Serrano-Lázaro, et al., A novel soft deposition methodology for textured ZnO:Al thin films as efficient transparent conductive oxide layers. Applied Surface Science Advances 9 (2022) 100255. https://doi.org/10.1016/j.apsadv.2022.100255

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Author approval:

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RENEWABLE ENERGY / 16

SYNTHESIS OF BOROPHENE NANOSTRUCTURES BY ULTRASONIC EXFOLIATION AS SUPPORT OF NOBLE METAL NANOPARTICLES FOR POTENTIAL H2 PRODUCTION

Authors: Eric Fernando Vázquez Vázquez[1]; Omar Solorza-Feria[1]; Oscar Eduardo Cigarroa-Mayorga[2]

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Borophene is a relatively new material nanosheet-like and is the lightest known 2D material. As boron is a neighbor of carbon it is expected to have similar properties to this material. Borophene synthesis remains an actual challenge due to the bulk bond configurations of boron. Theoretically, a triangular network could be more stable if it has periodic holes and it can grow on metallic surfaces such as Ag (111), Au (111), Cu (111) by chemical vapor deposition (CVD).

The present work aims to synthesize borophene nanosheets by the ultrasonic exfoliation method for the further decoration with noble metal nanoparticles to increase the photocatalytic activity of the nanosheets and enhance its activity in the hydrogen evolution reaction conducted by light absorption.

Borophene was synthesized following the reported method by Fu, Y. et al in which boron powder is added into 1-Methyl-2-pyrrolidinone (NMP). This mixture is then stirred and grinded, and then sonicated with a probe-type sonicator at 600 W, with a pulse on/off of 4 s for 4 h in an ice bath. The obtained solution was sonicated in an ice bath. Then it was centrifuged, and the supernatant was separated for another centrifugation to obtain the precipitate. The synthesized boron nanosheets were washed with distilled water, ethanol and acetone to remove the NMP.

TEM shows a few-layers nanosheets of borophene and SAED indicated good cistallinity. On the other hand, noble metals NPs were synthesized by wet chemical methods to have better control over the shape and size of the nanoparticles. UV-Vis spectroscopy demonstrates typical absorption bands due to longitudinal and transverse LSPR of the synthesized noble metal nanoparticles. SEM and TEM confirmed nanospheres shape.

Keywords:

borophene, noble metals nanoparticles, hydrogen production

Reference:

Y. Fu, et al Borophene-based mixed-dimensional van der waals heterojunctions for high-performance self-powered photodetector,Applied Surface Science, Volume 611, Part A, 2023,155668.

This work was supported by:

CONAHCyT Schorlarship

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RENEWABLE ENERGY / 345

EVALUATION OF THE PHOTOCATALYTIC DECOMPOSITION OF METHYL ORANGE, USING 3 TO 1 MOLAR MIXTURES OF BISMUTH OXYBROMIDE AND OXYCHLORIDE

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Given the growing usage and consumption of water resources, humankind needs to develop relevant and economic procedures to be able cleaning and purifying used water, in order to promote its reuse and possible reintegration into the environment, as well as to prevent its contribution to further contaminate soils. One could say that such is the wider purpose for the improvement of photocatalysts' efficiency in decontamination processes. Furthermore, they could play an important role in the cost-effective production of hydrogen for energy purposes. Heterojunction photocatalysts are pertinent contenders to achieve efficient visible light mediated photocatalytic processes. In this work, it is evaluated the performance in photocatalytic Methyl Orange degradation by four BiOBr/BiOCl composites, all with a molar ratio of 3 to 1, which are compared with a $BiOCl_{0.25}Br_{0.75}$ solid solution obtained by a simple precipitation route (sample M5). Three different processing methods were used to prepare four 3:1 composite samples starting from pure BiOBr and BiOCl obtained by precipitation; one by hydrothermal treatment (M1), and one by dry milling process of the mixtures (M2), and two by precipitation of BiOY (Y: Br, Cl) in the presence of BiOX (X: Cl, Br) (M3 and M4). The hydrothermally treated sample resulted in the formation of a solid solution $BiOCl_{1-x}Br_x$ (x ~ 0.8). On the other hand, the precipitation of BiOCl over BiOBr, resulted in the diffusion of chlorine ions into oxybromide lattice; more evident than bromine into oxychloride's. Meanwhile, the manually milled sample has the presence of both pure bismuth oxyhalides, as far as XRD and Raman spectroscopy results show. The photocatalytic activity of the samples under UV illumination was comparable to that of commercial TiO2, specially for samples M5, M4 and M1; otherwise, despite poorly active under visible light, samples M3, M4, and M1 had best results.

Reference:

Opcional

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Keywords:

Composites, BiOBr, BiOCl, Photocatalysis

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RENEWABLE ENERGY / 32

Bismuth Oxyhalloys: enhanced photocatalytic performance of novel BiOXY (X, Y= Cl, Br, I) alloys.

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Photocatalysis has always been a promising alternative in the remotion of pollutants from air and water, and even for clean energy production, such as hydrogen-based fuels. Nonetheless, there is not an ultimate photocatalyst with low recombination times, high quantum efficiency, chemical stability, non-toxicity and low cost. In order to face said drawbacks, bismuth-based materials, particularly bismuth oxyhalides (BiOX, X=Cl, Br, I), have demonstrated to be suitable for this application. Their photocatalytic behavior can be enhanced by a number of techniques, including, doping, morphological modulation, facet tailoring and, alloying. In this work, it is presented the enhanced photocatalytic activity of bismuth oxyhalide alloys (BiOXY, X, Y= Cl, Br, I) on the degradation of a reference contaminant (Rhodamine B 'RhB'). These materials were synthesized by a conventional hydrothermal reaction (160 ℃, 12 h, pH=2) using as reagents bismuth nitrate (Bi(NO3)3) and halogen salts (KCl, KBr, KI) in a stoichiometric ratio of 1:1. Characterization of the samples was performed by X-Ray diffraction (XRD), Diffuse Reflectance Spectroscopy (DRS), Volumetric Absorption of N2, and Scanning Electron Microscopy (SEM). The photocatalytic activity was measured by the diminution of the characteristic peaks of the absorption spectra of the contaminant as function of time. The obtained samples showed solid solution structures except for the Cl-I system due to difference between their ionic radii. The photocatalityc performance increased significantly in comparison to simple BiOX catalysts.

Keywords:

Bismuth oxyhalides, photocatalysis, solid solution, alloying, catalyst.

Reference:

R. Lu., A. H. Zahid, & Q. Han, Insight into the Photocatalytic Mechanism of the Optimal x Value in the BiOBr. Nanoscale 14(37). (2022). 13711-13721. https://doi.org/10.1039/D2NR03726B

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RENEWABLE ENERGY / 33

EXPLORING THE POTENTIAL OF H-Zn2GeO4 AS AN LI-ION HOST

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The demand for eco-friendly and efficient energy sources in industrial, portable, and wearable applications has driven extensive research into electrochemical storage devices. The lithium-ion batteries emerge as highly promising due to their exceptional physicochemical and electrochemical properties. To further enhance lithium-ion battery performance beyond conventional graphite-based anodes, there is ongoing exploration of advanced nanomaterials with specific chemical compositions and crystalline structures capable of facilitating reversible and rapid conversion and alloying reactions, thus enabling superior Li-ion storage capacity 1. In this context, our study focuses on employing hexagonal Zn2GeO4 nanoparticles as a Li-ion host material. The synthesis of h-Zn2GeO4 in a willemite-like phase is done by using the facile Pechini method. the charge-discharge curves show that the h-Zn2GeO4 delivers a specific capacity of 900 mAh/g with a Coulombic efficiency of 97%. The experimental analyses were complemented by computational simulations using Density Functional Theory (DFT) and Ab Initio Molecular Dynamics (AIMD) to delve into atomic-scale interactions between Li ions and the h-Zn2GeO4 crystal structure. The results evidence the chemical reactions observed in the experiment; besides the theoretical gravimetric capacity is 1400 mAh/g in agreement with experimental measurements.

Keywords:

Li-ion battery, DFT calculations, anode material, Zn2GeO4

Reference:

1 Chen, X., Ma, B., Li, W., Zhang, Y., & Tang, Y. (2014). ChemInform Abstract: Rational Material Design for Ultrafast Rechargeable Lithium-Ion Batteries. https://doi.org/10.1039/c4cs00442f

This work was supported by:

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RENEWABLE ENERGY / 39

EXPLORING PHOTOCATALYTIC ACTIVITY OF BISMUTH OXYHALIDES BIOX (X= CL, BR, I) ON DEGRADATION OF EMERGING POLLUTANTS

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The auge of semiconductors in the second half of the 20th century brought a fast and without precedent technological advancement, characterized by high-speed communications and faster and more efficient processing devices. All this, was powered by already known semiconductors like silicon, germanium, and metal oxides, but also by novel and outstanding materials like the well-known families of II-VI, III-V semiconductors and alloys like mercury-cadmium telluride (HgCdTe). Elements like As, Hg, Cr, Te and so on were released without control to the environment and some highly contaminant semiconductors continue being produced. To mitigate this situation, alternative materials and techniques are employed to solve energetic and pollution issues, this is the case of bismuth-based materials and photocatalysis. Bismuth oxyhalides (BiOX, X=Cl, Br, I) are known for their ability to remove conventional pollutants due to their interesting properties including, a layered structure, band gap modulation, visible light absorption, suitable band edges potentials and cheap production methods. In this work, we explore the photocatalytic activity of BiOX on the degradation of harmful emergent contaminants such as ibuprofen and ciprofloxacin. The synthesis of these photocatalysts was achieved by a conventional solvothermal reaction varying solvents used. Bismuth and halogen sources were bismuth nitrate (Bi(NO3)3) and potassium salts (KCl, KBr, KI) in molar ratio of 1:1. Samples were characterized by X-Ray Diffraction (XRD), Diffuse Reflectance Spectroscopy (DRS) and Volumetric Absorption of N2. The photocatalytic activity was performed by measuring the absorption spectra of a of common dye (Rhodamine B 'RhB') solution in order to find a relationship between solvent used and catalytic properties. The samples with the best performance on RhB were tested on ibuprofen and ciprofloxacin. Results indicated that BiOX removed approximately 40 % of ibuprofen in 240 minutes, and ciprofloxacin about 60 % in the same time.

Keywords:

bismuth oxyhalides, photocatalysis, emerging pollutants, solvothermal synthesis, water treatment

Reference:

H. Zhang, L. Liu, and Z. Zhou, Towards better photocatalysts: first-principles studies of the alloying effects on the photocatalytic activities of bismuth oxyhalides under visible light, Physical Chemistry Chemical Physics (2012) 1286-1292. https://doi.org/10.1039/c1cp23516h

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RENEWABLE ENERGY / 353

Synthesis and electric characterization of the thermoelectric materials Bi0.5Sb1.5Te3 and Bi1.5Sb0.5Te3 alloys

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Co-authors: Angel Eduardo Cerda-Frutis [2]; Francisco Gómez-López [2]; Misha Jessica Del Castillo-Aguirre [2]; Sergio Armando Tomás Velázquez [3]; Usiel Omar Garcia Vidal [2]

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Energy is likely to be the major scientific challenge in decades to come. The solution to the climate and environmental problems rests on a concerted effort to broaden our energy resources. New and improved functional materials are important components in efforts to effectively harvest energy from alternative energy sources, and to use the available energy more economically and environmentally friendly. One alternative energy source can be thermoelectric devices, which represents a clean energy. They are able to generate electrical energy from the waste heat, which is produced by computers, factories, household appliances, etc.
In this work we present the synthesis of Bi2-xSbxTe3 and BiTe3-xSex, as well as electric charecterization.

Keywords:

SPS, Thermoelectric Materials, Coefficient Seebeck

Reference:

Bed Poudel, Science 320, 634 (2008)

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RENEWABLE ENERGY / 41

Impact of Metallic Contact Selection on the Efficiency of Sb2S3/CdS Solar Cells

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Solar cells are essential for the transition to renewable energy, enabling the direct conversion of sunlight into electricity through the photovoltaic effect. In this context, the efficiency of the cells is crucial, and metal contacts play an essential role in optimizing their performance. These contacts extract and conduct the generated electrons, significantly influencing the efficiency and stability of the cell. The featured study examines the impact of various metal contacts on Sb2S3/CdS-based cells, highlighting how the proper choice of these materials affects the device's effectiveness. Electrical characteristics such as open-circuit voltage (Voc), short-circuit current (Jsc), fill factor (FF), and efficiency (η) were evaluated using the SCAPS simulation tool. Metals such as Silver (Ag), Iron (Fe), Silicon (Si), Molybdenum (Mo), Tellurium (Te), Beryllium (Be), Cobalt (Co), Gold (Au), Tungsten (W),

Nickel (Ni), and Platinum (Pt) were selected based on their work functions, which are compatible with the Sb2S3/CdS heterojunction. This compatibility facilitates better extraction and transport of charges. The metals were chosen according to values suggested by flat band alignment calculations. The results showed that platinum contacts, with an efficiency of 30.29%, improve efficiency by 15% compared to silver, which has an efficiency of 14.32%. This underscores the importance of meticulous selection of metal contacts. These findings highlight how careful choice and optimization of metal contacts can significantly improve the efficiency of solar cells, contributing to the economic and technological viability of solar energy and promoting the development of more sustainable energy technologies.

Keywords:

solar cells, metallic contact, scaps 1D

Reference:

Numerical Simulation and Performance Optimization of a Solar Cell Based on WO3/CdTe Heterostructure Using NiO as HTL Layer by SCAPS 1D. José Carlos Zepeda Medina, et al. Coatings, 13, 1436 (15 de agostos 2023).

This work was supported by:

Benemérita Universidad Autónoma de Puebla

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RENEWABLE ENERGY / 358

DESIGN, SIMULATION AND CONSTRUCTION OF A HELICAL SAVONIUS ROTOR FOR POWER GENERATION IN RURAL HOUSING

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In this work a detailed study of a helical Savonius rotor (HSR) was investigated to obtain the optimal characteristics for the generation of renewable energy. The designed and assembly of the HSR was developed in a CAD software. Simulations of the interaction between the flow of air and the HSR blades were developed through finite element analysis. Results of these simulations shows the velocity distribution of the profile designed blades. In the same way, it was obtained the profile pressure due the velocity's profiles. The formations of vortices were studied with the finality to improve the performance in the HSR. Simulations results show the best geometry to optimize the power coefficient (Cp) in the HSR. From the simulation results it was built a prototype Savonius wind rotor at scale and probe in a wind tunnel according to simulation done; field tests will be performed to check the amount of energy obtained with the changes implemented.

Keywords:

wind energy, power coefficient, off-grid system, energy storage.

Reference:

R. D. Maldonado, E. Huerta, J. E. Corona, O. Ceh, A. I. León-Castillo, M. P. Gómez-Acosta, E. Mendoza-Andrade, Energy Procedia, 57 (2014) 691 –697.

This work was supported by:

UNIVERSIDAD ANAHUAC MAYAB

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RENEWABLE ENERGY / 42

Numerical simulation of a solar cell based on a double CdTe/FeSi2 absorber layer and an AZO window layer with an efficiency of 26.34 %

Author: Enrique Rosendo Andrés[1]

Co-authors: Crisóforo Morales Ruíz [1]; Eduardo Camacho Espinosa [2]; José Carlos Zepeda Medina [1]; Leticia Treviño Yarce [1]; Reina Galeazzi Isasmendi [1]; Román Romano Trujillo [1]

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Solar Cell simulation serves to reduce the number of work hours and optimize the resources dedicated to carrying out experiments. Simulation of solar cells based on AZO as window layer, cadmium telluride (CdTe) like first absorber layer and FeSi2 like second absorber layer with the structure (Al/AZO/CdTe/FeSi2/Ni) using the Cell Capacitance Simulator solar-1D (SCAPS-1D) has been carried out. The effect of the thickness and carrier concentration of the first and the second absorber layer was studied. The thickness and concentration of carriers for the CdTe layer varied from 0.4 to 1 µm and from 〖10〗^13 to 〖10〗^15 cm^(-3) respectively, it was found that PCE decreases 0.22% with increasing thickness. The thickness and concentration of carriers in the second absorber layer varied from 0.1 to 1 µm and from 〖10〗^14 to 〖10〗^18 〖cm〗^(-3), respectively. It was observed that by increasing the thickness of the FeSi2 layer from 0.1 to 1 µm, PCE increased by 7.66%, while by increasing the concentration of carriers from 1014 to 1018 cm-3 in this layer, PCE increased by 2.81%. It was also observed that by increasing the defect density at the FeSi2/CdTe interface from 1010 to 1017 cm-2, PCE decreased by 22.1%. Finally, a maximum power conversion efficiency (PCE) of 26.34% is achieved with an open circuit voltage (Voc) of 0.62 V, short circuit current density (Jsc) of 51.43 mA/cm^2 and a fill factor (FF) of 82.24 %, obtained with a thickness and concentration of carriers of 1 µm and 〖10〗^18 〖cm〗^(-3) for the FeSi2 layer and for the CdTe layer the thickness and concentration of carriers was 0.4 µm and 〖10〗^15 cm^(-3), respectively. The above results provide design guidelines for a solar cell based on two absorber layers CdTe and FeSi2 and window layer of AZO with high efficiency.

Keywords:

solar cells simulation, two absorber layer, SCAPS-1D

Reference:

Performance simulation of solar cell based on AZO/CdTe heterostructure by SCAPS 1D software. José Carlos Zepeda Medina. Heliyon, 9 (marzo 2023) e14547

This work was supported by:

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RENEWABLE ENERGY / 45

Microplastic removal from Water Using Biodegradable Green Solvents

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Microplastics (MP) are tiny plastic particles (<5mm in size), that come from various sources, including synthetic textiles, tires, cosmetics, fragmentation of larger plastics (bottles, food containers, pvc pipes, etc.) and industrial processes. These complex compounds have become a mayor environmental concern due to their widespread presence and potential risk to human health and organisms1. Many attempts have been made to address this issue, technologies such as membrane filtration systems, electrocoagulation, plastic-eating enzymes, etc., offer unique approaches for the removal of microplastics, yet still face obstacles like high costs, limited scalability, environmental consequences, partial removal efficiency, and generation of more waste as filters have life cycles1. Additionally, microplastics are complex molecules, posing significant challenges for detection and complete elimination due to their small size and diverse composition, making it difficult to develop solutions to address the issue. Therefore, this work assesses said problematic by employing green solvents (GS) derived from renewable sources, as an eco-friendly alternative for microplastic in water pollution control. By harnessing the low toxicity, biodegradability, versatility and compatibility, GS can mitigate the environmental impact of microplastics pollution. In this work, two decanoic-based GS were synthesized, characterized and evaluated on the removal of PET (Polyethylene terephthalate) and Polyesterene (PET), and a mixture of both. The removal process was assessed using UV-Vis spectroscopy and infrared spectroscopy techniques. Overall results revealed a remarkable 99% removal of PET/PS mixture within 180 min. Total Organic Carbon measurements were also conducted to assess microplastic removal efficacy and to detect any potential contamination from the GS into the solution. This study demonstrates the effectiveness of GS in removing PET, PS and mixtures, achieving significant removal rates in short timeframes, confirming the potential of GS as promising solutions for microplastic pollution mitigation, promoting ecosystem health and contributing to a more sustainable management of our natural resources

Keywords:

Microplastics, Green solvents, Water Pollution, Emerging contaminants, Environmental remediation

Reference:

1 Iyare, Paul U., Sabeha K. Ouki, and Tom Bond. "Microplastics removal in wastewater treatment plants: a critical review." Environmental Science: Water Research & Technology 6.10 (2020): 2664-2675.

This work was supported by:

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RENEWABLE ENERGY / 51

EFFECT OF PH ON THE STRUCTURAL, OPTICAL AND MORPHOLOGICAL PROPERTIES OF COPPER SELENIDE THIN FILMS DEPOSITED BY CHEMICAL BATH DEPOSITION

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Co-authors: Anai Zavala Franco [2]; Edgar Arturo Chávez-Urbiola [3]; Iker Rodrigo Chávez Urbiola [4]; Pavel Vorobiev [5]; Yurii Vorobiev [2]

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Abstract
Copper selenide thin films (Cu2-xSe) were deposited onto soda lime glass via chemical bath deposition technique using our free ammonia process at different pH values ranging from 6.3 to 8.3. The thin films obtained were characterized by XRD, SEM, EDS and UV-Vis spectroscopy. It was found that the morphological and optical properties of the films were directly influenced by the pH conditions: the optical bandgap exhibited a blue shift from 1.91 to 2.15 eV and the crystallite size increased from 63 to 90 Å with increasing pH. Additionally, the stoichiometry Cu/Se ratio increased from 1.57 to 1.87, resulting in the formation of Cu1.87Se. This formation did not require high temperatures or any gas to modify the atmosphere, such as in the sputtering technique. Thus, the thin films obtained of Cu1.87Se only by modifying the pH represent a cost-effective option for use as solar cells.

Keywords:

pH effect, ammonia-free, CBD

Reference:

1 Nathan, A., Kumar, A., Sakariya, K., Servati, P., Sambandan, S., & Striakhilev, D. (2004). Amorphous silicon thin film transistor circuit integration for organic LED displays on glass and plastic. IEEE Journal of solid-state circuits, 39(9), 1477-1486.

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RENEWABLE ENERGY / 359

Construction of a Hybrid Photovoltaic System Connected to an Air Conditioner and Utilization of Wind and Solar Light Reflection for Cooling an Enclosed Space

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The main objective of the research is to design a closed space
and project the necessary modifications to decrease its temperature and reach a suitable temperature for human comfort through wind, reflection of sunlight, and an air conditioning unit solely for cooling, powered by electricity from solar panels. To achieve this objective, an air conditioning unit is selected that can decrease the temperature within the working volume. Additionally, solar panels with a performance greater than 16% and a solar charge controller are determined to supply the electrical energy required by the air conditioning unit.Photovoltaic application batteries and a solar power inverter are also selected for the storage and conditioning of the electrical charge from the solar panels. To develop this system,studies were conducted using solar atlases from the National Aeronautics and Space Administration and various wind databases to understand the environmental characteristics of the working area (Northern Zone of Mexico City).
An On/Off control is developed for the energy system, programmed on ARDUINO UNO, which allows us to switch the electrical supply from the solar panels to the grid distribution system used as a final backup for electrical energy after the batteries. Additionally, a simulation of the photovoltaic energy system is performed with each of the selected components to verify the system's functionality (Matlab Simulink student version). It is stated that the temperature difference generated by the air conditioning unit, with the help of the characteristics of the enclosed space, ranges from 3.5℃ to 4.5℃ within a timeframe of 20 to
30 minutes, and 6 to 10 minutes in cases where the intermediate wall was used.

Keywords:

Electrical energy, Solar panels, Temperature reduction

Reference:

Y. Li, G. Zhang, G.Z. Lv. (2015, mayo). "Performance study of a solar photovoltaic air
conditioner in the hot summer and cold winter zone". Institute of Refrigeration and Cryogenics.China.

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RENEWABLE ENERGY / 60

Ink-jet perovskite films for photocatalytic CO2 reduction and H2O decomposition

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Perovskite materials are one of the most promising photocatalysts for generating clean, energetic vectors and solar fuels. One of the main barriers to its massive production is the high cost and complicated deposition techniques. As an alternative, this work sought solutions to manufacture large-area printed films with high-throughput rates and minimal waste by ink-jet printing. This technology promoted the formation of crystalline and porous films with heterogeneous morphology, which absorb UV and Visible light. Two sets of perovskites were explored based on oxides: ABO3 (A=Na, Li, K, B=Na, Nb) and halides: KMgI3, which were evaluated as photocatalysts in the H2O and CO2 reduction to produce energetic vectors and solar fuels, respectively. The energy conversion efficiency was calculated to verify the efficiency of the studied systems, reaching values up to 7%. Furthermore, the stability and reuse of the perovskite ink-jet films were demonstrated after consecutive cycles of photocatalytic evaluation.

Keywords:

Perovskites, Ink-jet printing, CO2 reduction, H2O splitting, Photocatalysis, Solar fuels.

Reference:

Fuel 320 (2022) 123934.
Materials Letters 361 (2024) 136066.

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RENEWABLE ENERGY / 46

USE OF AGROINDUSTRIAL WASTE TO OBTAIN GRAPHENE OXIDE FOR VARIOUS APPLICATIONS

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Graphene oxide (GO) is a useful and promising carbon nanomaterial for applications in electronics, optics, chemistry, energy storage, and biology. Due to the presence of hydroxyl, carboxyl, and epoxy functional groups in the basal and edge plane of GO, this material is easily dispersed in aqueous solvents, which makes it more convenient to process and use. GO is usually obtained by the Hummers´

method by oxidizing graphite, in which a considerable volume of strong acid residue is generated. For this reason, currently the use of green chemistry in nanomaterials research aims to decrease and eliminate the presence of toxic and polluting compounds during GO synthesis. The use of peanut and coffee crop residues to produce nanomaterials can be an alternative for their final disposal, thus obtaining a value-added product in different science areas.
In the present work, we produced GO through pyrolysis of different agro-industrial wastes, which are: peanut shells, post-use commercial, and artisanal coffee, and were compared with GO produced by the Hummers method. Subsequently, GO from different materials was functionalized with magnetite by chemical coprecipitation for use as a catalyst. The functional groups present in the obtained nanomaterial are used as nucleation centers for the formation of metal oxides. Therefore, a higher number of functional groups present on the surface will lead to the formation of metal oxide nuclei, obtaining metal oxide nanoparticles with good dispersion on GO films for energy and environmental applications such as biofuel generation, adsorptive removal of dyes in water and antimicrobial activity in wastewater treatment plants.

Keywords:

Graphene oxide, agro-industrial wastes, nanoparticle, renewable, magnetite

Reference:

Somanathan, T., Prasad, K., Ostrikov, K., Saravanan, A., & Krishna, V. (2015). Graphene Oxide Synthesis from Agro Waste. Nanomaterials, 5(2), 826–834. MDPI AG.

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RENEWABLE ENERGY / 52

Optimization of ZnO nanorods thin film photocatalyst for hydrogen production

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To avoid ZnO photo-corrosion, In-doped ZnO nanorods were grown using the chemical bath deposition technique, varying the In concentration (0.5, 0.75, and 1 mol%). The increase in the indium load enhanced the photocatalytic activity in the hydrogen production, evolving ten times more hydrogen in the ZnO-NRD/1-In (1% In) sample. Unfortunately, after the recyclability cycles (three cycles), the ZnO-NRD/1-In film decreased its photoactivity by 90%, and the ZnO-NRD/0.5-In film (0.5% In) kept constant its gas evolution, evidencing stability. This decrease in the photocatalytic efficiency in the samples with larger load of In could be associated with the presence of In3+ species, which can act as electron scavengers that trap electrons in the ZnO CB and form oxidant species, causing the ZnO photo-corrosion. Finally, the photocatalytic stability of ZnO-NRD/0.5-In film (0.5% In) was tested for 72 hours, reaching a maximum hydrogen evolution at 48 h (up to 90 µmol). Despite this, during the third day of the irradiation, the hydrogen production did not increase, possibly due to a loss in the film surface caused by the turbulence in the reaction media. Additionally, after 72 hours

of irradiation, it is possible to observe the presence of In over the film surface (EDS results), while the XPS results show that the film has the presence of In3+ species, which could contribute to the photocatalyst deactivation, decreasing the hydrogen production of the film.

Keywords:

ZnO nanorods, photocorrosion, hydrogen production, photocatalysis.

Reference:

M. R. Alfaro Cruz, L. F. Garay-Rodríguez, Leticia M. Torres-Martínez, Analysis of the photocatalytic efficiency of ZnO–ZnO nanorods films deposited by two-step chemical methods in hydrogen generation, J Sol-Gel Sci Technol 103 (2022) 267–279.

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RENEWABLE ENERGY / 165

GREEN SYNHTESIS OF COBALT-BASED METAL-ORGANIC FRAMEWORK AND ITS POSSIBLE USE AS SUPERCAPACITOR ELECTRODE

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Metal-organic networks (MOF) are crystalline materials characterized by the coordination of metal centers with organic ligands. This class of material stands out for its properties such as high specific surface area, porosity and easy functionalization. The field of application of MOFs has ranged from gas separation/storage, adsorption/desorption of toxic gases and vapors, catalysts, drug delivery to, recently, their use as electrocatalysts for hydrogen production, as electrodes in Li-ion batteries, and in supercapacitors. However, the synthesis of MOFs often involves the use of aggressive and polluting solvents (DMF, ethanol, etc.). The use of water as a solvent in the synthesis and purification of MOFs is an attractive strategy for the reduction of pollution caused by the processing of these materials. In this work, we synthesized a Co-based MOF using only water as solvent and purified the product. Co-MOFs exhibit high electrochemical reversibility, a feature that is not common in MOF materials. Taking advantage of this feature, together with its structure, especially its redox centers, we studied this material for its application as a supercapacitor electrode.

Keywords:

Metal-organic frameworks; supercapacitor; Co-MOF; green-synthesized; electrode

Reference:

Yang J, Xiong P, Zheng C, Qiu H, Wei M. J Mater Chem A Mater. 2014;2(39):16640-16644.

This work was supported by:

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RENEWABLE ENERGY / 96

STUDY OF PHYSICOCHEMICAL PROPERTIES OF BIO-OIL

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One way to give new life to vegetal residues, which lead to pollution or take a long time to degrade, is using them as raw materials to obtain biomaterials and methane that can be used in several ways, reducing the degradation time. On the other hand, citrus is a highly consumed product worldwide with an estimated market of 28 billion US dollars, whereas orange stands out from it. In this work, orange residues, locally obtained, were mixed with water in a 1:1 ratio. Water acts as a fatty acid catalyzer. The hydrothermal conversion process is as follows: the mixture is heated from 180° to 290° C using a 5 MPa pressure. An aqueous solution is obtained with solid and liquid fractions. The liquid fraction containing fatty acids is then obtained by filtering, resulting in bio-oil. It is important to know its characteristics, such as absorption spectrum, thermal properties, and biochemical parameters, to know beforehand if the bio-oil obtained from the reactor is suitable for various uses. Some of the features obtained from the bio-oil are PH=3.36 (considered acid), total solids =2.57, volatile solids=78.68, total chemical oxygen demand =57.28, soluble chemical oxygen demand =51, ash of 17.37 and moisture of 97.42%. With thermal parameters thermal effusivity=1561 Ws^1/2/ mK, ρ= 0.001026985 Kg/m^3 and an absorption spectrum where the higher absorption is observed in the ultraviolet region. Therefore, the bio-oil can be used as fertilizer, feed for bioreactors, or extract fatty acids by various methods, and it has a high aroma.

Keywords:

Bio-Oil, Thermal properties, Biochemical, Hydrothermal conversion

Reference:

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RENEWABLE ENERGY / 360

SYNTHESIS AND CHARACTERIZATION OF HOLLOW Co Fe2 O4 MICROSPHERES WITH POTENTIAL APPLICATION IN ENERGY HARVESTING

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Co-authors: Antonio Serguei Ledezma Pérez [1]; Arxel de León Santillán [1]; Carmen Natividad Alvarado Canche [1]; Juan Carlos Anaya Zavaleta [1]

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Energy harvesting technologies have attracted considerable attention today. Various nano or microgenerators based on piezoelectric, triboelectric, and electromagnetic effects are becoming popular to design and realize many self-powered applications (1). Electromagnetic generators (EMG) offer numerous advantages, including possible architectures and nanostructured materials for device fabrication.
In this work, the synthesis of hollow CoFe2O4 microspheres was carried out using carbon microspheres as sacrificial structures. The synthesis was carried out in three steps. The first step is the hydrothermal synthesis of carbon microspheres from anhydrous dextrose, and the second step is the incorporation of the precursor salts of cobalt ferrite (2Fe(NO3)3·9H2O + Co(NO3)2·6H2O) in the presence of the carbon microspheres subjected to a solvothermal method for 15 hours with a controlled temperature of 150 ◦C, finally, the hollow microsphere is obtained from the calcination of the sacrificial structure in a muffle with a heating ramp of 1 ℃/min until reaching 500 ℃. The temperature is maintained for 4 h. The morphological characterization of the microsphere was done by scanning electron microscopy (SEM), observing spheres with average diameters of 4 μm, consistent with the sizes of the sacrificial structures. Regarding the magnetic nature of the cobalt ferrite microspheres, a remanent magnetization of 2.85x10-3 emu and a coercivity of 32.5 Oe were achieved, typical values of a ferromagnetic material.

Keywords:

Co Fe2 O4, energy harvesting, hollow microspheres, synthesis, characterization

Reference:

(1) Oh, Y., Sahu, M., Hajra, S. et al. Spinel Ferrites (CoFe2O4): Synthesis, Magnetic Properties, and Electromagnetic Generator for Vibration Energy Harvesting. J. Electron. Mater. 51, 1933–1939 (2022). https://doi.org/10.1007/s11664-022-09551-5

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RENEWABLE ENERGY / 98

CHARACTERIZATION OF INDIUM-DOPED ZNO FILMS DEPOSITED BY ROOM TEMPERATURE SHAVINGS REACTIVE MAGNETRON SPUTTERING (SRMS) FOR PHOTOVOLTAIC APPLICATIONS

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The finding for new low-toxicity materials to be used in photovoltaic devices is of great importance to meet the energy demand without harming the environment. In recent years, CdTe/CdS solar cells have attracted much attention due to the remarkable increase in efficiency from 16% to 22% [1,2]. Recent studies show that the CdS film has a parasitic absorption, which does not contribute to the photocurrent of the cell and has its toxicity as a drawback. Therefore, it is proposed to search for new n-type materials that can be coupled to the heterostructure of cells with CdTe. In this work, suitable conditions for the deposition of IZO thin films were found by applying a new methodology called shavings-reactive-magnetron sputtering (SRMS) at room temperature. This procedure consists of placing metal chips on a base target, thus varying the concentration of the deposited films, and it is advantageous compared to other methods because it allows the deposition of ternary materials without the need to fabricate or use different targets. The structural, morphological, optical and chemical properties of the obtained IZO films were investigated. XRD and RAMAN results show that with increasing indium concentration the ZnO structure is lost and the ternary compound Zn2In2O5 starts to form. In addition, XPS confirms that the IZO films are composed of the ternary compound Zn2In2O5.The obtained IZO films have a uniform and smooth surface with roughness (~1-2 nm) and bandgap from 3.02 to 2.82 eV. Finally, the high transmittance obtained from the IZO films (99% of λ= 450-530 nm) shows that their application as a window layer in photovoltaic applications is possible.

Keywords:

Thin film, sputtering reactive, window-layer, IZO, TCO

Reference:

Gupta, A., Parikh, V. and Compaan, A.D. (2006) 'High efficiency ultra-thin sputtered CdTe solar cells', Solar Energy Materials and Solar Cells, 90(15), pp. 2263–2271. Available at: https://doi.org/10.1016/j.solmat.2006.02.029.

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RENEWABLE ENERGY / 102

ZnO photocatalytic spheres obtained by Thermal oxidation of metallic Zn

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In recent years, photocatalytic materials based on semiconductor metal oxides have been extensively studied due to their vast potential in applications such as environmental remediation and protection, including air purification, disinfection, and water purification, as well as the destruction of harmful

compounds, etc. Among all photocatalytic oxides, TiO2 and ZnO stand out because they are excellent photocatalytic materials with high photosensitivity, no toxicity, and a large bandgap. Although TiO2 is universally accepted as a very good photocatalyst, ZnO is a very good alternative because it has a very similar bandgap and is low cost. Additionally, it has been reported that ZnO possesses better quantum efficiency and higher photocatalytic activity than TiO2. Furthermore, ZnO can be fabricated with numerous nanostructured morphologies such as wires, rods, tubes, sheets, columns, hedgehog-like structures, etc.
In the present work, the thermal oxidation of metallic Zn spheres is carried out with the intention of obtaining ZnO photocatalytic spheres. A Raman study is conducted to determine the times and temperatures at which the wurtzite phase of ZnO is obtained. Different obtained morphologies were studied using Scanning Electron Microscopy (SEM), as well as an elemental analysis using EDS to determine the purity of the obtained material.

Keywords:

ZnO, thermal oxidatiom, Raman Spectroscopy

Reference:

J. Y U, and X. Y U; Hydrothermal Synthesis and Photocatalytic Activity of Zinc Oxide Hollow Spheres; Environ. Sci. Technol. 2008, 42, 4902–4907; DOI: 10.1021/es800036n

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RENEWABLE ENERGY / 141

INFLUENCE ON DEPOSITION CYCLES OF AG-DOPED ZNO THIN FILMS PREPARED BY THE SILAR METHOD AND THEIR ANALYSIS IN PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE.

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Zinc oxide thin films as semiconductor catalysts have been studied recently due to the promising treatment of contaminated water, mainly from industrial wastes. The present work studies the influence of SILAR deposition cycles of Ag-doped ZnO thin films on glass substrates for the degradation of methylene blue under UV-Vis light irradiation. This method involves immersing a substrate in different cationic and anionic precursor solutions, resulting in a deposition cycle. ZnSO4, AgNO3, and NH4OH were used as cationic precursors, and hot deionized water at 90 ℃ was used as an anionic solution. The obtained Ag-doped ZnO thin films experienced a thermal treatment to remove

moisture and homogenize the surface. Structural, optical, morphological, and electrical properties were analyzed using X-ray diffraction (XRD), Ultraviolet-Visible Spectroscopy (UV-Vis), Scanning Electron Microscopy (SEM), and I-V measurements, respectively. The photodegradation analysis of methylene blue using Ag-doped ZnO thin films was executed by considering different SILAR deposition cycles.

Keywords:

Photodegradation, methylene blue, zinc oxide, sustainability.

Reference:

M. Khiari, M. Gilliot, M. Lejeune, F. Lazar, and A. Hadjadj, (2021). "Effects of ag nanoparticles on zinc oxide photocatalytic performance,"Coatings, vol. 11, no. 4, pp. 0–15, doi: 10.3390/coatings11040400.

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RENEWABLE ENERGY / 139

INTERACTION OF LASER PULSES IN LASER SCRIBING PROCESSES FOR APPLICATIONS IN PHOTOVOLTAIC AND ELECTRONIC DEVICES BASED ON CDTE AND CIS

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This work presents a study and analysis of laser scribing processes in thin-film semiconductor materials such as SnO2: F, CdTe and CIS, with possible applications in photovoltaic and electronic devices. The process carried out is with an Nd: YAG laser system that operates at a wavelength of 532 nm at a frequency of 50 Hz, the way in which laser scribing is done is with a pulse system mode, where only 1 pulse is emitted at a certain power. Due to the characteristics of the laser system, the only parameter modified for these experiments was the power of the pulses emitted and the number of pulses in each area in each of the materials. With the experimental processes carried out, profiles of each of the damages caused by the laser pulses are obtained in a superficial way, as well as profiles where the width and depth of the same damage is observed in each of the SnO2: F, CdTe and CIS materials. As a result, laser scribing processes are associated with a laser-material interaction in which surface damage is presented in each of the materials, which are associated with the values of power, fluence, energy densities that were used, an analysis is also made regarding the amount of ejected material with respect to the energy used in each of the materials. Other factors that are analyzed are the thermal and stress phenomena present in laser scribing processes. The characterizations that support the results of this work are based on profiles obtained by profilometry, 3D profilometry, optical microscopy, SEM and EDS.

Keywords:

Laser scribing, Thin films, Laser pulse, CdTe

Reference:

Wang, H., Hsu, S., Tan, H., Yao, Y. L., Chen, H., and Azer, M. N, Predictive Modeling for Glass-Side Laser Scribing of Thin Film Photovoltaic Cells, OCTOBER 2013, Vol. 135 / 051004-1. https://doi.org/10.1115/1.4024818

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RENEWABLE ENERGY / 361

LASER SCRIBING OF Sb2Se3 THIN FILMS FOR PHOTOVOLTAIC APPLICATIONS

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Sb_2Se_3 is a promising absorber material for photovoltaic applications due to its band-gap value (~ 1.2 eV), strong optical absorption, simple phase and composition, and earth-abundant and non-toxic constituents, reasons why Sb_2Se_3 has emerged as a potential candidate to be incorporated as high-efficiency and low-cost absorber material in thin film solar cell technology. The Sb_2Se_3 based solar cells has the possibility of its cells being interconnected in series by the laser scribing technique using 3 laser scribes steps called P1, P2 and P3 that are carried out in a sequential process by depositing each of the thin films that constitute the cell solar.
In this work, the P1 and P2 laser scribes steps were implemented in the structure glass/SnO2:F/Sb_2Se_3 using a 532 nm pulsed laser. Parameters such as laser energy, pulse repetition frequency and spot overlap percentage were optimized to obtain suitable channels for the electrical interconnection of Sb_2Se_3 solar cells. The resulting laser scribes were evaluated by optical microscopy, UV-VIS spectroscopy, profilometry, composition analysis and electrical conductivity measurements, thus validating the quality of the P1 and P2 processes.

Keywords:

Sb2Se3, P2 laser scribing steps, 532 nm laser, solar cells.

Reference:

N/A

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RENEWABLE ENERGY / 144

PROCESSING OF INDIUM SULFIDE AND CADMIUM SULFIDE THIN FILMS BY SPUTTERING-RF AT OXYGEN ATMOSPHERE FOR APPLICATIONS IN OPTOELECTRONICS DEVICES

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Co-authors: Adán Fierro [2]; Gerardo Contreras [2]; Jorge Aguilar [2]; Jorge Sastré [2]; Rogelio Mendoza [3]

[1] *Instituto Politécnico Nacional*

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One of the important physical properties to consider in a semiconductor window is the value of its band-gap Eg. In2S3 and CdS have typical Eg of the order of 2.42 and 2.62 eV, respectively; that is, their absorption window is in the visible light region. In this work, different configurations of these semiconductors were processed by means of the processing technique Magneto-Planar Cathode Sputtering in Radio Frequency mode (Sputtering-RF) in an Ar+O2 atmosphere, such as: In2S3/CdS, In2S3 :O2/CdS, In2S3/CdS:O2 and In2S3:O2/CdS:O2; with the purpose of studying the change in the optoelectrical properties of these window Semiconductors. In2S3 and CdS semiconductors, when deposited together sequentially in Sputtering-RF in an Ar atmosphere with the parameters: RF source power (Pot = 150 and 100 W, respectively), substrate temperature (Ts = 250 and 225 ℃, respectively) and deposition pressure (P = 10 and 12.5 mTorr, respectively), has a thickness of approximately 150 nm (In2S3 = 50 nm and CdS = 100 nm) and an average deposition rate of approximately 6 nm/min; whereas, when these same semiconductors are deposited in an O2 atmosphere with a flux of 1.0 sccm (5% of the total Ar+O2 flow entering the deposition chamber, approximately). As results we obtained that the mentioned configurations and with these same deposition parameters; the thickness decreases around 125 nm (average deposition rate of 5 nm/min); as well as other optical and morphological changes, such as: the absorption window is shifted towards the UV region (370 nm), for the In2S3 :O2/CdS:O2 configuration; attractive properties for the mentioned applications.

Keywords:

Window materials, Thin films, Sputtering-RF

Reference:

Materials Research Express
Inclusive Publishing Trusted Science, find out more.

Purpose-led Publishing, find out more.

Incorporation of an efficient β-In2S3 thin film as window material into CdTe photovoltaic devices Mater.Res.Express6(2019)125510 https://doi.org/10.1088/2053-1591/ab5508

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RENEWABLE ENERGY / 174

PHOTOCATALYTIC DEGRADATION OF RHODAMINE B POLLUTANT USING A BISMUTH FERRITE CATALYST.

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Water pollution is generated by the discharge of effluents from different sectors of industry, containing heavy metals, organic toxins, lubricants, solid dyes and chemicals. Research shows that, between 2007 and 2021 the presence of emerging organic pollutants (EOCs) and endocrine disruptors (ED) has significantly increased, becoming a serious health risk to humans and ecosystems 1. In Mexico, compounds like Rhodamine B, are known to be present in various water sources, as a result of inclusive use in the textile industry. Various water treatment strategies like Advanced oxidation process (AOPs), have been explored and aimed at removing dyes and pollutants present in water. Each of these methodologies offers different approaches and levels of efficiency in the removal of dyes present in polluted water, with photocatalysis being one of the most applied methods in recent years. This technology requires, the development use of heterogeneous catalysts, such as bismuth ferrite ($BiFeO_3$), a non-stoichiometric substance belonging to the family of perovskites (ABX3), exhibits promising photocatalytic properties, thanks to its suitable bandgap (~2.2 eV). In this work, the green synthesis by combustion method, of a $BiFeO_3$ catalysts and its removal efficiency and kinetics,were evaluated using Rhodamine B as a test molecule. As a result, a catalyst was obtained and characterized via xray difration, scanning electron microscopy and N2 adsorption-desorption. The Rhodamine B solution exhibited a degradation of 60% within a period of 60 minutes, indicating a substantial degradation of the Rhodamine B dye under the given experimental conditions. This suggests that the catalyst and method used were effective in reducing the concentration of Rh-B in a relatively short amount of time.

Keywords:

Rhodamine B, Bismuth ferrite, Photocatalysis.

Reference:

J. Halder and N. Islam, "Water Pollution and its Impact on the Human Health,"J. Environ. Hum., vol. 2, no. 1, pp. 36–46, 2015, doi: 10.15764/EH.2015.01005.

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RENEWABLE ENERGY / 176

TROUGH-BOND APPROACH ENHANCED CONDUCTIVITY OF A POROUS METAL-ORGANIC COORDINATION POLYMER: HIGHLY ELECTROCHEMICAL-REVERSIBLE ELECTRODE SUPERCAPACITOR PERFORMANCE

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Next generation materials for electronic-electrochemical applications are expected to move on from purely inorganic towards organic and hybrid inorganic-organic materials, because inorganic materials have clear drawbacks such as scarcity of usable inorganic ions and limited tailoring of structural design. Metal-Organic Coordination Polymers (MOCPs) are self-assembled crystalline materials which are constituted of metal ions or metal clusters coordinated with organic bridging ligands forming defined framework structures. These materials are easily designed with tailorable structures and functional tunability due to its molecular nature. Despite these interesting features, in general, the vast majority of metal-organic coordination polymers are insulators and exhibit very low electrical conductivity. An approach to enhance the electronic properties of metal-organic coordination polymers is to improve the orbital overlap in the coordinate bond between the ligand and the metal ions (through-bond approach). In this research work, a novel Porous Metal Organic Coordination Polymer, named Co-BDBA, was synthesized. To synthesize Co-BDBA, Benzene-1,4-diboronic acid and Cobalt were used as linker and metal center, respectively. Co-BDBA possess an energy gap (Tauc plot) of 3.41 eV, then, this material might be classified as a semiconductor. To take advantage of the semiconductor feature, Co-BDBA was investigated as a possible Supercapacitor electrode. Electrochemical outcomes indicate that this metal-organic coordination polymer has a pseudocapacitive behavior, showing two redox reactions, and its charge-discharge mechanism is controlled by surface processes. The most remarkable feature of Co-BDBA as a supercapacitor electrode is that, after 2000 galvanostatic charge-discharge cycles, it presents a capacitance retention of ~110 %, due to its high electrochemically reversibility, better than previously reported coordination polymers.

Keywords:

Semiconductor, supercapacitor, metal-organic, electrochemical-reversibility

Reference:

Tang X, Zhang Y, Sun W, Wang Y. Carbonyl functional group modified metal–organic coordination polymer with improved lithium-storage performance. ACS Appl Energy Mater. 2020 Nov 23;3(11):11378–87

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RENEWABLE ENERGY / 182

DEVELOPMENT AND CHARACTERIZATION OF PVDF/BaTiO3 COMPOSITES FOR SUSTAINABLE ENERGY HARVESTING

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Energy harvesting from renewable sources through advanced materials offers a sustainable option to reduce dependency on fossil fuels while meeting increasing energy demands. This study proposes an advanced piezoelectric polymer composite consisting of polyvinylidene fluoride (PVDF) and barium titanate (BaTiO3). The composite aims to combine piezoelectric and elastic properties for efficient energy conversion. BaTiO3 powders were synthesized via the sol-gel method using barium acetate (Ba(CH3COO)2) and titanium isopropoxide (Ti(OC4H9)4) as precursors with deionized water (H2O) and methanol (CH3O) as solvents, followed by thermal treatment at 1300℃ for 2 h. Additionally, cubic BaTiO3 powder from Aldrich was subjected to the same thermal treatment. Structural characterization using X-ray diffraction (XRD) and scanning electron microscopy (SEM) revealed an asymmetric tetragonal phase with an irregular morphology. PVDF films were synthesized via the solvent-casting method and characterized using XRD and Fourier-transform infrared spectroscopy (FTIR), identifying the predominance of the beta phase. Two composites were developed: one with synthesized BaTiO3 and one with BaTiO3 from Aldrich. Electrical characterization was performed using an impedance analyzer to obtain capacitance curves as a function of frequency, from which the dielectric constant (k) was calculated by comparing the results of both cases. The experimental results confirmed that the synthesized BaTiO3 exhibited enhanced piezoelectric properties and sufficient mechanical elasticity in the PVDF/BaTiO3 composite for effective deformation and energy conversion, suggesting its effective application in sustainable energy harvesting technologies.

Keywords:

Energy harvesting, piezoelectric composite, polyvinylidene fluoride, barium titanate

Reference:

C. Wan and C. R. Bowen, Multiscale-structuring of Polyvinylidene fluoride for energy harvesting: The impact of molecular-, micro- and macro-structure, J. Mater. Chem. A, 5, (2017), 3091. https://doi.org/10.1039/c6ta09590a

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RENEWABLE ENERGY / 193

INFLUENCE OF THE GLASS AND POLYMERIC NANOSTRUCTURED MATERIAL SUBSTRATE ON ZNO THIN FILMS DEPOSITED BY THE SILAR METHOD AND THEIR ANALYSIS IN PHOTODEGRADATION.

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The degradation by using catalysts, especially metal oxides as thin films has been recently a novel method for proper treatment of air and water contamination. Additionally, the thin films deposited on flexible substrates provide light weight, easy bending, and low-cost processing. The zinc oxide (ZnO) as a p-type semiconductor with a direct bandgap energy of 3.3 eV is a promising material for photocatalytic activity, which it makes it active under UV-Vis light irradiation, for this reason, the influence of the substrate on ZnO thin films has been studied on the degradation of methylene blue. In the present work, ZnO thin films were deposited on glass, and polymeric nanostructured materials (polyethylene/graphene) substrates using the Successive Ionic Layer Adsorption and Reaction (SILAR) method. This method involves sequential immersions of the desired substrate in different cationic and anionic precursor solutions, getting a cycle of ion adsorption, rinsing, reaction, and other rinsing. The cationic precursor consists of ZnSO4, complexed with triethanolamine (TEA), the anionic precursor was hot deionized water at 90℃, and deionized water for rinsing. Structural, morphological, and optical properties were analyzed using X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Ultraviolet-Visible Spectroscopy (UV-Vis), respectively, where the ZnO has a hexagonal phase formation with grain sizes in the order of 36.8-48.7 nm, bandgap values around 2.77-3.7 eV, and homogenized surface over the different substrates. The photocatalytic evaluation was performed by considering ZnO thin films deposited on the different substrate (glass or nanostructured polymer).

Keywords:

Photodegradation, zinc oxide, SILAR, nanostructured polymer, sustainability.

Reference:

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RENEWABLE ENERGY / 203

Polymers Design for Thermal Management in Solar Panels.

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Photovoltaic panels are one of the most popular means of producing renewable energy, mainly because of the innovations that have been made to improve properties such as mechanical flexibility, lightness, and semi-transparency. However, the conversion efficiency of photovoltaic cells is still low (below 30%) compared with conventional generators. Much of the solar energy received by PV modules is converted into heat, which increases their operating temperature. This contributes not only to reducing the PV module's efficiency (between 0.4% and 0.65% per °C), but also to its degradation (reduced service life). Several techniques already exist in the literature to dissipate heat in solar panels, such as the use of free or forced convection at the back of the panels, or the use of phase-change materials... In this talk, we will discuss the experimental results of the device we have developed, which consists of the incoparation of two thin layers of two special polymers that act as heat sinks and significantly regulate the operating temperature of the PV module. Details of the synthesis and characterization of the two polymers used will also be presented.

Keywords:

Polymers, solar panels, heat sink, van der waals heterostructures

Reference:

without references

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RENEWABLE ENERGY / 367

Enhancing Energy Efficiency through Advanced Polystyrene-Based Waterproofing Agents

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Climate change poses significant challenges for building maintenance in regions like the South-Southeast of Mexico, characterized by high humidity and extreme heat. This study introduces a novel approach to address these challenges by developing and testing recycled polystyrene-based waterproofing agents fortified with fiberglass, titanium oxide, and polyurethane. Formulations (M1 to M5) were evaluated for their UV and IR rejection properties using spectrophotometric analysis.

Results indicate that formulation M5 achieves exceptional UV rejection (>99.5%) and significant IR rejection (99.3%). Moreover, simulated tests in irradiation chambers demonstrate that M5 effectively reduces thermal differentials by up to 16 ℃ compared to uncoated surfaces, potentially offering substantial energy savings.

This research contributes to the field by presenting a practical and effective solution to enhance building durability and energy efficiency in humid and hot climates. Further physical testing is

recommended to assess adhesion and resistance to environmental degradation, validating the long-term viability of these formulations for widespread application in building materials.

Keywords:

energy saving, waterproof coating, recycled polystyrene

Reference:

P.W. Collin, J.A. Cassia, A.N. Walsh, J.H. Jackson y C.M. Reddy, Sunlight converts polystyrene to carbon dioxide and dissolved organic carbon, Environ. Sci. Techol. Lett, 6 (11)

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RENEWABLE ENERGY / 376

CONSTRUCTION OF CHEMICALLY MODIFIED ELECTRODES TO DESIGN ELECTROCATALYTIC, PHOTOVOLTAIC DEVICES AND ELECTROCHEMICAL DETECTORS

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The main goal of this talk is to describe how the systemic concept of chemistry nano-architectures has been employed as the main strategy for designing chemically modified electrodes that have been utilized for attending to alternative energy, environmental, and public health problems. In this way, it will share with the audience some relevant results obtained in my laboratory for preparing dendrimers-modified nanoparticulate TiO2 photoanodes for constructing efficient dye-sensitized solar cells, Ni(II) cyclam-modified nanocrystalline TiO2 anodes for urea oxidation and simultaneous H2 evolution on Pt cathodes, optically transparent electrodes modified by Ag, Cu or bimetallic Ag|Cu nanoclusters for CO2 electrochemical reduction to CO, stainless steel mesh electrodes modified by TiO2|carbon nanocomposites for CO2 photoconversion to ethanol, and glassy carbon electrodes modified by dendrimers-caped Au nanoparticles for the amperometric detection of human serum uric acid and its application to the early diagnosis of hypo/hiper-uricemia and gestational preeclampsia.

Keywords:

chemically modified electrodes, systemic chemistry, nanoarchitectures, electrocatalysis, photovoltaics, electroanalysis.

Reference:

J. A. Banda-Alemán, G. Orozco, E. Bustos, S. Sepúlveda, J. Manríquez, J. CO2 Util. 27 (2018) 459-471. https://doi.org/10.1016/j.jcou.2018.08.016

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RENEWABLE ENERGY / 377

MODIFIED SURFACES FOR ENVIRONMENTAL ELECTROCHEMISTRY, AS AN ALTERNATIVE TO THE SUSTAINABLE DEVELOPMENT AND CIRCULAR ECONOMY IN THE REMOVAL OF POLLUTANTS IN AIR, WATER AND SOIL MATRIX

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We are experiencing essential changes in the environment that are a consequence of the increase in anthropogenic activities, such as the excessive use of natural resources and the consequent generation of polluting emissions that seek to satisfy the needs of human beings, but at the same time affect the different strata of the environment: water, soil, and air. Different research groups are developing technologies that reduce pollutant emissions into the environment and destroy existing ones, using individual and combined biological, physical, chemical, and physicochemical treatments. Within the latter, we find electrochemical treatments, which are based on the exchange of electrons to promote electronic transfers between a substrate (electrode) and the medium (organic, aqueous, or aqua-organic) in the presence of an electrolytic conductive species in solution (support electrolyte). Currently, work is being done on the construction of modified electrodes with properties that can form the basis of new electrochemical applications with innovative technological developments, where the substrate or material of an electrode to be modified can be titanium, steel, platinum, gold, graphite, glassy carbon, tin or indium oxide, which can be modified with different techniques; this molecular organization of the electrodes promotes a better electronic transfer that increases the percentages of removal of contaminants in air, water, and soil in less time.

Keywords:

modified surfaces, environmental electrochemistry, sustainable development, and circular economy.

Reference:

Do not apply.

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RENEWABLE ENERGY / 378

PHENOL ADSORPTION ON A PERMEABLE REACTIVE BARRIER (PRB) OF ACTIVATED CARBON IN VARIOUS pH CONDITIONS

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Phenol is a toxicant from the petrochemical, resin, and pharmaceutic sectors and pollutes soil and water bodies. This work aimed to investigate the applicability of activated carbon (AC) as a material for a permeable reactive barrier to remove phenol from groundwater flow. Filtration tests were conducted through the AC layer using 1 mM phenol solution in vertical and horizontal reactors. The probes in the vertical reactor of 50 mL were conducted with AC mass of 1.3 g, solution volume of 50 mL, and flow velocity of 0.0015 L/min during ~30 min, whereas 10 g of AC and 500 mL of phenol solution were used in trials of ~220 min with the horizontal reactor of 36 cm3 at optimum velocity of 0.002 L/min. The influence of pH (3, 7, 11) was studied. The remaining phenol concentration was determined by UV-Vis spectrophotometry in a 1-cm width quartz cuvette. For the vertical reactor, the average phenol removal at pH 3, 7, and 11 was 92%, 95%, and 83%, respectively. Phenol retention increased for pH 3 until 15 min (87% to 94%), then remained almost unchanging (93%). It was close to constant for pH 7, varying between 93% and 96%. Oppositely, it decreased nearly monotonically for pH 11 from 93% to ~73%. In the horizontal reactor, phenol removal changed with time, almost like in the vertical one. The average phenol removal for acidic, neutral, and basic conditions was 94%, 92%, and 90%, respectively. In an additional test at pH=3 with the higher flow rate (0.02 L/min), the maximum and average retention decreased to 90% and 88%, respectively. Finally, a test with "soil:AC"ratio of 50:1 and AC mass of 1.3 g was conducted in the horizontal reactor. Phenol removal did not exceed 5% in that case.

Keywords:

adsorption, phenol, activated carbon, permeable reactive barrier.

Reference:

None.

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RENEWABLE ENERGY / 379

GENERATION OF HYDROXYL RADICALS FOR THE REMOVAL OF AMOXICILLIN IN AQUEOUS MEDIA USING DSA-TYPE ELECTRODES AND CONSTANT AIR FLOW

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Water pollution is a primary environmental concern that poses significant human and animal health risks. Various contaminants in water sources can lead to severe health issues. Despite using different techniques to remove impurities, traditional wastewater methods only sometimes effectively eliminate emerging pollutants, leading to continued water contamination. Electro-oxidation is an effective technique used for the degradation of pharmaceuticals in water. This method uses electric currents to break down contaminants, making it a valuable tool in the fight against water pollution. This study aims to investigate the effectiveness of electro-oxidation using an IrO_2-Ta_2O_5|Ti anode by comparing three different configurations. The configurations involved titanium mesh and carbon cloth with and without constant airflow as cathodes. Additionally, the generation of H_2O_2 and •OH radicals were measured to evaluate the performance of each configuration. The electro-oxidation process was carried out at a cell voltage of 2.5 V for 120 minutes, with samples taken at various intervals (3, 6, 9, 12, 15, 30, 60, and 120 minutes) to monitor progress. UPLC-UV-Vis identified the removal of the model molecule amoxicillin (AMX) at a wavelength of 229 nm. Two different media, 0.1 M NaCl and 0.1 M Na_2SO_4 were used to compare the generation of H_2O_2 and •OH radicals. The results showed higher levels of H_2O_2 and •OH radicals were produced in the 0.1 M Na_2SO_4 medium. However, the removal of AMX was similar in both media, suggesting that the degradation pathway of amoxicillin may differ. Specifically, it is believed that •OH radicals promote AMX removal in the 0.1 M Na_2SO_4 medium, while in the 0.1 M NaCl medium, removal is thought to be encouraged by active Cl_2.

Keywords:

electro-oxidation, hydroxyl radical generation, amoxicillin.

Reference:

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RENEWABLE ENERGY / 381

MULTISTAGE SYSTEM TO DEGRADE TOLUENE IN POLLUTED AIR

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One of the main factors influencing environmental problems is the constant increase in emissions of pollutants into the atmosphere, highlighting volatile organic compounds (VOCs) such as toluene. In the first stage of this project, a continuous system used in the toluene removal study was studied by boiling a synthetic solution of 100 ppm toluene in ethanol, which was initially passed through the adsorption column with activated carbon reactor (AC), followed by the electrochemical reactor (EC), and finally, photolytic reactor (P), for 60 min. The AC contained activated carbon (HYCEL, PM 12.01) packed in a 6 cm long column with a diameter of 2.5 cm. The EC consisted of a cylindrical PVC reactor (30 x 10 cm), stainless steel cathode, and TiO2,nt|Ti anode; the P was made of stainless steel and equipped with a 358 nm UV lamp. The toluene removal was evaluated by gas chromatography with a BID detector (Shimadzu, Nexus GC-2030). In the project's second stage, a cylindrical High-Density Polyethylene (HDPE) reactor was designed and built. This reactor, housing the study electrodes, was used to process a sample of air from Mexico City with a toluene concentration between 117-100 ppb. A constant potential of 2 V was applied to the system for 3 hours, and samples were collected at the reactor outlet for mass gas chromatography. The individual toluene removal efficiencies were AC-50.29%, EC-44.38%, and P-52.71%. However, the most impressive result was when the three reactors were coupled in a multistage system (AC+EC+P), achieving a remarkable toluene removal efficiency of 99.58%.

Keywords:

adsorption, activated carbon, electro-oxidation, photolysis, toluene.

Reference:

None.

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RENEWABLE ENERGY / 380

PROMOTING MAGNETOSTRICTION IN GRAIN BOUNDARIES OF NANOSTRUCTURATED TiO2 FILMS SUPPORTED ON STAINLESS STEEL ELECTRODES FOR CONTROLLING THE PHOTOGENERATION OF HOLES AND HYDROXYL RADICALS

Author: Juan Manríquez[1]

Co-authors: Jesús Israel Valdez-Nava [1]; Erika Bustos [1]; Laura Lupita Martínez-Rodríguez [1]; Gabriel Trejo-Cordova [1]; Fabricio Espejel-Ayala [1]; Selene Sepúlveda-Guzmán [2]

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The study of ferromagnetism (FM) in non-cubic semiconductor oxides such as defective TiO2 is attractive due to their applications in photocatalysis. FM can be activated in TiO2 nanomaterials by promoting oxygen vacancies (VO) located in paramagnetic defected sites Ti3+VOTi4+. In this context, the VO can induce in Ti3+-doped TiO2 structures remarkable magnetic anisotropy energy

(MAE) of 6.51x106 erg/cm3, thus indicating the magnetic saturation should be achieved at magnetic fields (MFs) of ⊠425 gauss. Therefore, magnetostriction can be observed in ferromagnetic TiO2 films as a phenomenon in which their dimensions and shapes are changed when they are magnetized. In this work, stainless steel mesh electrodes (ss) were modified by nanoparticulate TiO2 films (ssTiO2) enriched by Ti3+VOTi4+ sites, to gain an understanding of the effects of magnetostriction on the photocatalytic properties of ferromagnetic TiO2 electrodes. MFs having intensities (H) of 125, 250, 500, 1000, and 2000 gauss were applied to the ssTiO2 electrodes for 80 min under UV light illumination for increasing the number of Ti3+VOTi4+ sites. Our results revealed that the magnetic lines promoted compression in the grain boundaries of the TiO2 structure when achieving pressures p>4.67 GPa for H>425 gauss (equation p=1/2(MAE/4⊠ gauss2)H2 describes the relationship between p and H). Consequently, the proportion of TiO2(anatase)/TiO2(beta) and the photogeneration of trapped holes (h+) and hydroxyl radicals (•OH) were simultaneously controlled as a function of the MFs intensities. In this way, it was observed a significant increase of h+ able to carry out the direct photocatalytic oxidation of aqueous orange G (without electron scavenger's assistance, e.g. gaseous O2) at the lowest H values, whereas the photogeneration of •OH radicals decreased at the highest H values. Finally, it was also interesting to observe that the Hinshelwood-Langmuir kinetics constants for the orange G oxidation were improved as H was increased.

Keywords:

ferromagnetic TiO2, magnetostriction, photocatalysis.

Reference:

Y. Bian et al., RCS Adv.,11 (2021) 6284. https://doi.org/10.1039/D0RA08359C

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RENEWABLE ENERGY / 382

EFFECT OF THE MAGNETOSTRICTION INDUCED ON THE CRYSTALLINE STRUCTURE OF NANOPARTICULATE TiO2 PHOTOANODES AND THEIR RELATIONSHIP WITH THE PHOTOVOLTAIC RESPONSE OF BLACK-DYE SENSITIZED SOLAR CELLS

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The study of ferromagnetism (FM) in semiconductor oxides having non-cubic crystalline structures (e.g. TiO2) is attractive due to their applications in spintronics. FM can be activated in TiO2 nanomaterials by promoting oxygen vacancies (VO) in paramagnetic defected sites Ti3+VOTi4+. In this context, the VO can induce in Ti3+-doped TiO2 structures remarkable magnetic anisotropy energy

(MAE) of 6.51x106 erg/cm3, thus indicating the magnetic saturation (Ms) should be achieved by applying external magnetic fields (MFs) of ⊠425 gauss. Therefore, magnetostriction can be observed in ferromagnetic TiO2 films containing Ti3+VOTi4+ sites as a phenomenon in which their dimensions and shapes are changed when they are magnetized. In this work, black dye-sensitized solar cells (BD-SSC) were prepared using TiO2 nanoparticle films enriched by Ti3+VOTi4+ sites, to gain an understanding of the effects of magnetostriction on the photovoltaic responses of BD-SSC. In this way, photocurrent density-cell potential plots were obtained for the BD-SSC in the absence and presence of MFs having intensities of 125, 250, 500, 1000, and 2000 gauss. MFs lines were parallel applied to the surface of the BD-sensitized TiO2 photoanodes. Our results indicated that the photogenerated electron transport through the dyed TiO2 photoanodes was not limited by electron transfer to I3- anions at the electrolyte in the absence or the presence of MFs, because all the values for the open-circuit potential (-Eoc ⊠ 0.553⊠0.014 V) remain constant. On the contrary, the obtained values for the short-circuit current density Jsc and the global conversion efficiency revealed that both parameters increased as a function of the MFs intensities, thus indicating that the magnetic lines were responsible for decreasing the degree of disorder (0<⊠<1) of the electron-traps at the intra-bandgap state's distribution of the TiO2 film (Jsc is proportional to Q1/⊠ where Q is the number of trapped electrons).

Keywords:

ferromagnetic TiO2, magnetostriction, dye-sensitized solar cells.

Reference:

M. Stiller et al., Front. Phys., 11 (2023)1124924. https://doi.org/10.3389/fphy.2023.1124924

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RENEWABLE ENERGY / 383

ELECTROCHEMICAL TREATMENT OF HEMODIALYSIS WASTEWATER FROM A CLINIC USING MODIFIED SURFACES WITH TRANSITION METAL OXIDES

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Hemodialysis is an extracorporeal kidney replacement procedure to remove impurities or waste products from the blood. It is used to treat kidney failure and go out into wastewater. This research considered synthetic water from hemodialysis under acid and basic conditions. To better simulate the presence of organic compounds, 10 mg/L of amoxicillin (AMX), an antibiotic commonly present in wastewater from clinics and hospitals, was added. Electro-coagulation (EC) and electro-oxidation

(EO) were combined sequentially to treat hemodialysis wastewater. EC was performed using a cylindrical SS-304 bar electrode (f = 0.8 cm) as an anode and a concentric Ti mesh as the counter electrode. A 3.0 V cell potential was maintained over one hour of electrolysis in acidic pH (pH = 5.06, ⍰ = 227 mS/cm). This treatment yielded a removal efficiency of 86 ± 1.25 % of AMX contaminate (pH = 8.21, ⍰ = 217.26 mS/cm, i = 11.36 mA, E = 0.568 kWh/m3). After EC, it was necessary to include a filtration or separation process to remove the Fe(OH)3 and [AMX-cation-AMX] sludge generated (2.3 g). This separation employed a settler. Subsequently, the supernatant was placed in an EO cell to remove residual organic compounds as AMX. It used a similar cell arrangement as in EC but changed the anode to IrO2-Ta2O5|Ti (70:30) (f = 0.5 cm) to perform the EO of the pharmaceutical product. During this step, the team achieved an overall removal efficiency of AMX of 100 % (pH = 8.14, ⍰ = 179.83 mS/cm, E = 500 kWh/m3). EO was performed using a continuous 10 mA cell current for 2 h. EO generated reaction products ADP 1, ADP 2, and ADP 3. Additionally, this process decreased the content of 'salty'cations, Na+, K+, Ca2+, and Mg2+, while generating Cl2 gas at the electrode.

Keywords:

hemodialysis wastewater, electro-coagulation, electro-oxidation, amoxicillin, clinic.

Reference:

None.

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RENEWABLE ENERGY / 385

Influence of grown conditions on the synthesis of Vanadium Oxide thin films by Ultrasonic Spray Pyrolysis

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In recent years Vanadium (V) has attracted great interest because it is an abundant element on the planet, which has different vanadium oxides as: VO, VO2, V2O3, V6O13, V3O7 or V2O5, each of which has different properties. In particular, Vanadium pentoxide (V2O5) presents greater interest due to its chemical stability and its photocatalytic properties. V2O5 has an energy bandgap of ~2.3 eV, which favors photocatalytic reactions for the decomposition of contaminants in water under visible light, hydrogen production or its use as hole transport layer in solar cells 1. Different physical and chemical methods have been used to deposit VOx thin films, including spray pyrolysis [2]. In

particular, spray pyrolysis is a low-cost and versatile method where the materials selection (solvent, precursors, additives, substrate) and the parameters optimization (molarity of solution, flow rate and spray generation) have great influence in the final properties of the films, which offers several advantages to control the morphology and growth of material [3]. In this work, nanostructured VOx thin films are deposited by ultrasonic spray pyrolysis and the influence of precursor solution, substrate, molarity and substrate temperature is correlated with structural and optical properties. Structural and morphological properties are analysed by X-ray diffraction and scanning electron microscopy. The optical band gap was calculated from UV-vis measurements. Thickness was evaluated by profilometry, and the electrical properties was measured by a four points method. As grown samples are crystalline, but different phases are present. A thermal annealing was performance to the samples to improve the crystallinity and decrease the presence of secondary phases. The increase of molarity increases the thickness of film but decrease the homogeneity. The increase of substrate temperature from 350 to 400 ℃ increase the thickness and the crystallinity of films. Morphology and conductivity are dependent on the substrate used.

Keywords:

Vanadium Oxide, Spray Pyrolysis, hole Transport layer, solar cells, nanomaterials

Reference:

1. M. Imtiaz et al., Environ. Int., 2015, 80, 79.
2. M. Benkahoul, et al., J. Alloys and Compounds 2017, 704, 760
3. I. Zumeta Dubé, et al., Sci. Reports 2021, 11, 2006.

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SCIENCE OUTREACH / 232

Plásticos centelladores: una forma de detectar rayos cósmicos

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Los rayos cósmicos son partículas cargadas con altas energías que chocan continuamente con la Tierra. Su interacción con la atmosfera produce cascadas de partículas secundarias, las cuales nos proporcionan información de las propiedades físicas, en particular, la energía de la partícula primaria. La detección de estas partículas se realiza mediantes el estudio de su interacción con diversos materiales. En este trabajo se muestra un sistema desarrollado localmente que usa como material revelador un plástico centellador de síntesis propia. Se compara con simulaciones realizadas en GEANT4, lo que permite visualizar este tipo de fenómenos con fines didácticos.

Keywords:

Rayos cósmicos, PMTs, centelladores, GEANT4

Reference:

Ros, G., Sáez-Cano, G., Medina-Tanco, G. A., & Supanitsky, A. D. (2018). On the design of experiments based on plastic scintillators using GEANT4 simulations. Radiation Physics and Chemistry, 153, 140–151. https://doi.org/https://doi.org/10.1016/j.radphyschem.2018.09.021

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SCIENCE OUTREACH / 347

CATALIZADORES PARA LA PRODUCCIÓN DE BIOENERGÉTICOS Y EL TRATAMIENTO DE AGUA

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El consumo de combustibles fósiles, las plantas industriales, el transporte automotor, la deforestación, las actividades antropogénicas, entre otras, han contribuido al incremento de gases de efecto invernadero (GEI), al incremento de la temperatura global del planeta y al desabasto o contaminación de recursos naturales como el caso del agua. Un enfoque prometedor para mitigar los problemas ambientales y de energía es el uso de nuevos materiales cerámicos, como catalizadores, que puedan ser usados en varias aplicaciones y que ofrezcan respuesta a los retos que actualmente enfrentamos. Esta charla versará sobre la síntesis, caracterización y aplicación de materiales tipo óxidos laminares como catalizadores heterogéneos, desde una perspectiva de economía circular. Se presentarán tres casos de estudio en la producción de bioenergéticos, tratamiento de agua y captura de CO2, con el objetivo de desarrollar nuevas tecnologías y disminuir su impacto ambiental.

Keywords:

Catalizador, bioenergéticos, tratamiento de agua, biodiesel, bioetanol

Reference:

Mijangos G. Cuatli C, Romero-Ibarra I., Vazquez-Arenas J., Santolalla-Vargas C., Santes V., Castañeda-Galván A., Pfeiffer H. Renewable Energy, 2022, 184, 845.

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SCIENCE OUTREACH / 38

Explorando el Futuro del Agua: Tecnologías Emergentes en Tratamiento y Purificación

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En la actualidad, la escasez de agua y la contaminación hídrica se han tornado en desafíos críticos, donde la demanda de agua limpia "segura"para consumo humano, agricultura e industria, entran en conflicto con la limitada disponibilidad de recursos hídricos de calidad. Además, la existencia de contaminantes emergentes, como productos farmacéuticos, disruptores endocrinos y productos químicos industriales, plantea nuevas amenazas para la salud pública y el medio ambiente. En este contexto, el uso de tecnologías emergentes como la fotocatálisis y la sonocatálisis, surgen como una respuesta efectiva y prometedora para abordar la problemática del agua. Estas innovadoras tecnologías, aprovechan la luz solar o la radiación ultravioleta para activar catalizadores, en el caso de fotocatálisis, y la irradiación ultrasónica, en el caso de la sonocatálisis, para favorecer la descomposición de contaminantes presentes en el agua. Estas tecnologías ofrecen ventajas significativas, incluida una mayor eficiencia en la remoción de contaminantes, tiempos de tratamiento más cortos y menores costos operativos en comparación con los métodos convencionales. Además, su aplicación puede adaptarse a una variedad de contextos, desde sistemas de tratamiento de aguas residuales hasta la purificación de agua potable a pequeñas escalas. En esta conferencia, dirigida al público en general, exploraremos cómo estas tecnologías emergentes representan un paso adelante en la lucha contra la crisis del agua, abordando temas tanto de importancia, escasez y como la contaminación. Analizaremos el funcionamiento de las técnicas, sus aplicaciones prácticas, ventajas y su potencial para impulsar un futuro más sostenible en términos de un subministro de hídrico seguro y sostenible.

Keywords:

Escasez de agua, Sonocatálisis, Fotocatálisis, Tecnologías emergentes, Contaminación hídrica.

Reference:

N. Morin-Crini, et.al., "Worldwide cases of water pollution by emerging contaminants: a review,"Environmental Chemistry Letters, vol. 20, no. 4, pp. 2311–2338, 2022, doi: 10.1007/s10311-022-01447-4

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SCIENCE OUTREACH / 48

LA NANOTECNOLOGÍA EN TU VIDA DIARIA

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La nanotecnología es un campo de la ciencia que estudia la materia a una escala extremadamente pequeña, a nivel de átomos y moléculas. Un nanómetro es tan pequeño que se necesitarían mil millones de ellos para hacer un metro. Surgió a partir de la idea de manipular estas partículas individualmente, propuesta por el físico Feynman en el año de 1959. El término "nanotecnología" fue acuñado por primera vez en 1974 por Taniguchi. Posteriormente, en 1985, los químicos Kroto, Smalley y Curl descubrieron los fullerenos, una forma de carbono con una estructura esférica cerrada, seguidos en 1991 por el descubrimiento de los nanotubos de carbono por Sumio Iijima. Estos hallazgos marcaron el inicio de la nanotecnología moderna. En el año 2004, los físicos Geim y Novoselov aislaron el grafeno, un material bidimensional de una sola capa de átomos de carbono, abriendo la puerta a una gama amplia de aplicaciones. Además del grafeno, otros materiales bidimensionales, como el disulfuro de molibdeno, y las nanopartículas, también tienen propiedades únicas que están siendo estudiadas. Los materiales nanométricos están presentes en varios aspectos de nuestra vida, aunque a menudo no nos demos cuenta. En la electrónica, los componentes en la mayoría de los dispositivos se han miniaturizado para mejorar su rendimiento. En la medicina, la nanotecnología se utiliza en el desarrollo y liberación de fármacos, así como en el tratamiento y diagnóstico de enfermedades como el cáncer. También existen textiles tratados con nanopartículas para hacerlos repelentes al aceite y al agua, así como para adquirir propiedades antibacterianas; inclusive se pueden encontrar nanopartículas en diversos productos cosméticos y de cuidado personal, como los protectores solares. Estas son solo algunas de las formas en las que la nanotecnología impacta nuestras vidas diarias, y su influencia sigue creciendo a medida que la investigación y el desarrollo continúan avanzando.

Keywords:

nanotecnología, materiales, grafeno, materiales bidimensionales, nanopartículas

Reference:

Kumar, A., Jayeoye, T. J., Mohite, P., Singh, S., Rajput, T., Munde, S., ... & Parihar, A. (2024). Sustainable and consumer-centric nanotechnology-based materials: An update on the multifaceted applications, risks and tremendous opportunities. Nano-Structures & Nano-Objects, 38, 101148. https://doi.org/10.1016/j.nanoso.2024.101148

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SCIENCE OUTREACH / 40

EL HERALDO DEL PROGRESO Y CÓMPLICE DE LA CONTAMINACIÓN: METALES PESADOS COMO PROBLEMA, SOLUCIÓN, Y FUTURO

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Los metales pesados han sido la base del progreso humano en varios aspectos, como semiconductores, electrónica, maquinaria pesada, entre otros; sin embargo, la falta de manejo después de su vida útil, representa un grave problema ambiental que se está agravando por la constante extracción de mineral en las minas como consecuencia de esta 'era de los semiconductores'. La contaminación por metales pesados se ha convertido en una preocupación alarmante debido a su riesgo para la salud humana y de las formas de vida acuáticas, los suelos y los ecosistemas en general. Existen varios enfoques para abordar este problema, incluida la absorción, la extracción química, la separación por membranas, la electrocinética y la fitorremediación, por mencionar algunos de ellos. No obstante, estos métodos tienden a no ser tan eficientes, es por eso que se están desarrollando métodos innovadores e irónicamente, algunos de ellos se basan en metales pesados. El ejemplo más notable podría ser el uso de catalizadores que contienen bismuto, zinc o vanadio para eliminar el arsénico, el cadmio u otros metales del agua; si bien esta alternativa puede ser confiable, el uso de tecnologías emergentes como bigdata, aprendizaje automátizado y otras, puede aumentar notoriamente la tasa de eficiencia. En este trabajo revisamos las técnicas actuales para descontaminar el medio ambiente de metales pesados, centrándonos en estrategias que emplean metales pesados como ingrediente activo y potenciadas por tecnologías de la llamada 'cuarta revolución industrial'.

Keywords:

Metales pesados, contaminación, remediación ambiental, tecnologías emergentes

Reference:

J.BRIFFA, E. SINAGRA, R. BLUNDELL, Heavy metal pollution in the environment and their toxicological effects on humans. Heliyon 6 (2020). https://doi.org/10.1016/j.heliyon.2020.e04691

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SCIENCE OUTREACH / 129

La tecnología de los supercapacitores

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Los supercapacitores son dispositivos innovadores que almacenan energía de manera rápida y eficiente. A pesar de ser menos conocidos que las baterías, son extremadamente útiles en dispositivos electrónicos que requieren energía inmediata, como cámaras y computadoras. Se destacan por su capacidad para cargarse y descargarse en segundos, y su larga vida útil de hasta 20 años, con la capacidad de soportar más de 100,000 ciclos de recarga. Aunque almacenan menos energía que las baterías, lo hacen mucho más rápidamente.
Un supercapacitor está compuesto por electrodos (materiales conductores de electricidad), un separador dieléctrico (material no conductor) y un electrolito (como una solución salina). Estos componentes permiten el almacenamiento de energía mediante cargas eléctricas o reacciones químicas rápidas. Los supercapacitores se utilizan en tecnologías verdes, como en paneles solares para estabilizar la energía, y en vehículos eléctricos, donde facilitan la frenada regenerativa y proporcionan energía de forma instantánea.
Actualmente, la investigación se centra en desarrollar nuevos materiales, como el grafeno, para mejorar la eficiencia y las propiedades de los supercapacitores. Estos dispositivos representan una tecnología prometedora para el almacenamiento de energía rápido y eficiente, con numerosas aplicaciones futuras en tecnología y sostenibilidad energética

Keywords:

Energía, Supercapacitores, Electrodos, Nanomateriales, grafeno

Reference:

Libich, J. et al. (2018) 'Supercapacitors: Properties and applications', Journal of Energy Storage, 17(March), pp. 224–227. doi: 10.1016/j.est.2018.03.012.

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SCIENCE OUTREACH / 325

Entre la realidad y la ficcion de lo mas pequeño: NANOROBOTS, NANOMITES, NANOHORMIGAS, NANOSURFERS

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Algo que la ciencia de frontera puede agradecer al cine, televisión y series de streaming, es la difusión de nuevas ramas del conocimiento, como por ejemplo: la nanotecnología. El mundo lo infinitesimal. En el título de la platica se plasman palabras de uso muy reciente, todas con el prefijo "nano". Como tal vez hayas constatado en las películas, es realmente fantástico el mundo de posibilidades que se le

han adjudicado a estas nanocosas: maquinas minúsculas reparadoras de órganos humanos, restauradores del medio ambiente, combate de plagas, establecen batallas contra células cancerígenas y otras enfermedades, combaten el envejecimiento con radicales antioxidantes, son minúsculos mensajeros de entrega de medicina nano local, habilitan el intercambio de información ultrarrápida y de encriptación ultra-segura, son entes minúsculos pero a su vez demasiado fuertes en relación a su tamaño, hábiles surfeadores en torrentes sanguíneos, entre otras propiedades. Se insta a los asistentes en esta platica a imaginar nuevos escenarios reales, futuristas y/o imaginarios, compartiendo sus críticas y externando opiniones acerca de que si el cine sueña o enseña. El expositor como guía te expondrá entre otras cosas la dimensión de las cosas que se pretende dominar en esta nueva área de la Ciencia, se presentarán las posibilidades para manipular la materia a esta escala y algunos de los hallazgos y avances científicos reales

Keywords:

Nanotecnología, cine, nanomáquina, divulgación, nano medicina.

Reference:

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SCIENCE OUTREACH / 293

AMBIENTE EN CRISIS: SOLUCIONES CON SEMICONDUCTORES PARA UN FUTURO SOSTENIBLE

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Resumen

Sabemos que el ambiente está en crisis debido a varios fenómenos climáticos tales como sequías, inundaciones y huracanes, que están relacionados con el calentamiento global causado principalmente por el uso excesivo de combustibles fósiles de los seres humanos. A lo anterior se le suma nuestras actividades cotidianas que impactan negativamente al agua, contaminándola con residuos muchos de ellos de difícil degradación. Ante esto, es importante preguntarnos: ¿qué estamos haciendo para solucionar los problemas que nosotros mismos provocamos?, una de las respuestas a esta pregunta

va encaminada desde el punto de vista científico y tecnológico del área de la Ciencia e Ingeniería de materiales, recordando que a lo largo de la historia hemos utilizado diferentes materiales para crear herramientas y satisfacer diferentes necesidades. En la actualidad, uno de los esfuerzos más importantes de la comunidad científica es aprovechar las propiedades o desarrollar nuevas funcionalidades de los materiales, entre los cuales resaltan los semiconductores por sus propiedades ópticas y eléctricas especiales, que les permiten atender algunos problemas ambientales principalmente relacionados con el aprovechamiento de la energía solar y la remediación ambiental, así, pueden utilizarse en celdas solares (fuentes alternativas de energía) y también como fotocatalizadores (degradación de contaminantes en el agua). En esta plática se comentarán aspectos importantes para comprender mejor el tema de los semiconductores, sus propiedades y cómo estás se pueden aprovechar para desarrollar soluciones tecnológicas sostenibles que mejoren nuestro entorno, resaltando la importancia de la ciencia y tecnología de los materiales en la resolución de problemas reales.

Keywords:

semiconductores, desarrollo sostenible, aprovechamiento de energía.

Reference:

Favino, C. (2024, 6 febrero). The Role of Semiconductors in the Green Transition | Earth.Org. Earth.Org. https://earth.org/semiconductors/

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SCIENCE OUTREACH / 284

EL PAPEL DE LOS MATERIALES SEMICONDUCTORES EN LA REUTILIZACIÓN DEL AGUA

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Los contaminantes, como pesticidas, fármacos y colorantes, representan una amenaza significativa para el medio ambiente y la salud humana debido a su capacidad para resistir la degradación natural. Estos contaminantes persistentes pueden acumularse en los ecosistemas acuáticos afectando a la fauna y flora, por lo que su eliminación eficaz es crucial para garantizar la calidad del agua. Para ello, es necesario buscar alternativas para su degradación y que permitan reutilizar el agua residual producida por el ser humano; una de estas opciones es la fotocatálisis (un proceso avanzado

de oxidación que utiliza la energía de la luz para activar materiales semiconductores, generando especies reactivas capaces de descomponer contaminantes persistentes). Es decir, bajo la exposición a la luz, los fotocatalizadores producen radicales libres que atacan y rompen las moléculas de los contaminantes, transformándolos en compuestos menos dañinos. Los materiales semiconductores pueden ser aplicados en forma de recubrimientos sobre diversas superficies para ser usados como fotocatalizadores, lo que permitirá su implementación en sistemas de tratamiento de agua; entre sus ventajas se destacan su capacidad para degradar una amplia gama de contaminantes y su posible sustentabilidad al utilizar luz solar como fuente de energía. Sin embargo, existen desafíos técnicos y económicos que limitan su uso industrial, estos incluyen una baja eficiencia de los fotocatalizadores bajo condiciones de luz natural, la durabilidad y estabilidad de los recubrimientos, y el diseño de sistemas adecuados para su uso conocidos como reactores fotocatalíticos. A pesar de estos desafíos, el grupo de investigación de diseño y optimización de recubrimientos avanzados (DORA-Lab) así como distintos grupos de investigación estudian y proponen diferentes materiales para ser aplicados en procesos fotocatalíticos, los cuales prometen soluciones innovadoras y más eficientes para la purificación de agua en el futuro.

Keywords:

fotocatalizadores, semiconductores, recubrimientos, fotocatálisis, contaminantes persistentes

Reference:

Martínez-García, A. L., Montiel-González, Z., Ramírez-Esquivel, O. Y., & Mazón-Montijo, D. A. (2022). ¡A limpiar agua con óxidos! Química de materiales al servicio del ambiente. Revista Digital Universitaria, 23(5), 9.
https://doi.org/http://doi.org/10.22201/cuaieed.16076079e.2022.23.5.7

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SCIENCE OUTREACH / 185

La inteligencia artificial, desde resolver tus tareas hasta el desarrollo científico

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La inteligencia artificial se ha convertido en ese tema de moda que comenzamos a ver en todas partes, desde las entretenidas aplicaciones de chat, reconocimiento de voz, detección de imágenes, asistentes virtuales, mejora de fotografías, recomendaciones personalizadas y un sinfín de implementaciones mas con las que ya convivimos día a día.
Ya en la década de 1950 desarrolladores e informáticos soñaban con la posibilidad de crear maquinas que asimilaran tareas propias a las que es capaz de realizar un ser humano. Por años se avanzó a pasos lentos pero firmes en el desarrollo de algoritmos de aprendizaje automático, pero no fue hasta el año de 1997 cuando la sociedad realmente se interesaría en la inteligencia artificial, después de que la computadora "Deep Blue"derrotara al campeón mundial de ajedrez Garry Kasparov.
Una vez demostradas las capacidades de una computadora con inteligencia artificial su implementación

para una amplia cantidad de aplicaciones era solo cuestión de tiempo. Las computadoras que acostumbrábamos usar para automatizar labores ahora no solo podían realizar tareas que considerábamos propias de una mente humana, sino que, quedó demostrado que pueden hacerlo más rápido y pueden hacerlo mejor.
En el año 2023 se alcanzó otra gran hazaña en la historia de la inteligencia artificial, finalmente, el sueño de cualquier estudiante se había cumplido, una inteligencia artificial que pudiera resolver tus tareas en cuestión de segundos llegó al alcance de toda la humanidad. ChatGPT y algunos otros de los denominados "chatbots"han llegado para quedarse, pero este nuevo y gran avance nos pone nuevamente en duda, ¿Qué vendrá ahora?, ¿Hasta dónde podrá llevarnos la inteligencia artificial?
Imaginemos por un momento que logramos que las computadoras hagan ciencia por nosotros, y que, como en muchas otras tareas, son más rápidas y mejores haciéndolo.

Keywords:

Inteligencia artificial, aprendizaje automático

Reference:

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SCIENCE OUTREACH / 180

FOTOGRAFÍA HIPERESPECTRAL Y LA AGRICULTURA SUSTENTABLE

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La fotografía convencional con sensores RGB capta la luz dispersada desde un objeto iluminado en el rango óptico con gran calidad. Sin embargo, los sensores de las cámaras multiespectrales e hiperespectrales, captan imágenes en longitudes de onda más allá del espectro visible. Especialmente éstas últimas emulan y superan a las técnicas espectroscópicas usadas en ciencia de materiales, ya que con imágenes se escalan dichas técnicas que sólo sirven para caracterizar muestras muy pequeñas. En esta ponencia expondremos diversas imágenes multiespectrales en papaya, caña de azúcar y nopal. La agricultura de precisión hace uso de estas herramientas tecnológicas para monitorear campos de cultivo con el fin de mantenerlos en buen estado fitosanitario, con imágenes hiperespectrales es posible visualizar de manera certera lo que con el ojo humano no es posible realizar a simple vista. Fenómenos de diverso tipo como los sanitarios, hidrometeorológicos, químicos sobre los campos agrícolas son más fácilmente cuantificables que si no se tuvieran estas herramientas. Sin embargo, el diagnóstico no es suficiente y se requeriría alguna clase de solución que fuera amigable con el medio ambiente, por ejemplo cuando se tratara de un fenómeno sanitario. A saber, el control biológico de

plagas podría ser el siguiente paso cuando se tuviera un diagnóstico temprano de un fenómeno sanitario como plagas insectiles. En este caso, hablaremos del uso de microorganismos entomopatógenos insertados en micropartículas de zeolitas que sirven como plaguicidas que no tienen efectos adversos al medio ambiente y que atacan de manera específica los diferentes agentes biológicos que merman la productividad de un cultivo.

Keywords:

imagen hiperespectral, entomopatógeno, zeolitas, plagas insectiles, fenómenos sanitarios

Reference:

A. Terentev et al., Sensors 22, 757 (2022)

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SCIENCE OUTREACH / 368

Electricidad: un fenómeno maravilloso y útil en nuestra vida

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Nuestra vida cotidiana sería muy diferente sin la electricidad. Muchos de nuestros instrumentos como teléfonos, computadoras, tabletas, televisiones, aparatos del hogar e incluso automóviles la aprovechan para funcionar. En nuestros hogares y en todos los edificios se utiliza para la iluminación, acondicionamiento de aire, vigilancia, etc. Los fenómenos eléctricos están presentes también en la naturaleza; el ejemplo más notorio es el rayo. Pero también los impulsos nerviosos que nos hacen pensar y vivir funcionan en base a procesos de este tipo. Pero: ¿qué es la electricidad? ¿qué produce estos fenómenos tan maravillosos y tan útiles? En esta plática abordaremos estos temas. Empezaremos dando un contexto histórico, desde las experiencias de los griegos con el ámbar y la invención de la brújula en China, antes de la era cristiana, hasta el desarrollo de la tecnología más moderna. Comentaremos las aportaciones de científicos como Coulomb, Oersted, Ampere y Faraday que permitieron llegar al conocimiento clásico de la electricidad y magnetismo, sintetizado en las célebres ecuaciones de Maxwell. También explicaremos cómo se genera la electricidad que aprovechamos en nuestras vidas y daremos algunos consejos prácticos para no sufrir accidentes por descargas eléctricas. La plática se acompañará con algunos experimentos sencillos que ilustran algunos de los conceptos abordados.

Keywords:

Electricidad, magnetismo, historia de la ciencia

Reference:

A stident's guide to Maxwell's equations, Daniel Fleisch, Cambridge University Press, 2008.

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SCIENCE OUTREACH / 370

El Futuro Brilla con LEDs: Tecnología Eficiente que Cuida el Medio Ambiente

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Cada vez más personas apuestan por tecnologías eficientes, sostenibles y respetuosas con el medio ambiente. En esta línea, la iluminación con LEDs nos permite hacer una contribución significativa en el cuidado del planeta. Los diodos emisores de Luz (LEDs) son pequeños pero poderosos dispositivos formados por las uniones de materiales semiconductores que, al hacer pasar una corriente eléctrica a través de ellos emiten la luz que los caracteriza. Estas versátiles fuentes de luz se encuentran en una infinidad de dispositivos que usamos a diario, como radios, televisores, celulares, equipos de cómputo, electrodomésticos y automóviles. Las ventajas de la iluminación LED son múltiples y muy importantes: consumen mucho menos energía y tienen una vida útil mucho más larga que el sistema de iluminación tradicional, producen una luz nítida y brillante, y son más seguras para el medio ambiente al no contener mercurio. Además, las luces LED ofrecen una amplia variedad de colores y temperaturas, lo que las hace ideales en distintos ambientes. En esta charla, explicaremos de una manera sencilla el principio de funcionamiento de los LEDs, un poco de su historia y evolución, y exploraremos algunos materiales semiconductores que han sido claves en su desarrollo. También, destacaremos las aplicaciones más comunes y sorprendentes de estos dispositivos, y finalmente, presentaremos sus beneficios, el impacto ambiental positivo y su increíble potencial para el futuro.

Keywords:

LED, medio ambiente, semiconductores III-V

Reference:

HI Solís-Cisneros, et. al., Physical and technological analysis of the AlGaN-based UVC-LED: An extended discussion focused on cubic phase as an alternative for surface disinfection, Revista Mexicana de Física, Vol. 68, 2022, doi.org/10.31349/revmexfis.68.020301

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SEMICONDUCTORS / 283

OPTICAL CHARACTERIZATION OF III-N-V MULTI-QUANTUM WELLS IN INTRINSIC GaAs FOR OPTOELECTRONIC APPLICATIONS

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The Gallium nitride arsenide alloy (GaN_x As_(1-x)) is an outstanding semiconductor ternary material in the development of solar cell devices. For example, by adjusting the nitrogen content (%N) in the GaNAs, the bandgap energy (E-) can be tuned to optimize the absorption spectrum for energy harvesting applications. Nevertheless, there is a lack of information on the role of this III-N-V material on low-dimensional systems 1. In this work, two GaNAs/GaAs multi-quantum wells (MQW) sequences embedded on GaAs are explored where the GaAs barrier is kept at 18 nm while the GaNAs well is 6 nm for A-samples and 12 nm for B-samples, both with 15 periods of the quantum well sequence. Molecular Beam Epitaxy (MBE) was employed to fabricate the samples using an intrinsic GaAs-base (100) substrate, a 300nm-thick GaAs buffer layer, the MQW sequence, and a 100nm GaAs capping layer. High-resolution X-ray diffraction (HRXRD) is a useful technique to characterize the crystallinity and determination of nitrogen mole concentration in the alloy (%N), finding a value of 0.6 and 0.8 for samples A and B, respectively. A broadening in the diffraction peaks were found for sample B in contrast with sample A, indicating a degradation of the crystallinity caused by both the higher %N and upper volume of the GaNAs alloy in sample B. Satellite peaks were found in the HRXRD measurements indicating the presence of the MQW. The electric field strength and distribution along the samples was investigated using photoreflectance (PR) and the E- and GaAs band gaps were also determined at 1.3(1.2) eV and 1.42(1.42) eV for sample A(B). Spectral features associated to MQW were observed in the PR spectra. Ellipsometry was used to analyze the electronic band structure of both samples through the pseudo-dielectric function, finding that increasing the %N the strain effect on valence band increases

Keywords:

GaNAs alloy, multi-quantum wells, Ellipsometry, Photoreflectance, Molecular Beam Epitaxy.

Reference:

Cortes-Mestizo, I.E. et al. Overlapping effects of the optical transitions of Ganas thin films grown by molecular beam epitaxy', Thin Solid Films, 702(2022), p. 137969. doi:10.1016/j.tsf.2020.137969

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OPTICAL AND STRUCTURAL CHARACTERIZATION OF AlN/SI (111) THIN FILMS DEPOSITED BY PLASMA ASSISTED MOLECULAR BEAM EPITAXY

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In recent years, there has been much interest in studying Aluminum Nitride (AlN) because of its promising properties for fabricating electronics devices. It's high thermal conductivity and electron mobility make it suitable for the development of high frequency transistors and high-power diodes. AlN also possesses a wide band gap energy, making it ideal for applications such as light-emitting diodes (LEDs) in the ultraviolet region, having germicide and sterilization applications. In this study, we investigate the influence of substrate temperature has on the morphology, structure, and optical and thermal properties of in thin AlN films deposited on Silicon (111) using plasma-assisted molecular beam epitaxy technique (PA-MBE). We report estimated values of the band gap energy, thermal diffusivity constant as well as strain and stress within the films. Sush parameters were obtained through by using modulated spectroscopy, photoacoustic spectroscopy (PAS), X-Ray diffraction (XRD) and, Raman spectroscopy and photoacoustic spectroscopy (PAS)respectively. Morphology analysis was obtained using atomic force microscopy accompanied with scanning electron microscopy (SEM). Finally optical, thermal, and structural parameters were correlated to the growth conditions of the thin films.

Keywords:

AlN, molecular beam epitaxy, thin film, nitrides, substrate temperature

Reference:

1 General Properties of Nitrides, ch. 1, pp. 1–129. John Wiley Sons, Ltd, 2008
[2] M. Macias, Y.L Casallas and C.M Yee Rendon, Thermal properties of cubic GaN/GaAs heteroestructures grown by molecular beam epitaxy, 2020

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SEMICONDUCTORS / 50

EXPLORING THE IMPACT OF COUPLING SYNERGISTIC SEMICONDUCTORS α-Fe2O3 AND ZnO TO CONSTRUCT FEASIBLE BILAYER THIN FILM PHOTOCATALYSTS

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Exploration of proposals to address environmental issues, such as water decontamination, is a topic of significant interest. Advanced oxidation processes, such as heterogeneous photocatalysis, present feasible options for degrading organic pollutants in water. Thus, there has been a recent surge in research efforts focused on identifying ideal thin film photocatalysts. This study aimed to evaluate a semiconductor bilayer comprising nanostructured hematite (α-Fe2O3) layered over an ultrathin zinc oxide (ZnO) film. Two systems were studied labeled as α-Fe2O3/ZnO(5nm)/Glass and α-Fe2O3/ZnO(15nm)/Glass. The synthesis of ultrathin layers of ZnO was conducted using atomic layer deposition (ALD), whereas the deposition of the 200 nm α-Fe2O3 overlayer was carried out through chemical bath deposition (DBQ) with a subsequent thermal treatment. The photocatalytic behavior of each layer within the bilayer was individually assessed and then correlated with various factors, including crystalline structure, bilayer thickness, morphology, and optical properties of the systems. The primary findings revealed that while the intrinsic properties of hematite remained intact, significant morphological alterations were observed related to the different growth stages of hematite over each of the ZnO substrates. These variations also influenced the performance in indigo carmine degradation, where the bilayer featuring greater thickness of ZnO demonstrates the most favorable results. These outcomes underscore the high potential of the proposed bilayers for the degradation of persistent pollutants in water.

Keywords:

semiconductors, thin film photocatalyst, nanostructured hematite, ultrathin zinc oxide

Reference:

A. L. Martínez García, Evaluación de Evaluación de Fe2O3/ZnO como recubrimiento fotocatalítico para la degradación de contaminantes orgánicos en el agua, Tecnológico Nacional de México/Instituto Tecnológico de Nuevo León (2022).

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Proyecto interno CIMAV 25024-2023: Recubrimientos fotoactivos para combatir la contaminación ambiental y promover el uso eficiente de energía II.

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SEMICONDUCTORS / 90

STUDY OF ELECTRIC FIELD DISTRIBUTION ON p-i-n GaAs-BASED SEMICONDUCTOR STRUCTURE THROUGTH PHOTOREFLECTANCE SPECTROSCOPY

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The semiconductor p-i-n structures are one of the most important and useful photovoltaic architectures, being the GaAs-based devices one of the most employed semiconductor systems and still looking for strategies to obtain high-efficiency devices. In this task, the appropriate design and control of the built-in electric field is mandatory to solve problems such as recombination at surface and improve the photoelectric effect. In this work, a p++/p+/i/n GaAs-based semiconductor structure grown by MBE is studied through photoreflectance spectroscopy (PR) with the aim to determine the number of built-in electric fields along the sample. The electric field at surface is modulated by varying the p++ caping layer thickness, CLT. H2O2/HCl/H2O chemical wet etching was employed to vary the CLT from 0 to 120 nm, also modifying the carriers'distribution and the electric field strength (Eint). Franz-Keldysh oscillations (FKO) in PR spectrum were employed to evaluate the Eint. The total built-in electric field changes around 10 to 4% with the wet etching, suggesting a redistribution of the carriers and variations on the built-in electric fields along the sample. The ΔR/R intermediate-field spectrum was fitted utilizing the Aspnes and Studna model 1, finding 4 principal built-in electric field regions along the sample. Furthermore, the fast Fourier transformation (FFT) was used to evaluate the internal electric fields, detecting the presence of 4 frequencies in agreement with the fitting process. A numerical study of the built-in electric field distribution was conducted to contrast the experimental results against the theoretical ones. The modifications of the surface electric field induced by the wet etching made the identification of the origin of the PR signals as well as identification of the origin of the built-in electric field.

Keywords:

Photoreflectance, Built-in electric field, Fast-Fourier transform, MBE.

Reference:

D. E. Aspnes et al. "Schottky-barrier electroreflectance: application to GaAs." Physical Review (1973) 3-15 https://doi.org/10.1103/PhysRevB.7.4605

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SEMICONDUCTORS / 212

G-ZnO films for possible application in blood glucose measurement as test trips

Author: Raquel Ramírez Amador[1]

Co-authors: Haydee Patricia Martínez-Hernández [1]; Leonardo Morales de la Garza [2]; Raúl Cortés-Maldonado [1]; Salvador Alcántara-Iniesta [3]

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This work reports a study of Grphene-Zinc Oxide films deposited by Ultrasonic Spray Pyrolysis (USP) technique. The films were deposited on glass substrates at 460℃ with different thicknesses, respectively. The samples were characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), I-V measurements, and Hall Effect techniques, respectively. XRD results revealed that the G-ZnO thin films were polycrystalline with a hexagonal wurtzite ZnO phase and had preferential orientations along (002) planes. Therefore, films revealed a value of resistivity approximately (6.8x10-3Ω.cm). The glucose-sensing properties of the as-prepared G-ZnO thin film were investigated for various thicknesses. From sheet resistance, it was found that films present a change of their value when the measurement of glucose are done. The G-ZnO thin film exhibited a good response at room temperature.

Keywords:

Graphene-Zinc Oxide, Gluocose, Ultrasonic Spray Pyrolysis, Resistivity.

Reference:

1 Shehab, M., Ebrahim, S., & Soliman, M. (2017). Graphene quantum dots prepared from glucose as optical sensor for glucose. Journal of Luminescence, 184, 110-116.

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SEMICONDUCTORS / 135

EFFECT OF InGaAs UNDELAYING LAYER ON THE SELF-ASSAMBLING OF InAs QUANTUM DOTS GROWN BY MOLECULAR BEAM EPITAXY

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Quantum dots (QDs) have been receiving a lot of attention due to their optical characteristics and quantum confinement effects for various applications like optoelectronics, lasers, photodetectors, amplifiers, and solar cells 1. InAs QDs grown on InGaAs undelaying layers are studied in this study, varying indium (In) composition ($0 \leq x \leq 0.18$) with the aim to understand the effects of lattice mismatch between the InAs and InGaAs on the size, shape, and optical qualities of QDs. Molecular Beam Epitaxy (MBE) was employed to synthesize the semiconductor nanostructure GaAs buffer layer (150 nm), InxGa1-xAs (100 nm) layer, and finishing with self-assembled InAs QDs (2 ML). RHEED characterization indicated an inverse proportional relaxation time for QD formation as In composition increases, as well as their maximum intensity formation, the growth rate was also studied with this technique and their development of angle in QD RHEED structures, called chevrons. HRXRD showed the intensity profiles and evolution of the InxGa1-xAs layer. Atomic force microscopy analysis was used to measure QDs height, thickness and density, finding a relationship between the underlying layer and the QDs on top. The insights gained from this investigation allow us to study QD formation and growth mechanisms. This arrangement lets us explore how substrate composition affects QD nucleation, growth speed and interfacial characteristics. As indium composition increased, the QD formation time narrowed, decreasing the time for its formation and their height increased as composition. Aswell as their bandgap distribution. This allows us to fine tune the parameters of the QDs.

Keywords:

Quantum dots, MBE, Photoreflectance, ADM, HRXRD.

Reference:

: 1.-M. Al Huwayz, H.V.A. Galeti. Optical properties of self-assembled InAs quantum dots-based P–I–N structures grown on GaAs and Si substrates by Molecular Beam Epitaxy, Journal of Luminescence, Volume 251 (2022) 119155, ISSN 0022-2313, https://doi.org/10.1016/j.jlumin.2022.119155.

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SEMICONDUCTORS / 231

STRUCTURAL PROPERTIES AND CO2 SENSING MECHANISM IN TUNGSTEN OXIDE FILMS

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Growing urbanization, industry, agriculture, deforestation, production habits and energy consumption have generated the presence of substances that contaminate water, soil, vegetation, and the atmosphere. Sensors are analytical devices capable of detecting chemical species continuously and reversibly to measure concentrations and/or presence of gases in their environment at a certain operating temperature to overcome the ionization potential when detecting a gas. Today, there are several synthesis methodologies for this material. However, in this work, we synthesize WO3 using the wet coprecipitation method with ultrasonic irradiation, which allows us to achieve ideal temperature conditions and reduces the synthesis time.
X-ray diffraction, Raman spectroscopy, and photoluminescence previously characterized the synthesized material.. DRS, AFM, and SEM will be used to elucidate the structural, optical, and morphological properties. The WO3 films were obtained using the Doctor Blade technique, obtaining 5 µm thick films. Rietveld refinement was carried out based on XRD data, where a γ-monoclinic crystalline phase of WO3 was confirmed (Tan et al., 2021). The increase in temperature caused an increase in the size of the crystallites and a decrease in microdeformation and dislocation density, which caused variations in the intensity of the Raman peak, in addition to changes in optical coefficients, morphology, and gas detection. ; the 400 ℃ film sensor had the shortest response and recovery time (29.5 s). time (36.83 s) for CO2 detection, making it a promising sensor for closed sites. The 600℃ film sensor, with a detection response of 70.12% and sensitivity of 46.45%, is best suited for CO2 detection.

Keywords:

CO2 Detection, Gas Sensing, Doctor Blade, Tungsten Oxide, Sensor system.

Reference:

Tan, G. L.,(2021). Effect of heat treatment on electrical and surface properties of tungsten oxide thin films grown by HFCVD technique. Materials Science in Semiconductor Processing, 122. https://doi.org/10.1016/j.mssp.2020.1055

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SEMICONDUCTORS / 152

The properties of transparent conducting molybdenum-doped ZnO films grown by thermal evaporation

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Transparent conducting molybdenum-doped zinc oxide films are prepared by thermal vacuum evaporation from a mixture of powders of ZnO and MoO3. The MoO3 content in the evaporation boat varies from 0 to 5 wt%, and each film is poly-crystalline with a hexagonal structure and a preferred orientation along the c axis. The resistivity first decreases and then increases with the increase in MoO3 content. The lowest resistivity achieved is 9.2 × 10-4 Ω-cm, with a high Hall mobility of 30 cm2 ·V-1 ·s-1 and a carrier concentration of 2.3×1020 cm-3 at an MoO3 content of 2 wt%. The average

transmittance in the visible range is reduced from 80% to 60% with the increase in the MoO3 content in the boat.

Keywords:

molybdenum oxide, zinc oxide, thermal evaporation, transparent conducting oxides

Reference:

1 Gustafsson G, Cao Y, Treacy G M, Klavetter F, Colaneri
N and Heeger A J 1992 Nature 357 477

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SEMICONDUCTORS / 68

Exploring Graphene's role in III-V semiconductors growth.

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The advent of two-dimensional (2D) materials has instigated a paradigm shift in semiconductor growth methodologies, introducing innovative techniques such as quasy Van der Waals (QVdW) epitaxy, which exploit the weak out-of-plane bonds inherent in these materials 1. Among these materials, Gallium Arsenide (GaAs) and Aluminum Arsenide (AlAs) are semiconductor with unique electronic and structural properties, rendering them highly desirable for advanced device fabrication. Their compatibility with other III-V semiconductors facilitates seamless integration into complex heterostructures, enabling optoelectronic device engineering. Furthermore, the prospect of integrating AlAs with graphene (G) holds immense potential for the development of next-generation electronic devices with unprecedented functionalities [2].
In this study, we present a novel methodology for the epitaxial growth of GaAs and AlAs utilizing Graphene/GaAs(100) as a substrate during Molecular Beam Epitaxy (MBE) or Closed Space Vapor Transport (CSVT) processes. Specifically, a monolayer of graphene was meticulously transferred onto a GaAs substrate, serving as a template for subsequent AlAs and GaAs deposition. Through systematic investigation of GaAs and AlAs growth across a range of different conditions, we observed a discernible influence of Graphene on the morphology and crystallinity of the deposited layers, characterized by scanning electron microscopy and x-ray diffraction respectively. These observations underscore a significant interfacial interaction between graphene and the III-V semiconductors, suggesting the potential for enhanced control over the epitaxial growth process. Such insights into the influence of graphene on GaAs and AlAs growth dynamics hold promise for the precise engineering of advanced electronic devices with tailored properties. This study lays the groundwork for further

exploration into the utilization of graphene on the growth of various III-V semiconductors, thereby opening up new avenues for the advancement of electronic and optoelectronic technologies.

Keywords:

Graphene, AlAs, GaAs, MBE, CSVT

Reference:

1 Y. Alaskar, S. Arafin, et. Al., Adv Funct Materials, 24, 6629–6638 (2014).
[2] Shen, D., Zhu, et. Al., Chinese Sci. Bull., 57, 409-412 (2012).

This work was supported by:

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SEMICONDUCTORS / 258

Development of a Gallium Oxide Heterostructure for Enhanced UV Solar Blind Photodetector Applications

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This work aims to develop a gallium oxide (Ga_2O_3) heterostructure doped with magnesium on a silicon substrate for potential use as a UV solar blind photodetector. The growth process begins with the creation of a seed layer via plasma-enhanced atomic layer deposition (PEALD), utilizing trimethyl gallium and trimethyl magnesium as precursors, argon as a carrier gas, and oxygen for plasma generation. The growth temperature was maintained at 150℃. Structural properties were characterized using X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The process continues with ultrasonic spray pyrolysis (USP) to deposit a bulk layer, enhancing the capture of ionizing radiation. Gallium (III) nitrate hydrate ($Ga(NO_3)_3 \bullet xH_2O$) is used as the precursor in this stage. This study explores the potential to achieve a P-type material through PEALD and examines its influence on the subsequent growth of Ga_2O_3 by USP. Additionally, we investigate how temperature variations impact key performance metrics of the photodetector.

Keywords:

Gallium oxide, PEALD, Spray pyrolysis

Reference:

Z. Liua, Y. Huanga, H. Lia, C. Zhangb, W. Jianga y D. Guoc, «Fabrication and characterization of Mg-doped ε-Ga2O3 solar-blind photodetector,» Vacuum, vol. 177, p. 109425, 2020.

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Benemérita Universidad Autónoma de Puebla
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SEMICONDUCTORS / 192

Quantum dots faceting changes induced by misfit strain modulation

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In the last decade, quantum dots have demonstrated remarkable performance in advancing devices of great importance, with the potential to transform everyday life. This is due to their optical, structural, and electronic properties, providing groundbreaking applications such as quantum-based cryptography, spintronics, and light-emitting diodes. Given the substantial future technological advancement they are upheld of it is worthy to investigate basic but relevant issues that determine in a great deal most of the physical properties of the quantum dots, i.e. the self-assembly process. In particular, QDs are usually synthesized by the so-called Stransky Krastanov growth mode that takes place in the growth of lattice mismatched semiconductor crystals, such as InAs and GaAs. The strength of the misfit strain (fs) is a key factor in determining the QDs geometry, energy-free planes or facets build-up the QD as a result of minimizing strain during self-assembling. Four facets define a square pyramidal QD, whose vortex angle (α) can be monitored experimentally. In this work, we have grown the InGaAs/GaAs heterostructure to modulate the misfit strain prior to the InAs-QDs self-assembling. For QDs grown directly on InGaAs, the biaxial strain (εxx) above the apex increases linearly with α, while below the islands it decreases exponentially. We increase the epilayer/substrate misfit strain fs before InAs-QDs self-assembling and noticeable changes in QDs geometry were observed, inducing in this way changes in the strain fields that surrounds the QDs and within it. ⊠xx shows a linear dependence below both the QDs pyramidal base and GaAs layer with f. However, the strength of εxx, below QDs the tensil strain decreases with fs, while the compressive strain increases.

Keywords:

Molecular Beam Epitaxy, Strain, self-assembling, QDs, InAs

Reference:

J.P. Olvera-Enriquez, L.I. Espinosa-Vega, I.E. Cortés-Mestizo, C.A. Mercado-Ornelas, F.E. Perea-Parrales, A.Belio-Manzano, C.M. Yee-Rendón and V.H. Méndez-García, Journal of Vacuum Science & Technology A 41, 042714 (2023)

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SEMICONDUCTORS / 200

SYNTHESIS OF MIXTURES OF CuFeS2 AND ZnS (WURTZITE) USING MICROWAVES RADIATION

Authors: Gonzalo Viramontes Gamboa[1]; Isaí Raya Farías[1]; Pablo Agustín Calderón Franco[2]

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In this study, an extremely simple methodology is reported to synthesize high-purity CuFeS2 and CuFeS2 mixed with ZnS using microwave radiation from a conventional household microwave oven of 0.7 to 1.3 kW. For the synthesis of CuFeS2, stoichiometric amounts of 99.9 % pure Fe, Cu, and S powders are weighed and mixed thoroughly under a nitrogen atmosphere inside a glove chamber. Powders size ranges from 2 to 40 micrometers for Fe, 20 to 120 micrometers for Cu and 2 to 60 micrometer for S. The mixture is placed inside a closed glass container to avoid the presence of oxygen, and exposed typically from 5 to 10 seconds to the microwave radiation, until a sudden very highly exothermic reaction takes place. X-Ray characterization and electrochemical cyclic voltammetry show that following this method the mineral formed is CuFeS2. The formation of any other sulfurous phase containing these three elements is not observed, neither residue of the three starting elements. When 99.9% pure Zinc powder is gradually (increments of 1% of Zinc powder), added to the initial mixture, X-ray diffractograms show the formation of hexagonal (Zn,Fe)S Wurtzite together with CuFeS2. Optical and Scanning electron microscopy images show that the minerals synthetized following this method have a fractal sponge-like porous structure, with a measured BET surface area of 0.83 m2/g. This synthesis methodology has several advantages when compared to conventional hydrothermal methods, since it does not require using high pressure and high temperature autoclave. It also does not require long exposure times of weeks or months, neither chemical precursors other than elemental Cu, Fe, S and Zn.

Keywords:

Chalcopyrite, Wurtzite, microwave synthesis

Reference:

Gonzalo Viramontes-Gamboa, Berny Fernando Rivera-Vasquez and David G. DixonThe Active-to-passive Transition of Chalcopyrite. https://iopscience.iop.org/article/10.1149/1.2196007

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SEMICONDUCTORS / 354

Optical and morphological properties of ZnO thin films deposited by using a low-cost spray pyrolysis system

Author: Gerardo Alonzo[1]

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Zinc Oxide thin films were successfully deposited onto corning glass substrates. A "homemade" experimental system was implemented for spray pyrolysis deposition. The precursor solution was stirred at different times before spraying onto substrates previously heated to 400 ℃. After deposits of thin films, critical variation of the optical transmittance, band Gap energy, and microstructure of the films were observed as a result of variation of the stirring time. The results show that with the implemented system it is possible to obtain ZnO thin films with excellent and reproducible properties for different applications, e.g., gas sensors and TCO in optoelectronics and solar cells.

Keywords:

thin films, spray pyrolysis, optical transmittance

Reference:

M. Wang, S. H. Hahn, J. S. Kim, J. S. Chung, E. J. Kim, and K. K. Koo, "Solvent-controlled crystallization of zinc oxide nano(micro)disks"Journal of crystals growth, vol. 310, pp. 1213–1219, January 2008.

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SEMICONDUCTORS / 222

SYNTHESIS AND CHARACTERIZATION OF Li-DOPED POTASSIUM HEXATITANATE POTHOCATALYST

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Alkaline metal titanates with tunnel structure have attracted great attention both experimental and theoretical for model systems, for being fast ionic conductors, as well as for their high photocatalytic activities. In particular, potassium hexatitanate (PHT) is used as a reinforcing agent for polymers and metal alloys and it is a photocatalyst, which has been extensively investigated in the production of hydrogen through photocatalytic water splitting using UV e Vis irradiation. The aim was to synthesize and characterize Li-doped K2Ti6O13 in order to modify the band gap and evaluate its performance as a photocatalyst. PHT was produced by flux growth according to the methodology proposed by Ponce-Peña et al., (2015) and then doped with LiSO4 solutions at different concentrations. Materials were characterized by MP-AES, XRD, BET, UV-Vis and SEM. The main results confirmed that PHT doped with variable amounts of lithium was obtained, with a band gap in the range of 3.15 to 3.25 eV and surface area between 5.95 and 10 m2/g; these characteristics could make them attractive for use as photocatalysts for hydrogen production.

Keywords:

potassium hexatitante, photocatalyst, Li-doped

Reference:

P. Ponce-Peña, M.A. Escobedo-Bretado, P.deLira-Gómez, E. García-Sánchez, E. Rivera, and L. Alexandrova, Synthesis and characterization of potassium hexatitanate using boric acid as the flux, Ceram. Int. 41 (2015) 10051-10056. http://dx.doi.org/10.1016/j.ceramint.2015.04.093

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SEMICONDUCTORS / 296

Enhanced Solvent Sensing with Mesoporous Layer in MIS Capacitors

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This work investigates solvent sensing using a Metal-Oxide-Semiconductor (MOS) capacitor with a mesoporous layer as the insulator. Solvent sensors are crucial for various applications, including environmental monitoring, industrial processes, and safety, due to their ability to detect harmful solvent vapors and prevent potential hazards. We present electrical measurements taken under solvent exposure, from which we extract variations in the primary MOS capacitor parameters. The use of mesoporous material as the insulator in the Metal-Insulator-Semiconductor (MIS) capacitor demonstrates significant potential for developing high-sensitivity solvent sensors, bypassing the need for complex functionalization processes. Our results highlight the advantages of mesoporous insulators in enhancing sensor sensitivity and performance, making them highly effective for reliable solvent detection.

Keywords:

Solvent Sensing, Mesoporous Insulator, MOS Capacitor, High-Sensitivity Sensors, MIS Devices

Reference:

Panecatl, et al., Chemistry Select, Volume8, Issue12, March 28, 2023, e202204636

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SEMICONDUCTORS / 333

DESIGN OF A LATTICE-MATCHED InAs1-XSbX/AlIn1-YSbY QWs TYPE-I WITH TUNABLE EMISSION IN THE NEAR-INFRARED SPECTRAL RANGE (2-5 µm)

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The antimonide family has become one of the most potential semiconductor materials to develop a new generation of applications in the infrared, such as laser diodes and detectors. One of the most promising alloys is InAs1-ySby because its band gap energy (Eg) can be tuned in a range from near-infrared (NIR) (3.6 µm) to mid-infrared (MIR) (7.3 µm) and Al1-xInxSb with a Eg tunable from 0.52 µm to 7.3 µm. InAs1-ySby quantum wells (QWs) within Al1-xInxSb barriers can be in principle lattice-matched ($y = 0.1833 + 0.8167\ x$) in the NIR. For a given (x, y) composition the energy emission can be

modified by changing the QW width (Lw). However, to obtain a lattice-matched InAs1-xSbx/AlIn1-ySby QW type-I, the InAs1-xSbx/AlIn1-ySby band alignment requires to be studied, given that InAs1-xSbx/AlIn1-ySb interface can present type-I or type-II band alignment, depending on the alignment of the conduction and valence bands. The heterostructure type can be identified by using the electron affinity rule, in which the offset in the conduction band at the interface is equal to the difference of the electron affinity values of two compounds InAs1-xSbx/AlIn1-ySb. We have calculated the evolution of the valence and conduction band offsets as a function of In (x) and Sb (y) contents, and we found that the type-I for x≤0.40 and 0≤y≤1, for x>0.40 the antimony content (y) range can be found for 0.10<y≤1. While the type-II is allowed for x≥0.50 the antimony content (y) range can be found for 0.10<y≤1. To calculate the energy levels of the QWs type-I and the exciton binding energies we employed the matrix method formalism under the effective mass and envelope function approximations. Finally, with our calculations, we demonstrate that by modifying the Lw and (In, Sb) contents the spectral emission could be tuned in the 2-5 μm range.

Keywords:

InAsSb, AlInSb, quantum-wells, valence-band-offset, infrared.

Reference:

Effect of the Sb content and the n- and p- GaSb(100) substrates on the physical and chemical properties of InSbxAs1-x alloys for mid-infrared applications: Analysis of surface, bulk and interface, J, Alloys and Comp. 861 (2021) 1-10. https://doi.org/10.1016/j.jallcom.2020.157936

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SEMICONDUCTORS / 277

The obtaining of ZnO Nanoparticles with potential antibacterial activity

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In recent years, nanoparticles (NPs) have gained prominence as contrast agents for disease diagnosis, drug delivery systems, and treatments for cancer and bacterial infections, primarily due to their nanoscale size. The green synthesis of NPs combines nanotechnology with plant-derived metabolites such as sugars, terpenoids, polyphenols, alkaloids, phenolic acids, and proteins, which play a crucial role in reducing metallic ion. Zinc Oxide NPs (ZnO) are notable for their antimicrobial effects against pathogens like E. coli1.

This study aims to obtain ZnO NPs through a novel green synthesis method distinct from those commonly reported in the literature. Garlic extract was used along with a zinc nitrate solution as the precursor, followed by thermal processes. The resulting nanoparticles were characterized using techniques such as Dynamic Light Scattering (DLS), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and Energy Dispersive Spectroscopy (EDS). The antimicrobial

efficacy of the ZnO NPs was evaluated against E. coli.
The results demonstrated that ZnO NPs effectively inhibit E. coli bacteria, outperforming antibiotics such as cephalothin. This indicates that ZnO NPs possess significant antibacterial activity against E. coli, highlighting their potential as an alternative antimicrobial agent.

Keywords:

metallic nanoparticles, zinc oxide, natural extracts, antimicrobials, E. coli.

Reference:

1. M. Ali, M. Ikram, M. Ijaz, A. Ul-Hamid, M. Avais and A. A. Anjum, Green synthesis and evaluation of n type ZnO nanoparticles doped with plant extract for use as alternative antibacterials, Applied Nanoscience, (2020) 10(10), 3787-3803. doi:10.1007/s13204-020-01451-6

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SEMICONDUCTORS / 18

THE IMPACT OF SOLUTION ACIDITY AND BALL MILLING ON THE ELECTRICAL AND OPTICAL PROPERTIES OF FZO THIN FILMS DEPOSITED BY ULTRASONIC SPRAY PYROLYSIS

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This study investigates the effects of acetic acid concentration and ball milling on the zinc precursor in the initial solution for the deposition of zinc oxide (ZnO) thin films on glass substrates using the chemical spray deposition method. The substrate temperature was maintained at 450℃, and two different deposition times were employed. The milling process was used in a planetary ball mill at 500 rpm with a milling duration of one hour. The impact of acetic acid concentration and ball milling on the structural, morphological, and optical properties of ZnO thin films was examined. Results show that all samples exhibit a wurtzite-type ZnO structure and are polycrystalline. However, the concentration of acetic acid in the initial solution alters the preferred orientation planes, transitioning from (002) to (101). Surface morphology analysis reveals the formation of hexagonal grains, with their size increasing with higher acetic acid content in the initial solution. Films deposited with lower acetic acid content exhibit high optical transmittance in the UV-vis range. The band gap values ranged from 3.2 to 3.4 eV.

Keywords:

Zinc Oxide, Ball milling, Acetic acid, thin films, TCOs

Reference:

Jayaraman, V. K., Maldonado-Álvarez, A., Jimenez-Gonzalez, A. E., & de la Luz Olvera-Amador, M. (2016). Influence of precursor ball milling in enhancing the structural, morphological, optical and electrical properties of AIZO thin films. Materials Letters, 181, 52-55.

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SEMICONDUCTORS / 54

LIGHT SENSOR PERFORMANCE OF NdCoO3 PREPARED BY CO-PRECIPITATION METHOD.

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NdCoO3 has been studied for its relevant physical and chemical properties, which have applications in fields like photocatalysis and thermoelectrics conductivity. NdCoO3 is a p-type semiconductor material, possessing the perovskite-type structure. In this work, the detection of ultraviolet light (UV), as well as light of other wavelengths (λ), was investigated. For this purpose, polycrystalline NdCoO3 was synthesized by the co-precipitation method, using a concentrated solution of formic acid and Nd and Co nitrates. The identification of single-phase NdCoO3 was made by X-ray powder diffraction on samples calcined at 920ºC, in air. Measurements for detecting UV and light in the visible region were done at room temperature, using light emitting diodes (LEDs) at different optical irradiances (Ee). These measurements were done on a sintered pellet with silver wires as electrodes. The results show a uniform response pattern, characterized by an increase in photocurrent (Iph) under radiation. The quantitative detection of radiation was evaluated by varying Ee from 10 to 100 mW/cm2. The results indicate a non linear relationship between Iph and Ee. I–V curves were also performed on the pellet showing a linear (ohmic) variation. For other wavelengths, such as blue (449 nm), green (515 nm), red (642 nm) and white, reliable responses were also observed, noting that the change of Iph decreased by increasing λ. The results indicate that NdCoO3 can be used as a detector of radiation.

Keywords:

Neodymium, cobalt, oxide, Photocurrent, UV detector

Reference:

S. Kianipour, et al. NdCoO3 nanostructures as promising candidate photocatalysts for boosting visible-light-driven photocatalytic degradation of organic pollutants, J. Sci. Adv. Mater. Dev. 7 (2022) 100506. https://doi.org/10.1016/j.jsamd.2022.100506.

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SEMICONDUCTORS / 243

The accumulative death probability of free carriers in heavily doped semiconductors.

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Among the wide variety of sigmoidal forms or line shapes of growth, it shines a particular one, describes growth as being slowest at the start and end of a given period. This is the Gompertz function (GF), which can track asymmetric breakthrough curves exhibiting a moderate degree of tailing. It has frequently been used to statistically model growth phenomena across various research domains, particularly in demographic studies. When initially applied by Gompertz it was based on the assumption that the mortality rate increases exponentially as a person ages. The resulting function describes the number of individuals living at a given age as a function of age. The mathematical framework has been applied to several fields, for example,in biology describes the population in a confined space, as birth rates first increase and then slow as resource limits are reached. GF was used to predict the growth of tumors based on their initial size and growth rates, which facilitates the development of treatment schedules. In the medical field, these models also help anticipate the rates of spread and evolution of various diseases. By transitioning the concept to statistically describing phenomena and growth rates to solid-state physics, this function describes the growth of thin films during deposition, the stress relaxation process under constant strain, the diffusion of atoms or defects in a crystalline lattice, and the temperature dependence of electrical conductivity in certain materials. In this work, the relationship between the GF and another essential property of semiconductors is studied: the density of states (DOS). It is demonstrated that unlike the usual square of energy dependence of DOS for bulk materials, the random fluctuation of the impurity potential in heavily doped semiconductors, changes the number of states that are available in a system and the behavior can be described throughout the Gompertz function.

Keywords:

gompertz function, DOS, heaviy doped semiconductors, impurity potential, statistical approximation

Reference:

Mora-Herrera, M. F., Espinosa-Vega, L. I., Cortes-Mestizo, I. E., Olvera-Enriquez, J. P., Belio-Manzano, A., Cuellar-Camacho, J. L., Gorbatchev, A. Y., Del Rio-De Santiago, A., Yee-Rendón, C. M., & Méndez-García, V. H. (2024). Journal Of Applied Physics, 135(17). https://doi.org/10.1063/5.0193026

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SEMICONDUCTORS / 62

Optical characterization of GaN/SiO2 in Hexagonal phase synthesized by PLD

Author: Jesus Adrian Cano Salazar[None]

Co-authors: Cristo Manuel Yee Rendón ; Dainet Berman Mendoza ; Jose Guadalupe Quiñones Galván ; Rafael García Guitérrez

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In this work we present the results together with the analysis corresponding to the synthesis and characterization of gallium nitride thin films on quartz synthesized using prefabricated targets based on gallium nitride powders using the pulsed laser deposition technique, the results of photoluminescence indicate that we have the signal corresponding to gallium nitride in hexagonal phase[**1**] and XRD where we can see the planes corresponding to the wurtzite structure, showing that it is a viable way to synthesize this material by this method for gallium nitride, giving good future to other types of nitrides using prefabricated targets based on powders.

Keywords:

GaN, Laser, Ablation, Powders, Films, Photoluminescence

Reference:

Reshchikov, Michael A. 2022. "Photoluminescence from Vacancy-Containing Defects in GaN."Physica Status Solidi. A, Applications and Materials Science 220 (10). https://doi.org/10.1002/pssa.202200402.

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SEMICONDUCTORS / 280

Composition-graded InGaAs strain reducing layer as modulation strategy in InAs/InGaAs/GaAs semiconductor heterostructure

Authors: D. Corte Ponce[1]; I.E. Cortes-Mestizo[2]

Co-authors: A. Hernandez-Reyna [3]; K.L. Marquez-Antonio [3]; M.I. Bustos-Ibarra [1]; M.F. Mora-Herrera [3]; D. Lopez-Vilchis [3]; V.H. Mendez-Garcia [1]; L.I. Espinosa-Vega [1]

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The epitaxial semiconductor growth process presents significant challenges when synthesizing heterostructures from two different semiconductor materials due to the lattice mismatch's effect on crystallinity. Specifically, in the InAs/GaAs system, commonly used for the self-assembly of Quantum Dots (QDs), the residual strain caused by a 7% lattice mismatch leads to issues in the crystalline structure, degrading the optical and electronic properties. In this study, an InxGa1-xAs composition-graded layer (GL) is proposed as a strain reduction strategy. The semiconductor heterostructure under investigation consists of a (100) GaAs substrate, a 200 nm GaAs buffer layer, a 100 nm GL, an In0.5Ga0.5As underlying layer, and InAs QDs previously optimized for morphology. The GL layer transitions from 0 to 0.5 in In composition, matching the underlying layer's composition. Using Silvaco Atlas software, computer-based simulations were performed to fine-tune the optimal semiconductor heterostructure. The final structure was synthesized using Molecular Beam Epitaxy (MBE), which provides precise control over quantum dot growth and thickness adjustments during deposition, as well as the slope gradient of the ternary layer. Insights from this investigation reveal how the GL affects InAs QD devices for solar cell applications, marking a significant step forward in developing efficient emerging devices using quantum dots for further investigation in multi-staking.

Keywords:

Quantum dots, MBE, Photoreflectance, Silvaco.

Reference:

Li R, Liu F, Lu Q. Quantum Light Source Based on Semiconductor Quantum Dots: A Review. Photonics. 2023; 10(6):639. https://doi.org/10.3390/photonics10060639

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SEMICONDUCTORS / 349

Study of two energy level GaNxAs1-x system to build up symmetrical double-well and step graded quantum well confinement potentials.

Authors: JESUS ROLANDO PINSON ORTEGA[1]; Leticia Ithsmel Espinoza Vega[2]; Maria Fernanda Mora Herrera[3]; Daniel Lopez Vilchis[4]; Felipe Eduardo Perea Parrales[5]; C.M. Yee-Rendon[6]; Irving Cortes[7]

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Two of the most important potentials in quantum mechanics and semiconductor physics are the symmetrical double-well (SDW) potential and the step graded quantum well (SGW) structure. The first one consists of a potential with two minima separated by a barrier. In the classical limit one expects that an initial state prepared in one well is stable. Quantum tunneling allows the possibility to escape from one side to the other passing under the classically forbidden region. For the second potential, symmetrical intermediate potentials are set aside of a deep well. In this work we present an alternative to construct simultaneously an SDW and SGW confinement potentials throughout highly mismatched alloys (HMA) like GaNAs. For this material the decoupling in electronegativity and size of the atomic radii of the N with Ga, generates a splitting conduction band (CB) letting unaltered the balance band (VB). The low and high energy CBs after splitting have been called as E- and plus E+ bands, respectively. Using these bands, a new quantum well heterostructure is proposed where the GaNAs/GaAs/GaNAs heterostructure is sandwiched between AlGaAs barriers. Under these conditions, the GaAs may act as barrier between E- bands in SDW, and as the deepest well between E+ bands for a SGW. 3d finite element model was employed to determine the confinement quantum states. Some eigenfunctions of both bands are found to be overlapped depending on the Al content in the AlGaAs barriers. In spite that the activation of bands was corroborated by photoreflectance spectroscopy, there was not clear experimental evidence of quantum confined states related with E+, suggesting that E- is the sole energy band that contributes to the quantum electron confinement. Controversy arose concerning to the meaning and functioning of double band HMA.

Keywords:

MBE, Quantum confinement, semiconductor, highly mismatched alloys, potentials

Reference:

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SEMICONDUCTORS / 136

OPTICAL AND NUMERICAL ANALYSIS OF SELF-ASSEMBLED InAs QUANTUM DOTS GROWN ON InGaAs VIA MOLECULAR BEAM EPITAXY

Authors: A. Hernandez-Reyna[1]; I.E. Cortes-Mestizo[2]

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Currently, research on quantum dot (QD) semiconductor heterostructures is at its peak due to the need to improve their structural and optical characteristics, because they have unique properties that are used in a wide variety of device applications 1. In this project, the self-assembly of InAs QDs is studied by modifying the lattice mismatch between the InAs QDs and the InGaAs undelaying layer to explore changes in the structural and optical properties. Molecular beam epitaxy was employed to growth the (200nm) GaAs/(100nm) InxGa1-xAs/(2.9ML) InAs heterostructure. The $0 \leq x \leq 0.18$ mole concentration range was explored. The growth process was analyzed in situ through RHEED method considering the chevron angle (φ) modification by the quantity of InAs monolayers deposited. A relationship between the φ and the QDS morphology was determined, being increased as the QDs size is bigger, according to AFM measurements. With the aim to explore the structural properties of the samples Raman spectroscopy was engaged. A modification on the TO and LO InAs- and GaAs-like vibrational modes was determined as result in modification on the crystallinity by lattice mismatch and InGaAs composition. Band-structure characterization was obtained by photoreflectance spectroscopy, being the InGaAs and GaAs spectral features modified by the effect of strain. Numerical simulations of the heterostructures were made to determine the effect of the InGaAs underlayer on the strain distribution and the band structure of the samples under study. In this numerical study the sample's geometry and the InGaAs composition obtained from its experimental characterization were considered as input data

Keywords:

Quantum dots, Raman, Photoreflectance, MBE, Numerical analysis.

Reference:

: W. Zhou and James J. Coleman, Semiconductor Quantum Dots, Current Opinion In Solid State & Materials Science, 20(6), 352-360. https://doi.org/10.1016/j.cossms.2016.06.006

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SEMICONDUCTORS / 216

Analysis of the initial thermodynamic conditions to grow GaAsSb epitaxial layers by Liquid Phase Epitaxy (LPE) on GaAs substrates

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Sb-containing III-V semiconductor materials are interesting for the fabrication of optoelectronic devices for the mid- and far-infrared range of electromagnetic waves. In this work, the initial thermodynamic conditions for the growth of GaAsSb epitaxial layers on GaAs substrates from liquid phases with liquidus temperatures of 560, 610 and 650 C are analyzed. The system under consideration is characterized by the existence of a broad area of immiscibility of solid solutions, inside this area, not considering the elastic energy, thermodynamic conditions for the formation of solid phases of diverse compositions from one liquid phase at the same liquidus temperature are reached. On the other hand, with supersaturated liquid phases, regions appear and expand, as supersaturation increases, in which thermodynamic conditions for the formation of epitaxial layers are not achieved. The miscibility gap becomes wider at lower temperatures. Nevertheless, its boundary on the GaAs side lies past the limiting compositions of solid phases achieved experimentally by the LPE growth. The presence of elastic energy stabilizes the composition of the solid phase and should lead to the growth of epitaxial layers of single composition strongly shifted to the GaAs-rich side. So, the estimated GaSb content does not exceed 0.12 molar fraction in the solid phases to be formed from ternary liquid phases having the liquidus temperature of 560 C in the whole range of their compositions. Thus, it is quite probable that the presence of elastic energy serves as a major limiting factor in the LPE growth of GaAsSb epitaxial layers with high Sb content on GaAs substrates. The thermodynamic analysis was done with the CALPHAD method using SGTE data.

Keywords:

LPE growth, CALPHAD method, Sb-containing III-V semiconductors

Reference:

V. Donchev et al., J. of Crystal Growth 574 (2021) 126335, Low-temperature LPE growth and characterization of GaAsSb layers for photovoltaic applications

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SEMICONDUCTORS / 224

PHOTOCATALYTIC PRODUCTION OF CO2 TO HYDROCARBONS WITH UV AND VISIBLE LIGHT BY TiO2/GRAPHENE QUANTUM DOTS

Author: Miriam Béjar Sánchez[1]

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The photocatalytic conversion of CO2 and H2O to hydrocarbons, also called artificial photosynthesis represents a CO2 reduction instrument in the environment and a sustainable fuel production method. For good energy and conversion efficiency it is desirable that the photocatalyst has a low band gap value and can carry out fuel production in the visible light range and take advantage of the solar renewable energy source. In recent years quantum dots have been used as photocatalysts because of their optical properties which are due to a quantum confinement effect and have been shown to have good conversion of CO2 to fuels such as CH4 and C2H6 even in visible light. This research aims to synthesize photocatalysts from TiO2 quantum dots with graphene and graphene nano-ribbons having low band gap value and photocatalytic activity in the visible light range for the production of fuels such as CH4 and C2H6. The photocatalysts were synthesized by the hydrothermal method, obtaining the anatase phase of TiO2 with different amounts of graphene and graphene nano-ribbons. And their photocatalytic production of fuels is tested using UV and visible light lamps. It should be noted that in this test not only C1 and C2 hydrocarbons have been obtained, but also C6 hydrocarbons have been produced with band gap values within the visible range and fuels have been obtained in the same way within this range of light. Likewise, it is observed that by having a lower amount of graphene and graphene nano-ribbons in the photocatalysts, a higher fuel production rate is obtained and likewise a lower band gap value.

Keywords:

artificial photosynthesis, quantum dots TiO2/graphene, visible hydrocarbons production

Reference:

Reduced TiO2 quantum dots/graphene for solar light driven CO2 reduction into precisely controlled C1 vs C2 hydrocarbon products without noble Co-catalyst

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SEMICONDUCTORS / 233

SYNTHESIS OF PINK EMISSION CsPbBr_x〖I〗_(3-x) PEROVSKITE NANOCRYSTALS THROUGH A SHORT-LENGTH CHAIN LIGANDS APPROACH

Authors: Fernando Edsel Guerra Vega[1]; Héctor Juárez Santiesteban[1]; José Alberto Alvarado García[1]; René Pérez-Cuapio[1]

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All-inorganic perovskite materials significantly impacted the scientific community due to their intrinsic electronic and optical properties, which provide them with enough versatility to have them in a variety of optoelectronic devices such as solar cells, LEDs, photodetectors, and lasers. In this work, CsPbBr_x〖I〗_(3-x) perovskite nanocrystals using short-ligand chain and low toxicity solvents with low boiling point are synthesized through Ligand Assisted Re-precipitation (LARP) method as a fast and simple procedure to acquire perovskite nanocrystals at room temperature with well controlled size and shape. It is worth mentioning that this methodology has been previously reported only

for CsPbBr3 perovskite nanocrystals. The structural, optical, and morphological properties of the particles were studied through X-ray diffraction (XRD), UV-vis spectroscopy, photoluminescence spectroscopy (PL), and scanning electron microscopy (SEM) and energy-dispersive spectroscopy (EDS). By analysing the XRD patterns, there is a notable shift in the main peaks when the 〖Br〗^- concentration is reduced and replaced by I^- indicating an ion substitution within the crystalline lattice. Optical characterization showed a band edge absorption at ~620 nm and a narrow emission peak at ~600 nm with a full maximum high width of ~20 nm suggesting a reasonably monodisperse particles. It should be noted that the synthesized particles showed a pink emission when irradiating with a UV lamp. SEM images showed urchin-like, agglomerates and tubular morphologies in the micro scale as well as undefined nanoparticles morphology. Finally, EDS analysis indicated that the atomic composition varies in each morphology, being the ones at microscale the more accurate in terms of atomic distribution.

Keywords:

Perovskite, Synthesis, Nanocrystals, CsPbI_x 〖Br〗_(3-x)

Reference:

Ye, J., et al. Elucidating the role of antisolvents on the surface chemistry and optoelectronic properties of CsPbBrxI3-x perovskite nanocrystals. J. Am. Chem. Soc. 2022, 144, 12102-12115

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SEMICONDUCTORS / 240

Impact of Precursor Concentration and Annealing Temperature on the Photocatalytic Efficiency of SnO2 Nanoparticles for Degrading Organic Pollutants.

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In recent years, semiconductor oxides have been widely used in photocatalysis for the water degradation pollutants. Specifically, SnO2 has been applied to degrade organic dyes. In this work, we synthesized SnO2 nanoparticles by the sol-gel method at 60℃ for 2 h using tin chloride as precursor at several concentrations, polyvinylpyrrolidone and distilled water as surfactant and solvent respectively. To study their evolution in size, morphology, structural and optical properties a thermal treatment was done at 200, 400 and 600° C. X-ray diffraction results displayed a mixture of phases at lower annealing temperatures. As the annealing temperature increases, the SnO2 nanoparticles crystallized in tetragonal structure. Also, we saw a high influence over crystallite size by the precursor

concentration and annealing conditions. The UV-Vis measurements showed a strong absorption in the ultraviolet region, with a slight shift to wavelength shorter at lower annealing temperatures. The PL spectrum displays emissions in UV and visible region due to edge transitions as well as the due intrinsic defects, respectively. SEM images exhibit that the size and morphology of the nanoparticles are highly dependent on the synthesis conditions. Preliminary results showed that the degradation efficiency of methylene blue is directly associated to the nanoparticles synthesis conditions, and their structural, optical, and morphological properties.

Keywords:

Photocatalysis, Nanoparticles, SnO2, Thermal treatment, Sol-gel

Reference:

Patel, Gauravkumar & Chaki, Sunil & Kannaujiya, Rohitkumar & Parekh, Zubin & Hirpara, Anilkumar & Khimani, Ankurkumar & Deshpande, M.. (2021). Sol-gel synthesis and thermal characterization of SnO2 nanoparticles. Physica B: Condensed Matter. 613. 412987. 10.1016/j.physb.2021.412987.

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SEMICONDUCTORS / 250

OPTICAL PROPERITES OF KESTERITE Cu2(Sn1-xGex)S3 THIN FILMS

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Cu₂SnS₃ (CTS) kesterites are semiconductors with suitable optical properties for solar cells, due to their excellent absorption coefficient greater than 10⁴ cm⁻¹ and direct band gap between 0.9 and 2.5 eV. On the other hand, CeO₂ is a wide bandwidth semiconductor with optoelectronic properties that have allowed its recent application in photovoltaic structures. The heterojunction of Cu₂(Sn_{1-x}Ge_x)S₃ as p-type material and CeO₂:Gd as n-type film has potential as a thin film photovoltaic heterostructure. In this work, thin films of Cu₂(Sn_{1-x}Ge_x)S₃ were deposited in which the Ge composition was gradually increased by spin-coating with a maximum Ge of x=0.15, and they were also thermally treated to improve the crystallinity. The crystalline phase of the material was identified by Raman spectroscopy and x-ray diffraction. Additionally, spectroscopic ellipsometry measurements were performed in the range from 0.6 to 4.75 eV. Through a model that considers a Tauc-Lorentz dielectric function, it was possible to identify the energy of the optical gap and up to three maximum absorption features.

Keywords:

CTS, CeO2, kesterite, ellipsometry

Reference:

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SEMICONDUCTORS / 254

UNVEILING THE EFFECTS OF ANTIMONY (Sb) CRYSTALLINITY ON THE ANTIMONY TRISULFIDE Sb_2S_3 SYNTHESIS OBTAINED BY A TWO-STEP METHOD.

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Antimony chalcogenides are two-dimensional materials that have gained significant interest as absorber materials in thin film solar cells due to their high absorption coefficient, suitable direct band gap, earth-abundant and environmentally friendly constituents.
In this work, antimony sulfide Sb_2S_3 has been synthesized by a two-step method, studying the crystallinity effect of antimony (Sb) thin films on the sulfurization process. The Sb thin films were deposited by RF-Sputtering technique on glass/molybdenum substrates under different working conditions, varying the working pressure and the deposition time, to obtain both amorphous and crystalline phases. Then, the obtained films and the sulfur powder were placed inside a home-made graphite box, which was introduced in a tube furnace coupled to a vacuum pump. For the sulfurization processes, the pressure, time and temperature were varied until the appropriate stoichiometric Sb_2S_3 conditions were obtained.
The structural, compositional, morphological, and optical properties of the Sb_2S_3 thin films were studied. Results show that the working pressure variation in the Sb deposit allows for modification of the structure, obtaining a phase change from amorphous to crystalline. Moreover, the Sb_2S_3 show an orthorhombic crystalline structure, with an average crystallite size of 50 nm. Additionally, it has a stoichiometric composition close to the S/Sb ratio of 1.5 and a nanorod morphology. A band gap energy around 1.4-1.6 eV was measured, which suggest the Sb_2S_3 suitability as an absorber layer in photovoltaic devices.

Keywords:

Crystallinity, Sb2S3 thin films, 2D materials, sulfurization, two-step process.

Reference:

M. A. Farhana, A. Manjceevan, J. Bandara, Recent advances and new research trends in Sb2S3 thin film based solar cells, J. Sci.: Adv. Mater. Devices 8 (2023) 100533. https://doi.org/10.1016/j.jsamd.2023.100533.

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SEMICONDUCTORS / 281

NUMERICAL OPTIMIZATION OF NANOSTRUCTURED ANTIREFLECTIVE COATING LAYER FOR GaAs-BASED SOLAR CELLS

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The solar cells made from GaAs are scarcer and more expensive compared to silicon cells. Wherefore, efforts on optimizing the solar absorption through reducing the optical losses are mandatory with the aim to increase the GaAs solar competitiveness and availability in the solar cell market. The use of antireflective coatings has emerged as a relevant engineering tool to address this issue 1;they suppress light reflections and enhance the power conversion in GaAs photovoltaic devices. It is a common strategy to deposit Anti-Reflective coatings on light detecting devices to improve device quantum efficiency. These coatings rely on destructive interference of reflected waves to reduce overall reflection coefficient of light incident on the detecting device surface. In this work, Technology Computer-Aided Design was employed to design and optimize the conversion efficiency of GaAs solar cells by applying a nanostructured antireflective layer thereby improving the blue waves absorption. A numerical model was built using Silvaco Atlas to investigate the optimal thickness of antireflective layer over a p++/p+/p/i/n/n+ GaAs photovoltaic structure. The optimal thickness can be calculated by using the concept of destructive interference which minimizes reflection and maximizes light transmission into the solar cell.Furthermore, The Transfer Matrix Method was utilized to compute a light propagation through multilayered structures, considering phase and amplitude changes of light waves through each layer. Hafnium oxide,Indium oxide,and Gallium oxide were evaluated, with antireflective layer thickness ranging from 20 to 100 nm. Optimal values were identified typically between 50-60 nm. The study demonstrated significant enhancement in the spectral response of the solar cell by reducing reflections within the blue spectrum (450-495 nm), thereby increasing absorption efficiency and overall conversion efficiency. This research provides a practical configuration for AR layers in solar cell applications, offering a promising pathway for experimental implementation with epitaxial techniques such as ALD and MBE.

Keywords:

antireflective, Technology Computer-Aided Design, he Transfer Matrix Method, ALD

Reference:

Tenwar, Ankit Kumar, et al. “Anti-reflective nanostructures for efficiency improvement of GaAs based solar cells.” Materials Today: Proceedings (2022),58, 682-685. https://doi.org/10.1016/j.matpr.2022.02.163

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SEMICONDUCTORS / 323

FORMATION OF GaAs 3D structures THROUGH METAL-ASSISTED CHEMICAL ETCHING FOR APPLICATIONS IN INFRARED OPTOELECTRONIC DEVICES

Author: Marco Antonio Ramírez Orozco[1]

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The formation of GaAs 3D structures is crucial for advanced applications in optical communications, infrared sensors, and other semiconductor technologies because these structures offer enhanced efficiency and superior structural properties. Therefore, this study focuses on achieving controlled formation of GaAs 3D structures using metal-assisted chemical etching to enhance the geometric precision and spectral response of devices crucial for advanced optical communications and infrared sensors. Gold (Au) and nickel (Ni) were used as the metal for this process, deposited on GaAs substrates using high vacuum equipment. The concentration of the chemical etching solution and the immersion time of the metal-coated substrate in the solution for chemical etching were varied. The characterization by scanning electron microscope (SEM) and optical microscope confirmed the successful formation of GaAs 3D structure through chemical etching. By fine-tuning the etching process through the manipulation of solution concentration and etching duration, twe achieve a high degree of precision in the formation of the GaAs structures. . Overall, the findings from this study provide valuable insights into the optimization of metal-assisted chemical etching processes for the fabrication of GaAs-based 3D structures. Raman spectroscopy showed the LO (longitudinal optical which is found at a frequency of 292 cm^{-1}) and TO (transverse optical which is typically observed at a frequency of 268 cm^{-1}) modes of GaAs. A. T T

Keywords:

GaAs structures, Metal-assisted chemical etching, SEM, Raman, Optic Microscopy

Reference:

Han, H., Huang, Z., & Lee, W. (2014). Metal-assisted chemical etching of silicon and nanotechnology applications. Nano Today, 9(3), 271–304. https://doi.org/10.1016/j.nantod.2014.04.013

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SEMICONDUCTORS / 330

Delta doping band engineering in GaNAs/GaAs structures grown by MBE for THz applications

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THz technology has aroused great interest due to its wide range of applications in various fields in recent years. These applications include areas such as high-speed communications, security and, notably, healthcare. In this last area, significant advances have been made, such as the detection of diseases like diabetic foot.This radiation is generated by the excitation of a semiconductor material by an ultrafast pulsed laser that generates ballistic transport and acceleration of the electrons. Recently, studies on THz emitters indicate that the near surface band bending can improve the emission due to the modification of the surface electric field that provokes an increment in the charge carrier's acceleration. The band bending has been achieved by implementing along the growth of InGaAs variations of the In molar concentration. However, a barely explored technique is the use of near-surface delta doping. In this work, the band bending in GaNAs/GaAs structures is studied by incorporating a monolayer of silicon at different depths from the sample surface, process known as delta doping. The samples were grown by molecular beam epitaxy (MBE) and the analysis was supported through electric field simulations. With the intention of partially relax the strain in the samples and to improve the optical quality of the GaNAs alloys the samples were subjected to rapid thermal annealing (RTA) process. Then, the samples were characterized by HRXRD, revealing a nitrogen molar concentration near to 2%; Raman TO/LO ratio shows that the RTA improved crystalline quality compared to the as-grown films. Furthermore, delta doping will be studied by changes in the electric field using photoreflectance.

Keywords:

MBE. THz, band bending, semiconductors, Delta doping

Reference:

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SEMICONDUCTORS / 195

SYNTHESIS AND ANALYSIS OF CsPbBr3 PEROVSKITE NANOCRYSTALS OBTAINED UNDER DIFFERENT AMBIENT CONDITIONS

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All-inorganic perovskite materials have had a significant impact on scientific community due to their intrinsic electronic and optical properties which provide them with enough versatility for optoelectronic applications in devices such as solar cells, LEDs, photodetectors, lasers. In this work, a comparation between a colloidal synthesis of CsPbBr3 perovskite nanocrystals at room (RT) and low temperature (LT) conditions is done. Also, a stationary state nitrogen flow injection system at room temperature (RT-N) was added as a variable condition to observe its impact on the particle quality and stability. As for the synthesis, Ligand Assisted Re-precipitation (LARP) method was applied as a fast and simple procedure to acquire perovskite nanocrystals at room temperature with well controlled size and shape. Optical, and morphological properties were studied through X-Ray Diffraction (XRD), UV-vis spectroscopy, photoluminescence spectroscopy (PL), infrared spectroscopy by Fourier transformation (FTIR), and scanning electron microscopy (SEM). From XRD patterns it was determined the crystallite size that is strongly dependent to the temperature and ambient conditions, with a cubic and orthorhombic phase mixture in all three conditions. UV-Vis spectrum showed absorption bands at 510, 438, and 405 nm in all the samples. The presence of the last two bands can be related to a phase mixture backing up the XRD results. PL spectra showed an high emission from 511 to 522 nm, a decrease in the FWHM from 22.15 to 19.26 nm, is observed which may be due to the relationship between the phases present in each sample. The presence of ligand species is confirmed by the analysis of the FTIR spectrum. Finally, perovskite nanocrystals presented a homogeneous morphology showing various particle sizes being the LT sample the greatest and the RT-N the smallest according to the SEM images.

Keywords:

Perovskite, CsPbBr3, colloidal synthesis, nanocrystals, PL spectra.

Reference:

Liu, W.; Zheng, J.; Cao, S.; Wang, L.; Gao, F.; Chou, K. C.; Hou, X.; Yang, W. General Strategy for Rapid Production of Low Dimensional All-Inorganic CsPbBr3 Perovskite Nanocrystals with Controlled Dimensionalities and Sizes. Inorg. Chem. 2018, 57, 1598– 1603.

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SEMICONDUCTORS / 375

Magnetic and electric effects on low doped ZnO with Ni, experimental and DFT analysis

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This research aims to identify how the properties of ZnO change in relation to low amounts of Ni doping. It examines the magnetic and electric properties of low Ni-doping in ZnO-Wurtzite using experimental techniques and density functional theory (DFT) analysis. ZnO samples with varying Ni concentrations were synthesized and characterized. DFT calculations provide theoretical insights, supporting the experimental results and elucidating the mechanisms behind these changes.

Keywords:

DFT, ZnO, Semiconductor

Reference:

Xue, S.; Zhang, F.; Zhang, S.; Wang, X.; Shao, T. Electronic and Magnetic Properties of Ni-Doped Zinc-Blende ZnO: A First-Principles Study. Nanomaterials 2018, 8, 281. https://doi.org/10.3390/nano8050281

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SEMICONDUCTORS / 371

CHARACTERIZATION OF Ga(Mn)As DILUTED MAGNETIC SEMICONDUCTOR GROWN BY MOLECULAR BEAM EPITAXY

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Semiconductors with relatively high concentration of transition metals (between 0.5% and 6% molar fraction) are known as Diluted Magnetic Semiconductors (DMS) due to the arise of ferromagnetic response caused by, in this case, Mn incorporation in the crystalline structure. These materials are the cornerstone for the development and implementation of spintronic devices, which take advantage of the intrinsic magnetic moment of electrons. It is of great importance to study wether the incorporation of the transition metal takes place in interstitial sites or if it is substituting Ga ions in the crystal for the sake of obtaining the desired properties regarding DMS's. In this work, thin films of Ga(Mn)As were grown by the Molecular Beam Epitaxy (MBE) technique under different conditions. Parameters such as the low temperature GaAs buffer layer and the Mn cell temperature were changed in order to modify the incorporation of Mn in the semiconductor. Characterization techniques like XRD, Raman spectroscopy and photo-reflectance were carried out and results were analyzed to infer the quantity of Mn ions and its sites of occupancy in the crystalline structure. Concentrations of Mn in the GaAs thin films were of 1.3% and 2.71% respectively for both cases presented in this work.

Keywords:

thin films, gallium arsenide, III-V semiconductor, Manganese, diluted magnetic semiconductor

Reference:

1 Hideo Ohno, "(Ga,Mn)As: A new diluted magnetic semiconductor based on GaAs", Appl.Phys., vol. 69, no. 3, 1996

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SEMICONDUCTORS / 374

STRUCTURAL, CHEMICAL AND THERMOLUMINESCENCE CHARACTERIZATION OF MEXICAN MINERALS OF DAILY USE

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Mexican minerals (calcite, fluorite, danburite, topaz and aragonite) were structurally and morphologically characterized with X-ray diffraction (XRD) and petrographic microscopy, the blue and green calcites presented the rhombohedral crystalline system. Their chemical composition was analyzed

with electron probe microanalysis (EPMA) obtaining that the molecular formula of the green calcite shows a composition Ca1.95Mg0.05(CO3)2. Photoluminescence spectra of blue and green calcite minerals were also measured, the presence of rare earths such as Eu2+ with excitation transitions 8S7/2 → 6P7/2 and emission 6P7/2 → 8S7/2 was observed. The TL glow curve was measured after irradiating the minerals at a dose of 50 Gy with a beta source of Strontium-90 to evaluate its possible use as a retrospective dosimeter in accidental radiological events. The calcite minerals (blue and green) show a TL curve composed of two maxima, an intense one at 92 ℃ and a lower intensity one at 213 ℃. In the TL response of fluorite, three maxima were observed, one of high intensity at 271 ℃ and two other less intense ones at 85 ℃ and 168 ℃. Danburite shows a TL curve with an intense maximum at 211 ℃, and topaz shows a broad and intense TL maximum at 238 ℃.Finally, aragonite presents a TL curve composed of an intense maximum at 97 ℃ and one of lower intensity at 187 ℃. The TL brightness curve of the Mexican minerals (calcite, fluorite, danburite and topaz) can be useful for possible use in accidental dosimetry because it shows a good TL intensity with localized maxima at optimum temperatures between 180 and 250 ℃.

Keywords:

Thermoluminescence, Dosimetry, Calcite, Minerals, Radiation

Reference:

Dendy, P. P. (2004). "Retrospective assessment of exposures to ionising radiation", ICRU Report 68.

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SEMICONDUCTORS / 396

HIGH RESPONSIVITY AND NEW CAPABILITIES IN OPTOELECTRONICS WITH HYBRID GRAPHENE AND QUANTUM DOT PHOTODETECTORS

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Quantum dots and graphene offer high-quality optoelectronic properties in addition to offer some of the smallest surface/volume ratio and therefore an important route for high-performance and small footprint optoelectronic devices. In this talk, we will present significant improvements over the photoresponsivity and quantum efficiency of hybrid-graphene optoelectronic devices. This included a novel intercalated graphene-quantum dot architecture to increase light absorption and film thickness without sacrificing charge collection. This allows achieving near full-absorption and high-quantum efficiency, which has been one of the major limiting factors for quantum dot optoelectronics. We also show the use of ZnO as an electron collection layer, which is critical to obtain graphene-quantum dot photovoltaic devices. Finally, we will show how the intercalated architecture enables novel capabilities for optoelectronics. In particular, we will show a multispectral photodetector in which intercalated graphene layers have independent electrodes, allowing to detect individual spectral bands that can open the path for thin-film spectral analysis devices.

We will also present a route for integrating sensing, power harvesting, and remote communication for autonomous nanosensors.

Keywords:

Optoelectronics, Graphene, Photodetectors, Quantum Dot

Reference:

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THEORY AND SIMULATION OF MATERIALS / 357

STRUCTURAL, ELECTRONIC AND MAGNETIC PROPERTIES OF GAAS BIDIMENSIONAL: AB INITIO STUDY

Author: Abigail del Pilar Valdés Guajardo[1]

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GaAs is a semiconductor of the III-V family that is distinguished by its properties such as high electronic mobility, this property allows transistors to work at high frequencies. It also has a larger band gap than Si, so it maintains its properties at higher temperatures. However, by reducing the dimensionality of GaAs, the semiconductor behavior changes. In this work the structural, electronic and magnetic properties of two-dimensional GaAs are studied using Density Functional Theory as implemented in Quantum Espresso software. A PBE functional was used to model the correlation and exchange interactions. A conventional wurzite-type unit cell was used for the bulk energy calculations. In the case of two-dimensional GaAs, a 4x4x1 supercell was used. A cutoff energy of 40 Ry was used for the wavefunction expansion. A Monkhorst-Pack 7x7x5 lattice was used for the energy in the bulk and 7x7x5 for the energy in the two-dimensional system. DOS calculation was performed. Total energy calculations were also performed for the system with different vacancies: As vacancy and Ga vacancy. PDOS of the system with Ga vacancy presents a small shift in the energies of up and down spins.

Keywords:

DFT, GaAs, bidimensional

Reference:

Cipriano, Luis & Di Liberto, Giovanni & Tosoni, Sergio & Pacchioni, Gianfranco. (2020). Quantum Confinement in Group III-V Semiconductor 2D Nanostructures. Nanoscale. 12. 10.1039/D0NR03577G.

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THEORY AND SIMULATION OF MATERIALS / 356

ELECTRONIC PROPERTIES OF GRAPHYNE AND GRAPHENE MODIFIED WITH VACANCIES AND SUBSITUTINAL MN DOPING: A DFT STUDY

Author: Otniel García Domínguez[1]

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Graphyne and graphene are two allotropes of carbon. Both are bidimensional materials but they have different electronic properties. We have performed spin polarized first principles calculations to study the doping effects on the electronic and structural properties of graphene and graphyne. Graphene layers have been modeled using the 4x4 periodic supercells. Vacancies and Stone Wales defects were considered. Different geometries of graphyne were considered. Calculations have been done within the periodic density functional theory as implemented in PWscf code of the Quantum Espresso package.A substitutional doping is explored considering Mn atoms. Results show that Mn atoms induces electronic states in Fermi level in both, graphene and graphyne hexagonal systems.

Keywords:

DFT, Graphyne, graphene

Reference:

Li, Z., Smeu, M., Rives, A. et al. Towards graphyne molecular electronics. Nat Commun 6, 6321 (2015). https://doi.org/10.1038/ncomms7321

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THEORY AND SIMULATION OF MATERIALS / 82

PBOH AND PB(OH)2 ADSORPTION ON SRTIO3(111) A DFT STUDY

Author: Reyes García Díaz[1]

Co-authors: María Teresa Romero de la Cruz [2]; Víctor Eduardo Comparán Padilla [3]; Aracely del Carmen Martínez Olguín [4]; Gregorio Hernández Cocoletzi [5]

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Water polluted by lead (Pb) produces health problems. At high levels of exposure to lead the brain and central nervous system can be severely damaged. Lead in human being can produce coma, convulsions and even death. Currently, pollution is an important global problem that have motivated several groups to develop experimental and theoretical investigation using different methods for removing contaminants. Adsorption is a suitable process that can be used to remove dangerous contaminants such as heavy metals like Pb. One of the Pb compounds found in water is lead hydroxide, Pb(OH)2. On the other hand, strontium titanate (SrTiO3) is a perovskite type material with good chemical stability and catalytic properties. This study focuses on the adsorption of lead species (Pb(OH)2 and PbOH) on SrTiO3(111) surface. Calculations were performed using the PWscf code of the quantum ESPRESSO package. The adsorption energy was calculated at different high symmetry sites founding strong interaction with the surface for the PbOH. This is useful for PbOH removal from water. Structural and electronic properties of selected systems are reported and compared with those encountered in the literature. The understanding of the adsorption mechanism may help to propose systems to fabricate improved sensor devices that may guide scientist to more efficient pollutant removal.

Keywords:

Lead species, water pollution, strontium titanate, adsorption, DFT

Reference:

A. L. Wani, A. Ara, J. A. Usmani. Lead toxicity: a review. Interdiscip Toxicol. 2015; Vol. 8(2): 55–64. doi: 10.1515/intox-2015-0009

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THEORY AND SIMULATION OF MATERIALS / 351

AlAs(001) surface reconstruction. Atomistics insights

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Co-authors: Jonathan Guerrero Sanchez [1]; Rodrigo Ponce Perez [2]

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The III-V semiconductors are often used to growth technologies like molecular beam epitaxy. Moreover, the interest in the structure and stability of the (001) surfaces has also been caused by the rich variety of surface reconstructions. The large number of surface reconstructions observed on III-V (001) surfaces have prompted attempts to classify and understand them from a more general point of view. This study attempts to classify the surface reconstruction of AlAs from the (001) surface by first-principle method. There are shown the dimerization and trimerization atomic structures of some different reconstructions.

Keywords:

Surface reconstruction, Semiconductor, AlAs

Reference:

A.M.Dabiran, P.I.Cohen: Journal of Crystal Growth, 1995, 150[1-4], 23-7

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THEORY AND SIMULATION OF MATERIALS / 328

COMPUTER SIMULATION OF THE IRRADIATION OF (BI, PB)-2212 SUPERCONDUCTING THIN FILMS WITH IONS FOR THE CREATION OF MAGNETIC VORTEX PINNING POINTS

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Superconducting materials are capable of carrying electric current densities four orders of magnitude greater than that of a copper wire. A promising method to enhance the critical current density (Jc) in High-Temperature Superconductors is the ion irradiation. The objective is to create imperfections into the crystalline structure of the material, which serve as pinning points for the magnetic vortices that emerge within the type II superconductors. As vortices begin to move within the material, Jc rapidly decreases to zero. The creation of pinning points and the subsequent reduction in vortex mobility serve to enhance the magnitude of Jc of the film. In this work, computer simulations of ion irradiation over a superconducting thin film were made using the software SRIM v. 2013.00 1. Films of the superconductor (Bi, Pb)-2212 (Bi1.6Pb0.4Sr2CaCu2O8) with thicknesses of 200, 500 and 1000 nm were simulated. The parameters of the irradiated ions were: Type of ion: He, C, Si, Cu, Ag and Au. Irradiation energy: 3 and 6 MeV. Angle of incidence: 0° and 45°. For each simulation, a single value was assigned to each of the aforementioned parameters. Each simulation consisted of 100,000 ions fired in succession. Considering that each atom displaced from its original position in the crystal lattice due to ion irradiation can be a pinning point, heavy ions such as Ag and Au were found to be the most efficient in creating pinning points (up to 15000 per ion). The irradiation of samples with lower atomic mass ions like C, Si, Cu, and Ag, resulted in the creation of fewer pinning

points. However, the sample is less likely to become amorphous due to the irradiation process. For an irradiation energy of 3 MeV the amount of ions trapped inside the film increases significantly and is not recommended.
Presenting author: fesanchez4@gmail.com

Keywords:

Computer simulation, High-Temperature Superconductors, Ion irradiation, Magnetic vortices, BSCCO

Reference:

J.F. Ziegler, J. Biersack, U. Littmark, "The Stopping and Range of Ions in Matter",
Pergamon Press, 1985. https://doi.org/10.1007/978-1-4615-8103-1_3

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THEORY AND SIMULATION OF MATERIALS / 307

Charge-density asymmetry in MoSO and MoSeO nanotriangles increases their reactivity towards the hydrodesulfurization reaction

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Co-authors: Luis Pellegrin [2]; José Paez [3]; Rodrigo Ponce [3]; Jonathan Guerrero [3]

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Transition metal dichalcogenides have garnered attention because of their unique physical properties. Janus monolayers with different chalcogen layers may increase their versatility and range of applications. Paez et al. 10.1038/s41598-021-00287-6 demonstrated that charge-density asymmetry generates curvature in MoSeS nanotriangles and, consequently, an increase in their reactivity. Considering such effect, in this work, we engineered the MoS2 and MoSe2 nanotriangles to generate MoSO and MoSeO via selective oxidation of one side of the monolayer, ending up with thermodynamically stable Janus monolayers. After that, we designed MoSO and MoSeO nanotriangles and analyzed the curvature generated by the difference in electronegativity between S/Se and O. Also, we analyzed the reactivity increase due to the induced curvature and discussed their potential in the hydrodesulfurization reaction.

Keywords:

Transition metal dichalcogenides, nanotriangles, curvature, charge density asymmetry

Reference:

M. V. Bollinger, et al. Physical Review B, 67, 085410, 2003.

This work was supported by:

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THEORY AND SIMULATION OF MATERIALS / 226

DFT STUDY OF GRAPHENE OXIDE INTERACTING WITH THE BATIO3(001) SURFACE

Author: Reyes García Díaz[1]

Co-authors: María Teresa Romero de la Cruz [2]; Víctor Eduardo Comparán Padilla [3]; Aracely del Carmen Martínez Olguin [4]; Gregorio Hernandez Cocoletzi [5]

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Ceramic composites with single-walled carbon nanotubes have proven a relevant increase in the mechanical resistance and thermal and electrical conduction. Graphene is a two-dimensional (2D) material with a very large surface area and good electrical conduction, among other properties. However, graphene oxide (GO) is a more accessible material to be synthesized with suitable properties for practical applications. There are reports in the literature of the inclusion of GO in a ceramic matrix of the perovskite barium titanate (BaTiO3) where an improvement in the mechanical, thermal, and electrical conduction is obtained. Unfortunately, in the literature, only a few models exist that explain the GO-perovskite interaction. Understanding the interaction could lead to modifications in the process, increasing the knowledge in the composite material properties. Adsorption energies and charge transfer are important properties in the GO-BaTiO3 interactions study. As part of the current study, the structural and electronic properties of selected GO groups (O, OH) are allowed to interact with the BaTiO3(001) surface, with the results reported and compared with those encountered in the literature.

Keywords:

graphene, graphene oxide, barium titanate, DFT

Reference:

D.W. Boukhvalov, I.S. Zhidkov, A.I. Kukharenko, S.O. Cholakh, J.L. Menéndez, L. Fernández-García, E.Z. Kurmaev. Interaction of graphene oxide with barium titanate in composite: XPS and DFT studies. Journal of Alloys and Compounds 840 (2020) 155747. https://doi.org/10.1016/j.jallcom.2020.155747

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DGTIC UNAM/CGSTIC CINVESTAV project 37-2023.

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THEORY AND SIMULATION OF MATERIALS / 292

AB-INITIO STUDIES OF THE INITIAL STAGES OF THE EPITAXIAL GROWTH OF GaN/GaP SUPERLATTICES IN GaP(hhl) SURFACES.

Authors: Javier Alanis Perez[1]; Esteban Cruz-Hernández[2]; Sandra Julieta Gutiérrez-Ojeda[3]; Gregorio Hernandez Cocoletzi[4]

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The III-Nitride (GaN, AlN, etc) exhibits unique properties that excel other III-V materials. These properties include the high dielectric breakdown voltage, wide bandgap, and high thermal conductivity. However, the monolithic integration of these compounds in Si substrates has been hindered by the mismatch in its fundamental physical properties such as their lattice constant, polarity and the formation of an amorphous SixNy interface 1. The main solution has been the growth of a buffer layer to overcome some of these problems and, in addition, it can also correct the Si surface defects [1,2]. The use of GaP as buffer layer for Si surfaces is a common occurrence due to the low cell parameters mismatch between them. Furthermore, the growth of III-Nitride heterostructures has been proof experimentally with interesting properties [3].
In this work, we present an ab initio study of the initial growth steps of different superlattices of GaN/GaP on GaP(111), GaP(110) and GaP(001) surfaces. The structural changes, energy density differences and interfacial energy were calculated by using density functional theory.

Keywords:

DFT, GaN/GaP, Heterostructures

Reference:

1 https://doi.org/10.1016/S0169-4332(97)00463-7
[2] https://doi.org/10.1063/1.4751024
[3] https://doi.org/10.1134/1.1187571

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Continuidad de Estancia Posdoctoral Académica (3) 2022.

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THEORY AND SIMULATION OF MATERIALS / 88

Determination of thermal properties in thermal insulating solids using Infrared Photothermal Radiometry (IPTR) and numerical simulation by COMSOL Multiphysics

Author: R. C. García Zúñiga[1]

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Currently, there are different photothermal techniques (PTT) for the characterization of materials that allow obtaining thermal properties from the evolution of temperature over time, based on the generation and detection of thermal waves (TW). The PTT used here is the one proposed for the first time by Nordal and Kanstad in 1979 1, which they called Photothermal Radiometry (PTR). This technique is based on inducing temperature changes on the sample surface through the incidence of a modulated light beam, producing TW, and detecting the thermal radiation emitted using an infrared sensor. This allows the detection of temperature changes and obtains information that enables the determination of the sample´s thermal properties [2-4]. Studies were realized using the PTR's back detection configuration on thermal insulating materials. An analytical model was developed and applied to the results of temperature change measurement, in vacuum and ambient temperature under two different modulation frequencies in the intensity of the light beam. Based on the finite element method, numerical simulations of temperature vs time of the PTR process using COMSOL Multiphysics software were obtained [3,4]. The correspondence between the experimental and numerical results demonstrates the usefulness of the developed model for the determination of thermal properties of thermal insulating solids.

Keywords:

Thermal properties; Numerical simulation; Photothermal radiometry

Reference:

1 Nordal, Kanstad, (1979). Physica Scripta 659.
[2] Martínez, K et al. (2015). International Journal of Thermal Sciences, 98.
[3] Suarez, V. et al. (2014) Applied Radiation and Isotopes 83.
[4] Wong, J. et al. (2019). Rev. Mex. Fis. 65.

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THEORY AND SIMULATION OF MATERIALS / 99

COMPUTATIONAL SIMULATIONS OF ANTICANCER DRUGS ENCAPSULATION IN MAGNETIC-DOPED BORON PHOSPHIDE NANOTUBES (BPNTS)

Authors: A. C. Martínez Olguín[1]; Gregorio H. Cocoletzi[2]; M.T. Romero de la Cruz[3]; R. García-Díaz[1]

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Currently, platinum coordination complexes are employed in treating diseases like cancer. These complexes act as anticancer by disrupting DNA configurations, thereby preventing cell damage. However, these drugs make no distinction between healthy and cancerous cells, which is crucial for cancer treatment. Encapsulating these complexes in nanotubes may potentially mitigate their interactions with healthy cells. In this work, we have investigated the encapsulation of anticancer drugs cisplatin, nedaplatin, and carboplatin in magnetic doped (14,0) boron phosphide nanotubes (BPNTs). We have explored different orientations and adsorption sites for drug encapsulation. First principles total energy calculations were performed using the density functional theory (DFT) as implemented in the Quantum ESPRESSO package. The generalized gradient approximation (GGA) with the Perdew, Burke, and Enzerholf (PBE) functional was used to treat exchange-correlation potential energies. Provided that the transition metal dopants contain 3d orbitals, we have included the Hubbard correction (GGA+U) to deal with the highly correlated electrons, and to perform a good description of the electronic and magnetic properties of the different systems. The electron–ion interactions are modeled with the Vanderbilt ultra-soft pseudopotentials. The density of states (DOS) and projected density of states (PDOS) were calculated to investigate the electronic properties. Finally, non-covalent interactions (NCI) were determined to study weak interactions. The results indicate that these nanotubes can encapsulate drug molecules, suggesting their potential use for drug transportation and delivery within biological systems.

Keywords:

Magnetic-dopants, Boron Phosphide Nanotubes, DFT, carboplatin, nedaplatin

Reference:

D. García-Toral, V. M. Vázquez-Báez, R. Mendoza-Báez, E. Chigo-Anota, A.Flores-Riveros , G. Hernández Cocoletzi, J. F. Rivas-Silva, "Structural Stability and Electronic Properties of Boron Phosphide Nanotubes: A Density Functional Theory Perspective", Symmetry 14(5) (2022) 964. https://doi.org/10.3390/sym14050964

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SIMULATION OF CHARGE TRANSPORT AND OPTICAL PROPERTIES IN THE DISTRIBUTION OF CARBON PARTICLES IN CARBON-TIO2 FILMS.

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In the last decades, photocatalysis has been extensively studied for applications in air and water treatment, water splitting, and antimicrobial purposes. Despite its potential, the practical application of photocatalysis remains limited by low photocatalytic efficiency and poor stability. Considerable efforts have been devoted to enhancing the photocatalytic to enhance charge transport under sunlight irradiation and prevent electron-hole pair recombination. However, the development of high-efficiency photocatalysts necessitates a thorough understanding of the photophysical processes involved, including: i) Photon absorption and electron-hole pair generation ii) Migration of charge carriers to the surface iii) Semiconductor-electrolyte interactions. In this study, we propose a computational approach to investigate these physical phenomena through simulations. We focus on the impact of carbon particle distribution within a TiO2:C composite material on charge transport, we analyzed three possible distributions of carbon particles: on the surface, within the structure, and in both locations. We used wxAMPS software to simulate charge transport and estimate surface current density for photocatalytic applications. Our results indicate that the optical properties of carbon particles significantly affect the generation of charge carriers on the surface and the best distribution of carbon particles occurred when they are inside the TiO2:C composite structure. Furthermore, the distribution of carbon nanoparticles plays a crucial role in enhancing charge carrier generation. This work highlights the importance of optimizing the distribution of carbon and TiO2 particles and demonstrates the utility of wxAMPS software for simulating and understanding charge transport in photocatalytic systems.

Keywords:

Photocatalysis, wxAMPS, carbon-TiO2 composites, simulation photocatalysis, distribution of carbon particles

Reference:

A new solar cell simulator: WxAMPS,Journal Article, (2011), DOI:10.1109/PVSC.2011.6186517.

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THEORY AND SIMULATION OF MATERIALS / 229

FIRST PRINCIPLES STUDIES OF THE SILVER DEPOSIT ON HIGH INDEX SILICON SURFACES

Author: Gregorio Hernandez Cocoletzi[1]

Co-authors: WILFRIDO CALLEJA ARRIAGA [2]; Reyes García Díaz [3]; Juan Carlos Moreno Hernández [4]; Aracely del Carmen Martínez Olguin [5]; Dolores García Toral [6]; María Teresa Romero de la Cruz [7]

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Silver (Ag) deposit on high index silicon (Si) surfaces is investigated using first principles total energy calculations within the density functional theory (DFT). Two surfaces are considered, namely Si(114) and Si(5512), and several Ag concentrations are used, starting with one Ag atom up to two monolayers. Special attention is paid on the atomic wire formation. The first step is to determine the total energy of each case, afterwards, the surface formation energy is calculated, then the electronic properties are explored. Concerning the electronic properties, the total density of states (DOS) and the projected density of states (pDOS) are calculated. According to the discussion of results, we have also performed ab-initio molecular dynamics (ABMD). Surface formation energy results show that the Ag deposit on the Si surfaces may produce stable atomic structures. Moreover, the ABMD results corroborate the SFE findings.

Keywords:

silver nanowires, high index silicon surfaces, DFT

Reference:

A. Bhukta, P. Guha, A. Ghosh, P. Maiti. Growth of Ag nanostructures on high-index Si (5 5 12) surfaces under UHV conditions: effect of prior surface treatment before deposition. Appl. Phys. A (2016) 122:356. DOI 10.1007/s00339-016-9929-6

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THEORY AND SIMULATION OF MATERIALS / 209

INFLUENCE OF GRAPHENE FUNCTIONALIZATION IN MANGANESE DIOXIDE ELECTRONIC PROPERTIES: A COMPUTATIONAL STUDY

Authors: Ana Karina Cuentas Gallegos[1]; Christian Alejandro Celaya López[1]; Elizabeth Fernández García[2]; Jesus Muñiz Soria[3]

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Metal oxides and carbon materials are exceptionally compatible material choices for electrode materials on supercapacitors due to their capacity to provide high pseudocapacitance and superior electrical conductivity. Among metal oxides, MnO2 possesses one of the highest theoretical pseudocapacitances, and birnessite layered polyphorm allows fast charge-discharge electrosorption. This compatibility, in turn, results in heightened specific energy and power, respectively. Nevertheless, the deposition of metal oxides onto various carbon allotropes presents several challenges when it comes

to harnessing the full potential of carbon's extensive specific surface area and electrical conductivity. Achieving the optimal metal oxide loading of a particular carbon allotrope surface is a key challenge. With this in mind, we are conducting an investigation into the interactions between carbon nanocomposite materials with functional groups (such as OH, COOH, NH2) and birnessite MnO2. Therefore, we introduce in silico models of carbon nanostructures with the mentioned functional groups and MnO2. Morse potential function calculations results indicate better affinity.

Keywords:

MnO2, Carbon nanomaterials, Functional Groups, Energy Storage, DFT.

Reference:

Huanping Yang, Jian Jiang, Weiwei Zhou, Linfei Lai,. Influences of graphene oxide support on the electrochemical performances of graphene oxide-MnO2 nanocomposites. Nanoscale Research Letters, 6:531 (2011). http://dx.doi.org/10.1186/1556-276X-6-531

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THEORY AND SIMULATION OF MATERIALS / 197

Experimental and theoretical assessment of the Eu3+ doped Bi4Ge3O12

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In this work, Bi4Ge3O12 doped with Eu3+ was investigated experimentally and theoretically. The synthesis of several samples with different Eu3+ concentrations was carried out by the polymeric precursor method. Photoluminescence spectroscopy was performed, and it shows the typical electronic transitions of Eu3+. FTIR interpretation of samples allows us to infer that Eu3+ substitutes not only Bi3+ but also Ge4+. This interpretation was corroborated by ab initio calculations as both substitutions were found to be thermodynamically stable. Eu3+ naturally takes on the Bi3+ sites, producing ferromagnetic alignment; but when Eu3+ takes on the Ge4+ sites the alignment becomes antiferromagnetic. Since rare earth elements are particularly important in modifying the magnetic and luminescent properties of host materials, our findings open a new way to give a bi-functionality to the Bi4Ge3O12 material through selective doping.

Keywords:

Eu doped, BGO, magnetism

Reference:

Journal of Alloys and Compounds 966 (2023) 171567

This work was supported by:

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EFFICIENT COMPUTATIONAL MODEL FOR PREDICTION OF CONTINUUM PERCOLATION THRESHOLD FOR SPHERICAL PARTICLES IN 3D POLYMER/CONDUCTIVE COMPOSITES

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Polymeric composite materials are among the most researched in the industry because of their excellent performance in several applications that combine the properties of metals or ceramics with the lightness and flexibility of polymers. Percolation theory is relevant in research on these materials because it allows the estimation of the percolation threshold f_c, which is the critical volumetric fraction at which phase transition occurs, where certain properties of the filler material begin to dominate those of the polymeric matrix. In this work is proposed an efficient computational model for the estimation of the electrical percolation threshold for spherical conductive particles in 3D composites using the continuum percolation approach, where the particles are dispersed freely in space. The particle distribution method is based on a simple reflex agent that distributes particles by following conditional rules to avoid an overlap between them. Percolation evaluation is performed by pathfinding conduction through the material, considering both the contact and quantum tunnelling conduction mechanisms. The A^* heuristic algorithm was used owing to its efficiency and capacity to find the shortest paths. Experiments were performed with different particle sizes ranging from 15 to 500 nm, considering a constant maximum tunnelling distance of 10 nm. The obtained results show percolation threshold values of $f_c = 0.06$ for the smallest particles and values of $f_c = 0.29$ for larger particles, indicating the effect of particle size on the percolation threshold. Similar results have also been reported in other studies

Keywords:

Percolation threshold, polymeric composites, continuum percolation

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THEORY AND SIMULATION OF MATERIALS / 160

Surface stability and magnetic arrangements of SrRuO3 surfaces

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The strontium ruthenate (SrRuO3) perovskite is a ferromagnetic material that crystallizes in three phases (tetragonal, orthorhombic, and cubic). This perovskite has been widely studied in the last fifty years due to its high conductivity, Curie temperature of 160 K, and because it is chemically inert. To this day, most studies focus on the orthorhombic bulk system, but less effort has been put into studying its different possible surfaces. In this work, we investigated the cubic and orthorhombic SrRuO3 surfaces at the atomic scale in the [001], [110], and [111] directions. For each direction, three different surface terminations were proposed. The surface formation energy formalism was employed to study the thermodynamic stability of these models and find the most stable surface. Besides, the magnetic properties of the surfaces were analyzed to determine if these surfaces show perpendicular magnetization anisotropy (PMA). Finally, the electronic band structure was calculated to determine if the surfaces present topological surface states (TSS), making them suitable for enhanced catalytical applications.

Keywords:

SrRuO3, surfaces, magnetic properties, DFT

Reference:

NA

This work was supported by:

DGAPA-UNAM projects IA100624, IG101124, IG101623. CACG thanks DGAPA for the postdoctoral grant. Calculations were performed in the Miztli supercomputer projects LANCAD-UNAM-DGTIC-368, LANCAD-UNAM-DGTIC-422, and LANCAD-UNAM-DGTIC-084. JGS acknowledges LNS-BUAP project 202201042N and THUBAT KAAL IPICYT supercomputing center project TKII-JGSA001.

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THEORY AND SIMULATION OF MATERIALS / 164

ANIONIC GOLD IN RARE EARTH OXIDES? IN SEARCH OF NEW ENVIRONMENTAL REMEDIATION AGENTS.

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The environmental impact caused by man has reached levels of no return. Among the problems of this nature are climate change and air pollution. The use of materials to remove contaminants has been widely studied. However, the search for new materials that improve efficiency in contaminant removal has been constant. In this sense, gold is known for its ability to improve various material properties. It facilitates the conditions to catalyze several reactions of high interest in environmental remediation. It is well known that gold behaves as a cation in a wide variety of materials of which it is a part or in which it is deposited or incorporated. However, the existence of anionic gold in some compounds has also been reported in the literature. Although it has been discussed in terms of experimental evidence, and it is known that it can exist in double perovskite-type structures, so far, there is no atomic-scale explanation of the interaction mechanisms, as well as the conditions that lead to the anionic behavior of gold in this type of structures and the potential applications it has in environmental remediation. Prominent candidates for finding anionic gold with great possibilities for application in environmental remediation are rare earth oxides since they have been shown as excellent catalysts for the CO oxidation reaction with great selectivity, in addition to the low electronegativity that f-block metals have. In this work, the modification of CeO2 with Au was simulated employing density functional theory (DFT) calculations. Surface models of (111) and (100) were constructed. The most probable adsorption sites were determined by electrostatic potential maps. Au adsorption was assessed by constructing several models. Determination of anionic gold behavior was carried out by Bader charge analysis.

Keywords:

anionic gold, rare earth oxides, CeO2, DFT

Reference:

T.A. Zepeda, R. Ponce-Pérez, A. Solis-Garcia, J. Guerrero-Sanchez, S. Fuentes, S.A. Gomez, Boosting oxygen activation in ceria-oxide via gallium addition, Appl Catal B 336 (2023). https://doi.org/10.1016/j.apcatb.2023.122936.

This work was supported by:

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THEORY AND SIMULATION OF MATERIALS / 183

First principles studies of the adsorption of short-chain aldehydes on 2D-As-P compounds

Author: Jose Mario Galicia Hernandez[1]

Co-authors: Jonathan Guerrero Sanchez [1]; Noboru Takeuchi [1]

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We have performed a first principles study based on the Density Functional Theory, focused on the adsorption of short-chain aldehydes on 2D-As-P compounds. The aim of the work is to test the catalytic properties of these 2D systems, as the proposed molecules own particular characteristics in their structure and chemical reactivity. In the study we use a selective hydrogenation of the 2D systems in order to facilitate the adsorption. On the other hand, we have included the presence of vacancies in order to induce active-sites to favor the adsorption. The study also considers the description and prediction of self-propagating reactions that can take place on the sheets, as a results of the adsorption of the molecules, in order to control and reduce the toxicity of these molecules. Besides, we have predicted that, as products of the chemical reactions, it was possible to obtain alcohols and other compounds which can be used in several industrial processes. Finally, we have included a study of the changes in the charge distribution by calculating the Bader population analysis, for a better understanding of the adsorption processes.

Keywords:

2D-Si-Ge, Aldehydes, adsorption

Reference:

Jiating Lu; Xi Zhang; Limeng Shen; Ya Nie; Gang Xiang, J. Appl. Phys. 127, 094302 (2020).

This work was supported by:

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COMPLEX BAND STRUCTURE OF THERMAL WAVE CRYSTALS: THE PLANE-WAVE METHOD

Author: César Augusto Romero Ramos[1]

Co-authors: Betsabe Manzanares Martinez [1]; Diego Soto Puebla [1]; Jesus Manzanares Martinez [1]

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In this paper, we present an extension of the plane-wave method (PWM) to compute the complex band structure of thermal wave crystals (TWCs). The structural periodicity of TWC allows the possibility to manipulate non-Fourier heat via wave interference. While the Cattaneo-Vernotte (CV) heat conduction theory accurately models oscillatory wave-like propagation of heat in TWCs, obtaining an eigenvalue equation for frequency using the CV wave equation is not possible. To overcome this limitation, we propose a novel approach that solves a complex eigenvalue equation for the Bloch wave vectors.

Keywords:

Heat, non-Fourier, Crystal

Reference:

A.-L. Chen, et al., Heat reduction by thermal wave crystals, International Journal of Heat and Mass Transfer 121 (2018) 215

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THEORY AND SIMULATION OF MATERIALS / 225

ELECTRONIC STRUCTURE OF NICKEL-DOPED LK-99 MATERIAL: AB INITIO CALCULATIONS

Authors: Ernesto Alonso Guerrero García[1]; Israel Omar Pérez López[2]; José Luis Enríquez Carrejo[2]

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In July 2023, researchers led by Sukbae Lee, et al., announced the creation of the first room-temperature superconductor (RTS) with a critical temperature (Tc) of 400 K. The material, named LK-99, is a lead phosphate apatite (Pb10P6O25) doped with copper ions (Cu2+). Theoretical studies have demonstrated the possibility of superconductivity in the crystal lattice of LK-99, especially with copper doping. However, transition metals like nickel and zinc, like copper, could also induce the superconducting state in LK-99. Simulation and density functional theory (DFT) calculations of nickel-doped LK-99 will allow for a better understanding of the effect of doping on the electronic structure and potential superconductivity, avoiding costly experiments and exploring different structural and electronic scenarios. This will serve as a theoretical basis for experimental research. The project aims to study the electronic properties of copper and nickel-doped LK-99 (Pb10-nXn(PO4)6O), with n = 1, 2, 3, using DFT calculations. The geometric optimization of the material and its copper-doped variant was carried out using CASTEP program. The Kohn-Sham equations were solved with the PBE-GGA functional, using a 5x5x5 k-point mesh in the first Brillouin zone for the self-consistent cycle. For the density of states calculations, the grid was expanded to 10x10x10. The band structure and state density calculations of pristine LK-99 and its copper-doped and nickel-doped versions were obtained to analyze and determine the presence of the superconducting state of the material and compare the results with those found in the literature.

Keywords:

Superconductivity, Electronic structure, Density functional theory, state density, band structure

Reference:

S. L., J.-H. K., Y.-W. K., "The First Room-Temperature Ambient-Pressure Superconductor". 2023.
S. M. G., "Origin of correlated isolated flat bands in copper-substituted lead phosphate apatite". 2023.

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THEORY AND SIMULATION OF MATERIALS / 213

UNDERSTANDING MOLYBDENUM DISULFIDE MONOLAYER REACTIVITY WITH ZINC OXIDE NANOBUBBLES: A THEORETICAL STUDY

Authors: Alan Miralrio[1]; Ana Karina Cuentas Gallegos[2]; Christian Alejandro Celaya López[3]; Daniel G. Araiza[4]; Eduardo Rangel[1]; Luis Enrique Sansores Cuevas[5]

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Over time, several research groups have focused on studying proposals to activate the surface of molybdenum disulfide (MoS_2) monolayer, which is almost inert in the pristine form 1. Herein, we present a theoretical study that investigates the conformational behavior and chemical reactivity of a $(ZnO)_{12}$ nanobubble attached to a MoS_2-S defective monolayer [2,3]. Our analysis reveals that the nanobubble attaches to the monolayer via an O atom and two Zn atoms, activating the surface chemically as previously hypothesized based on an Au_S defect.The adsorption energy, measured at approximately 3.38 eV, indicates strong chemisorption between the nanoparticle and the defective monolayer. Charge density difference maps illustrate significant charge transfer from the middle atomic layer of molybdenum atoms to the nanobubble. The moieties' primary contact points are Zn-S and Au-O bonds, with a bond length of 2.13 Å for Au-O. Analysis of the density of states (DOS) and projected DOS (PDOS) reveals overlapping orbitals of Au ($5d$), O ($2p$), and Zn ($3d$), indicating their involvement in the chemical bonding between the monolayer and the nanoparticle. The Zn-S bonds exhibit a covalent character due to charge accumulation. Also, surface functionalization with the semiconductor nanoparticle does not significantly alter the band gap in terms of magnetism. The incipient chemical activation of the MoS_2 monolayer, achieved by the extrinsic defect Au_S, was enhanced by the interaction with the semiconductor zinc-oxide nanobubble $(ZnO)_{12}$. A chemisorption process was evidenced after a conformational study carried out, within dispersion-corrected density functional theory (DFT).

Keywords:

DFT, MoS2, Zn12O12, CO adsorption

Reference:

1 Ouyang, et al. (2016). Chemistry of Materials, 28(12), 4390-4396.
[2] Miralrio et al. (2018). Applied Surface Science, 455, 758-770.
[3] Flores-Hidalgo et al. (2013). Journal of the Chinese Chemical Society, 60(8), 1082-1091.

This work was supported by:

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THEORY AND SIMULATION OF MATERIALS / 125

Engineering TiO2 surfaces to enhance the LP gas detection.

Authors: Jonathan Efrain Rodriguez Hueso[1]; Jonathan Guerrero-Sánchez[2]; Rodrigo Ponce[2]; Hugo Aejandro Borbon Nuñez[3]

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Understanding and manipulating materials at the atomic scale has become a fundamental aspect of engineering the materials involved in high-performance devices. In the present work, we report the sensing behavior and structural properties of the titanium dioxide surface (TiO2) of the optimized structures and describe the structural and electronic properties of the interaction between the molecules that integrate the LP gas (butane, propane, and methanethiol) and the anatase TiO2 surface. The aim was to evaluate the feasibility of this material in a high-performance LP gas sensor device. Results demonstrate that the methanethiol of LP gas was the most reactive molecule to the TiO2 surface. In addition, the electrical properties calculated show the need to induce oxygen surface vacancies or a rearrangement of the (101) surface TiO2 anatase to make the interaction with methanethiol detectable. Our results are a step further in the design of LP gas sensing devices with modified TiO2 substrates.

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Keywords:

TiO2, Surface, LP Gas, Gas sensor, DFT.

Reference:

Rodríguez-Hueso Jonathan E., Borbón-Nuñez H. A., Guerrero-Sánchez Jonathan, et al., Atomic-scale study of TiO2-GR nanohybrid formation by ALD: the effect of the gas phase precursor, Nanoscale Adv., 2023,5, 5476-5486, https://doi.org/10.1039/D3NA00729D

This work was supported by:

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Author approval:

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THEORY AND SIMULATION OF MATERIALS / 178

Water splitting mediated by proton transfer on defected BiOI surfaces.

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Co-authors: Eduardo Gerardo Pérez Tijerina [2]; Hector Noe Fernandez Escamilla [2]; Jonathan Guerrero Sanchez [3]; Rodrigo Ponce Perez [1]

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Hydrogen generation is complex because it requires high energy; an example is electrolysis, which needs 2.456 eV/particle to dissociate it 1. Different materials have been investigated to achieve water splitting. Bismuth oxyhalides (BiOX, X = Cl, Br, I) are constantly investigated due to their efficient catalytic properties, among them recently the material BiOI (2x1) has been studied, which by first-principles simulations proved to be stable [2]. It has vacancy-mediated channels that serve as catalytic points for water splitting. Using the BiOI (2x1) structure, it was possible to determine an energy barrier to dissociate water molecules, where a barrier of 0.106 eV. Two hydrogen atoms are displaced in the process, recreating a proton transfer effect—such an effect generates lower energy barriers than those required for electrolysis.

Keywords:

Water, BiOI, proton transfer, energy barrier

Reference:

Fernández-Escamilla, H. N., et al. "Bismuth and oxygen vacancies induce (2× 1) reconstructions in bismuth oxyhalide (BiOX, X= Cl, Br, I)(0 0 1) surfaces." Applied Surface Science 618 (2023): 156583.

This work was supported by:

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THEORY AND SIMULATION OF MATERIALS / 395

DFT in a Computational calculation of normal vibrational modes for rhodamine B.

Author: Carlos Alberto Carpio Amador[1]

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Density Functional Theory (DFT) is the best way to solve the Schrödinguer equation for a many-body system. Could be used to find the normal vibrational modes for a molecule, for a molecule assembled by many atoms the exact solution is hard to get. There are only a few articles with computational calculations of the vibrational modes of the markers, because the current development of the DFT theory is not sufficient and the computational requirements are highly expensive and not very accessible. For this reason, this work presents a general algorithm to use DFT and computational methods to solve this problem on vacuum. Comparing our results with experimental data, our percentual errors are minimal.

Keywords:

DFT, SERS, Ramman spectroscopy, rhodamine B.

Reference:

1. H. Watanabe, N. Hayazawa, Y. Inouye, S. Kawata.(2005). DFT Vibrational Calculations of Rhodamine 6G Adsorbed on Silver: Analysis of Tip-Enhanced Raman Spectroscopy. J. Phys. Chem. B 2005, 109, 5012-5020.

This work was supported by:

1. C.A.Carpio Amador (2024).Determinación experimental de los modos vibracionales de la rodamina B y su comparación con cálculos DFT como entrenamiento para su futura aplicación en biomarcadores de Cáncer de Ovario (Tesis de Maestria en física). CINVESTAV Unidad Zacatenco.

Author approval:

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THEORY AND SIMULATION OF MATERIALS / 115

THERMODYNAMIC STABILITY OF THE TaN/MgO INTERFACE

Authors: Victor Quintanar-Zamora[1]; Michelle Cedillo-Rosillo[1]; Oscar Contreras-López[2]; Jonathan Guerrero-Sánchez[2]; Rodorigo Ponce-Pérez[2]; Armando Reyes-Serrato[2]; Jesús Antonio Díaz[2]

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The present work studies the growth of TaN thin films by reactive pulsed laser deposition (PLD) on MgO (001) substrates. Cross-section micrographs acquired by transmission electron microscopy (TEM) reveal that the epitaxial relation between the TaN film and the MgO substrate is $[001]_{TaN}/[001]_{MgO}$. Furthermore, the films exhibit a lattice mismatch with the substrate around 3%. In addition to the experimental measurements, first-principles DFT calculations have been performed to find a thermodynamically stable TaN/MgO interface model by evaluating it with the interface formation energy

(IFE) formalism 1. These calculations determine the most feasible model for the interface, which is a tantalum oxide layer formed between the TaN and MgO layers. Finally, the electronic properties at the interface, such as density of states (DOS) and electron localization function (ELF), were calculated. The DOS reveals a metallic behavior, with Ta-dyz and Ta-dxz degenerated orbitals mainly contributing to the states at the Fermi energy (EF). Meanwhile, the ELF shows ionic-type bonding at the interface.

Keywords:

tantalum nitride, magnesium oxide, thermodynamic stability, TEM, DFT

Reference:

1 J. Guerrero-Sánchez, and Noboru Takeuchi, Formation of ferromagnetic/ferrimagnetic epitaxial interfaces: Stability and magnetic properties, Computational Materials Science, 144 (2018) 294-303. https://doi.org/10.1016/j.commatsci.2

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THEORY AND SIMULATION OF MATERIALS / 140

NUMERICAL APPROXIMATIONS FOR THE MADELUNG CONSTANTS AND THE BINDING ENERGIES FOR CRYSTAL LATTICES FCC, BCC AND HCP

Authors: David Peralez Olguin[1]; Jorge Luis Medrano Mendieta[1]; José David Lamas Medina[1]; Oscar Joel Castro Contreras[1]

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The Madelung constant is a geometric quantity related to the electrostatic potential energy of a crystal. It is the sum of all the ionic interactions in the lattice based on the three dimensional positions of the ions and takes into account the distance and charge of each ion. The Madelung constant is important in understanding the properties and behavior of crystals. In this work, a code which calculate the Madelung constant was implemented using Phyton as language programming. The code was implemented for structures like NaCl and CsCI. The methodology is based on concepts of crystallography and solid state which were implemented in the Phyton code. The calculations of the Madelung constant depend on the number of terms in the series. The calculations were performed using a N from 1 to 120. The constant Madelung value, is agree with values in the literature.

Keywords:

Madelung constant, Phyton code, NaCl, CsCl, NiAs

Reference:

McKelvy, J. P. (1993). Solid state physics for engineering and material science. Krieger Publishing Company.

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THEORY AND SIMULATION OF MATERIALS / 344

Strain effect on Cr2C MXene passivated surfaces: insight from first principles calculations

Authors: Ma. Guadalupe Moreno-Armenta[1]; Sandra Julieta Gutierrez Ojeda[2]

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structural, electronic and magnetic properties of passivated surface of Two-dimensional Cr2C MXene were studied by Density Functional Theory with spin polarization. The most possible surface termination after synthesis (Cl, F, O2 and OH) were considered. For this study high symmetry sites adsorption were considered and the biaxial and uniaxial strain, from -5% to 5% to represent compressive and tensile strain, were considered in the deformation effect study. Regarding with the electronic and magnetic properties these could be tunable and it could be a good candidate to employed in the spintronic area.

Keywords:

DFT, Cr2C MXene, Functional groups, strain effect

Reference:

…

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Correspondence should be addressed to sjulietago@fisica.unam.mx ,moreno@ens.cnyn.unam.mx We thank DGAPA-UNAM projects IG101124, IA100624, and IN101523 for partial financial support. Calculations were performed in the DGTIC-UNAM Supercomputing Center projects LANCAD-UNAM-DGTIC-150, LANCAD-UNAM-DGTIC-368, and LANCAD-UNAM-DGTIC-422.

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THEORY AND SIMULATION OF MATERIALS / 36

DFT+U STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF ZnO-O (0001) POLAR SURFACE

Author: Roberto Silva Gonzalez[1]

Co-authors: Daniel Olguin [1]; Jose Martin Yáñez [1]

[1] *CINVESTAV-QUERETARO*

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Density Functional Theory using the Hubbard correction (DFT+U), as well as the generalized gradient approximation (GGA) to the exchange-correlation part of the total energy, were implemented to investigate the structural and electronic properties of wurzite ZnO-O (0001) polar surface. To study the stability of the ZnO-O (0001) surface, we minimize the total energy as a function of different vacuum thicknesses for multiple constructed supercells. The Coulomb on-site interaction was considered to describe appropriately the stronger hybridization between Zn-3d states and O-2p states, the dispersion of Zn-4s states through the Fermi level, and the surface's conductivity type. The effective values of the U parameters were obtained in a self-consistent procedure, using linear response theory as it is implemented in Quantum ESPRESSO (QE) suite. Our obtained results are discussed and compared with available experimental and theoretical data.

Keywords:

ZnO-O (0001) polar surface, DFT+U, Semi-infinite media approximation, Quantum ESPRESSO.

Reference:

P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017)

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THEORY AND SIMULATION OF MATERIALS / 100

Ab-initio Assessment of Thermoelectric Properties of Cobalt-doped Zinc Oxide.

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In this study, the thermoelectric properties of $Zn_{1-x}Co_xO$ (x=0.03, 0.1, 0.4) have been investigated by using the first principles calculations based on the combination of the density functional theory model "QUANTUM EXPRESSO"with the semi-classical transport theory software "BoltzTraP". The DFT model has shown solid abilities to reproduce the electronic structure of the material of interest. The results input by the combined models show a clear reduction in the lattice thermal conductivity as the Co doping level is increased without affecting the electrical conduction. This enhances the dimensionless figure of merit zT of the material, which rises from 0.03 in the pure sample to 0.97

in the doped one at 400° C. It is also possible to note that Co-doping contributes to a considerable reduction in the bipolar effects that appear in the material at high temperatures.

Keywords:

First-principles calculations, Thermoelectric, Seebeck coefficients, figure of merit, zinc oxide

Reference:

we have not cited any reference in the abstract.

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THEORY AND SIMULATION OF MATERIALS / 206

First-principles calculations for structural, electronic, and phonon properties of H3S, D3S, MgB2 y Nb-bcc conventional superconductors under pressure

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In this work, we investigated the structural, electronic and phonon properties of H3S, D3S, MgB2 y Nb-bcc conventional superconductors using density functional theory. Our interest is focused on evaluating the effect of pressure on the electronic and phononic properties of some well-known superconducting compounds, with the idea of establishing possible correlations with observed patterns in the functional derivative of Tc with respect to the electron-phonon spectral function α2F(ω), δTc/δα2F(ω), as a function of Tc and pressure. These patterns have already been reported in the literature 1 and appear to have some relationship with the superconducting temperature Tc measured in these systems. This study aims to establish a potential mechanism for a Tc prediction based on the δTc/δα2F(ω).

Keywords:

First-principles-calculations, density-functional-theory, electronic-phonon-properties, conventional-superconductors, Eliashberg -theory

Reference:

J. Camargo-Martínez, F. Mesa, G González-Pedreros . Temperature effects on the calculation of the functional derivative of Tc with respect to α2F(ω), PLoS ONE 18(6) (2023) e0286855. https://doi.org/10.1371/journal.pone.028685

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THIN FILMS / 15

Nanoparticle formation in co-sputtered Cu-Ni films deposited by reactive RF-Sputtering*

Author: Luis Vega-Cano[1]

Co-authors: Leonel Sanchez-Garcia [1]; Alejandra Garcia-Sotelo [1]; Angel Guillen-Cervantes [1]; Miguel Melendez-Lira [1]

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Cu and Ni are metallic elements relatively abundant with important applications by their own. There are reports of catalytic applications for Cu-Ni bimetallic films and copper oxides and nickel oxides are semiconductor compounds. CuO is a p-type semiconductor with a narrow bandgap of approximately 1.3 eV to 2.1 eV. NiO is also a p-type is a ferroelectric semiconductor with direct allowed energy bandgap between 3.6 and 4 eV.
In this work Cu-Ni films were prepared by RF sputtering employing a Cu-Ni sputtering target employing RT, 100, 200 and 300 ℃ employing Ar and an Ar-O2 mixture . Also to produce nanoparticles a sequential process Cu-Ni oxide/Cu-Ni/Cu-Ni oxide was employed 1.
Results of morphological, structural, chemical and electronic properties are reported y results discussed in terms of their potential applications.

Keywords:

nanoparticles, semiconductor oxides, catalysis, thin films

Reference:

1 Avila-Meza, M.F., et al. Synthesis and Characterization of Self-Assembled ZnO Nanoparticles Embedded Within a SiO2 Matrix Deposited on (111) p-Type Silicon By Reactive RF Sputtering Using Metallic Zinc Target As Precursor. J. Electron. Mater. 47, 6607–6612 (2018).

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THIN FILMS / 21

GROWTH OF SMFE1-XCOX THIN FILM BY MOCVD AND EXITU DIFFUSION PROCESSES

Authors: Agustin Conde-Gallardo[1]; Karen Aguilar-Mendoza[2]

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Based on the viability of the method to grow other 1111 family iron-based compound polycrystalline superconductor thin films by MOCVD and exitu diffusion processes, in this work, we report studies details of the synthesis of the SmFe1-xCoxO thins films by MOCVD and exitu diffusion processes. The cobalt (Co) percentage is varied in the films, and different thermal treatments are explored to synthesize the superconducting phase with the highest transition temperature (Tc). Additionally, different annealing times and temperatures are investigated to optimize the superconducting transition once that the cobalt percentage at 10% is fixed. The X-ray diffraction, scanning electron microscopy, and the measurement of resistance as a function of the temperature show that the best results are for annealing at 1323K for 3 hours.

Keywords:

Superconductors, Resistivity, MOCVD,

Reference:

10.1088/1361-6668/ab098f

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THIN FILMS / 322

ELECTRICAL AND OPTICAL ANALYSIS OF ULTRA-THIN FILMS OF NANOMATERIALS VIA THZ TIME-DOMAIN TRANSMISSION SPECTROSCOPY

Author: Gustavo Hilario Perez[1]

Co-authors: Alfredo David Morales Vite [2]; Pablo Córdova Morales [1]; Adrián Martínez Rivas [3]; Alejandro Gonzalez Cisneros [4]; Jose Didino García Aguilar [5]; Ángel Adalberto Durán Ledezma [6]; Donato Valdez Pérez [2]

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The nanomaterials currently find numerous applications in optoelectronics, photonics, and nanophononics for the development of new ultrafast systems and the next generation of devices. In this report,

we present findings from an experimental assessment of ultra-thin films composed of graphene oxide (GO) and reduced graphene oxide (rGO), deposited onto glass substrates using the Langmuir-Blodgett (LB) technique. Using Scanning Electron Microscopy (SEM), we show the distribution of nanomaterials forming an ultra-thin film on the glass substrate. The optical and electrical properties, such as the refractive index, dielectric constant, and frequency-dependent complex conductivity, were analyzed employing terahertz time-domain spectroscopy (THz-TDS). Raman spectroscopy provided insights into film thickness, monolayer count, and vibrational modes, all contributing to the assessment of the graphene quality in the thin films. The results obtained in this assessment suggest that GO and rGO materials are promising for application in metasurfaces and for micro and nano-devices operating at THz frequencies, such as photoswitches, filters, and multiplexers/demultiplexers.

Keywords:

THz-TDS, Ultra-Thin films,

Reference:

Eda, Goki, and Manish Chhowalla. "Chemically derived graphene oxide: towards large-area thin-film electronics and optoelectronics." Advanced materials 22.22 (2010): 2392-2415.

This work was supported by:

Authors are thankful to CONHACYT (Number 1222922), SIP-IPN Project Number 20230447 and 20231556.

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THIN FILMS / 341

EXPLORING THE OPTOELECTRONIC POTENTIAL OF TWO-DIMENSIONAL MONOLAYERS ON FLEXIBLE SUBSTRATES: GAINING INSIGHTS FROM THZ MICROSCOPY AND SPECTROSCOPY ANALYSIS

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Co-authors: Gustavo Hilario Perez [2]; Pablo Córdova Morales ; Adrián Martínez Rivas [3]; Narciso Muñoz Aguirre [4]; Ángel Adalberto Durán Ledezma [5]; Jose Didino García Aguilar [6]; Donato Valdez Pérez [7]

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This study delves into monolayers of graphene oxide (GO), reduced graphene oxide (rGO) and derivatives deposited on a flexible substrate called polydimethylsiloxane (PDMS), using the Langmuir-Blodgett technique. The optical and electrical properties were examined using terahertz time domain spectroscopy (THz-TDS), which shows us information about the refractive index and absorption. Atomic force microscopy (AFM) provided details of the thickness and morphology of the samples. Scanning electron microscopy (SEM) revealed the distribution of the deposited graphene layers

using the Langmuir-Blodgett balance. The findings of this research highlight the potential of two-dimensional materials in the development of optoelectronic devices as flexible metasurfaces designed to operate in the THz region.

Keywords:

absorption, flexible, Langmuir-Blodgett, monolayers, terahertz

Reference:

Podzorov, A., & Gallot, G. (2008). Low-loss polymers for terahertz applications. Applied Optics, 47(18), 3254. https://doi.org/10.1364/ao.47.003254

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THIN FILMS / 104

NiCo2O4 thin films chemically deposited

Authors: Miguel Martinez Gil[1]; Fernanda Vega Panduro[1]; Frank Romo García[1]; Rafael Verdugo Miranda[1]; Wencel De La Cruz[2]

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A promising material used as an electrode in ion lithium batteries (LIBs) are the transition metals oxide (TMOs), due to the diverse oxidation states are suitable to form different materials, such as cobalt oxide (Co3O4), nickel oxide (NiO), manganese oxide (MnO), nickel cobalt oxide (NiCo2O4)/(NCO), and others. A unique feature of some TMOs is that they present a cubic spinel crystal structure. This type of crystal structure also benefits during the charge and discharge cycles [1,2]. In this work, we present the synthesis of NiCo2O4, obtained firstly from metal hydroxide thin films deposited by chemical bath deposition and subsequently into an annealing process in different temperatures of 200, 300, and 400℃. After the annealing process, the thin films exhibit a polycrystalline behavior at 400 ℃, and XRD patterns correspond to the PDF of NiCo2O4. Also, the morphology on the surface shows a porous area that increases directly when the annealing temperature is increased. Also, the chemical composition of the films of NCO was present in all samples, and EDS obtained a ratio of Co/Ni to 2:1. On the other hand, the electrical properties reveal that resistivity decreases when the annealing temperature is increased. NCO thin films are synthesized via chemical bath deposition and processed into annealing at different temperatures. The film which was annealed at 400℃ present a polycrystalline phase of ternary NiCo2O4.
Also, all thin films of NCO exhibit a porous morphology; this is an appropriate characteristic in the application of electrodes in LIBs. Finally, the electrical properties can be modulable depending on the annealing temperature, where the sample which was annealed at higher temperature shows the lower electrical resistivity.

Keywords:

NiCo2O4, Thin films, porous surface, XPS, Low resistivity

Reference:

1 Cao Y. et al. (2023). https://doi.org/10.1016/j.jpowsour.2023.232710
[2] Pan J. et al. (2023). https://doi.org/10.1016/j.ijoes.2023.100233

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THIN FILMS / 113

Effect of adding a cooling system in a hybrid plasma: magnetron sputtering and graphite anode

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In this work, titanium (Ti) thin films were deposited using a DC magnetron sputtering (MS) system and a graphite anode, both before and after the application of a cooling system to the second anode-type plasma, to analyze the differences in the hybrid plasma system and the resulting products. The method is based on exposing substrates for defined time intervals while varying the gas pressure (Ar), MS current, MS power, the voltage applied to the anode, as well as the application of the cooling system. The changes in the properties of the films were investigated based on these variables. For the analysis of the deposition process, profilometry measurements to obtain the deposition rate and TEM analysis were used.

Keywords:

Magnetron sputtering, Graphite anode, Cooling system, Profilometry

Reference:

R. Hippler, M. Cada and Z. Hubicka, A positively biased external anode for energy control of plasma ions: hollow cathode and magnetron sputtering discharge, Plasma Sources Sci. Technol. 30 (2021). https://doi.org/10.1088/1361-6595/abe0cc

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THIN FILMS / 126

Characterization of Zinc Oxide thin films deposited by the Ultrasonic Spray Pyrolysis technique for optoelectronic applications

Authors: Diana Elizabeth Vázquez Valerdi[1]; Jesus Moreno Gomez[1]; Leticia Avila Maximo[None]

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[3] *Centro de Nanociencias y Nanotecnología CNyN-UNAM*

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This work presents the optical and electrical characterization of ZnO thin films obtained by the Ultrasonic Spray Pyrolysis (USP) technique for potential use in optoelectronic devices, such as photodetectors. The transmittance spectra of the ZnO films deposited at 300℃ for 4 to 8 minutes were obtained using UV-Vis spectroscopy, revealing significant absorption in the UV region and high transparency in the visible region, exceeding 80%, which is desirable for such applications. Analysis using a rotating analyzer ellipsometer Woollam M-44 showed that the thickness and surface roughness of the films decreased from 200 to 120 nm and from 29 to 12 nm, respectively, as the temperature increased, which is related to grain and crystal size. These results confirm that film thickness can be controlled through deposition temperature. ZnO thin films deposited by USP typically exhibit relatively high electrical conductivity. In this context, it was noted that the film deposited at 400℃ had another preferential orientation (100) with a FWHM peak corresponding to the (101) orientation, indicating two possible orientations, which is very interesting for its electrical properties. Although this may pose some conductivity issues, it remains sufficient for practical use. The results indicate a well-defined crystalline structure, low surface roughness, high transparency in the visible spectrum, along with suitable resistivity and carrier mobility, suggesting a low defect density in the ZnO thin films. Results obtained from the Hall Effect measurement system show a resistivity of 4Ωcm and a carrier mobility of 238 cm^2/Vs. This is an expected result given the material nature. In conclusion, the characteristics observed in ZnO thin films allow us to confirm that they can be used in optoelectronic devices.

Keywords:

Zinc Oxide, thin films, Ultrasonic Spray Pyrolysis, photodetectors

Reference:

Muchuweni, E., Sathiaraj, T., & Nyakotyo, H. (2017). Synthesis and characterization of zinc oxide thin films for optoelectronic applications. Heliyon, 3(4), e00285. https://doi.org/10.1016/j.heliyon.2017.e00285

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THIN FILMS / 112

Photocatalytic H2 production on Zr-doped TiO2 thin films

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Zr-doped TiO2 thin films were deposited on glass substrates using a sol-gel dip coating methodology, evaluating the effect of Zr concentration (0.01, 0.05, and 0.1 mol%) on their properties and photocatalytic activity evolving hydrogen from the ethanol photo-reforming. The structural characterization confirms the introduction of Zr4+ cation into the TiO2 crystal structure, resulting in the formation of the Ti1-xZrxO2 phase. This phenomenon caused a slight decrease in the TiO2 badgap, reducing also the film's transmittance. Additionally, compare to bare TiO2, an increase in the Zr concentration resulted in a growth of larger and agglomerated particles, increasing the roughness of the films. The photocatalytic hydrogen evolution was also enhanced with the Zr incorporation on TiO2, resulting in a double production rate in the 0.1 Zr-TiO2 film (38 000 µmolcm-2) compared to pristine TiO2. In this context, the enhancement of the photocatalytic activity can be associated with the growth of a rougher surface that allows a greater adsoption of the reactants (alcohols), and the reduction of the recombination rate of the photo-generated charges.

Keywords:

TiO2, sol-gel, hydrogen production, photo-reforming

Reference:

Ahmed M. Bolbol, Omar H. Abd-Elkader, et al., The effect of Zr (IV) doping on TiO2 thin film structure and optical characteristics, Results in physics, 42, 2022, 105955. Doi: 10.1016/j.jnoncrysol.2006.12.017

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THIN FILMS / 114

CHARACTERIZING LEAD-FREE PIEZOELECTRIC THIN FILMS USING PULSED LASER PHOTOACOUSTIC WAVES FOR ULTRASONIC TRANSDUCERS

Author: Erick Benítez-Flores[1]

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Piezoelectric and ferroelectric materials play crucial roles in the electronic industry, finding applications in everyday devices such as actuators, sensors, and transducers. While lead zirconium titanate

(PZT) remains a widely used ferroelectric material due to its advantages, growing environmental concerns have prompted the search for lead-free alternatives. This study focuses on BTO($BaTiO_3$)-based and KNN($K_{0.5}Na_{0.5}NbO_3$)-based piezoelectric materials.
Our objective is to demonstrate that pulsed laser photoacoustic waves can effectively characterize piezoelectric films, proving their suitability as ultrasonic transducers. Additionally, we explore properties such as resonance frequency and bandwidth.
We employed a Nd:YAG pulsed laser system to generate photoacoustic (PA) waves on the thin film surfaces. By leveraging the direct piezoelectric effect, we captured the electric response of the ferroelectric films using an oscilloscope connected to both a bottom electrode (Pt substrate) and an upper electrode (Au, approximately 100 nm thick, deposited by DC sputtering). We also characterized the piezoelectric films using X-ray diffraction in grazing angle mode and Piezoelectric Force Microscopy. The thin films was synthesized by pulsed laser deposition on Pt/Si substrates.
All films were successfully characterized as ultrasonic transducers, exhibiting frequency responses ranging from 8 to 15 MHz with bandwidths of 5 MHz. The best frequency responses were observed in the thinnest films, approximately 200 nm thick.
Our findings demonstrate that pulsed laser photoacoustic waves can effectively characterize and prove the suitability of lead-free piezoelectric thin films as ultrasonic transducers, eliminating the need for additional characterizations. These lead-free materials exhibit superior ultrasonic response compared to their lead-based counterparts.

Keywords:

Transductor, Ultrasonic, Piezoelectric, lead-free, ferroeléctric

Reference:

R. Castañeda-Guzmán, M. Villagrán-Muniz, J.M. Saniger-Blesa, O. Pérez-Martínez, Photoacoustic phase transition of the ceramic BaTiO3, Appl. Phys. Lett. 73 (5) (1998) 623–625

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THIN FILMS / 218

MAGNETO-STRUCTURAL STUDY OF Ge(001)/Mn5Ge3Cx THIN FILMS GROWN BY MAGNETRON-SPUTTERING TECHNIQUE

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Semiconductor spintronics leads the development of information technology. Devices such as spin-FET transistors and STT-MRAM magnetic memories base their operation on tunnel magnetoresistance. It has been found that Mn_5Ge_3 is a ferromagnetic compound that increases its Curie temperature, T_C, up to ~450 K by carbon doping. The Ge/Mn_5Ge_3 interface behaves like a Schottky contact,

which allows spin injection by tunneling into IV-group semiconductors. Mn_5Ge_3 can be easily synthesized as a continuous thin film on Ge(111). However, Ge(111) is not compatible with the Si(001) technology. We present the growth of Ge(001)/$Mn_5Ge_3C_x$ thin films by magnetron-sputtering technique, using the solid phase epitaxy (SPE) method, which consists of the co-deposition of Mn+C at room temperature followed by thermal annealing at a substrate temperature, T_s = 450 °C. The epitaxial growth of Ge(001)/$Mn_5Ge_3C_x$ thin films allowed obtaining a continuous layer with homogeneous thickness and lower root mean squared (RMS) surface roughness, thus identifying a Frank-van der Merwe or layered growth mechanism. The SPE method favored more homogeneous grain growth in size and shape, which resulted in a significant decrease in RMS surface roughness of ~1nm. Elemental analysis by X-ray photoelectron spectroscopy presented a thin film with composition $Mn_5Ge_3C_x$. Carbon doping was responsible for the increase in T_C up to ~422 K. The addition of C induced a charge transfer from Mn_{II} atoms to C, thus offering the possibility of double exchange inducing a ferromagnetic order 1. On the other hand, magnetization measurements vs. the magnetic field, M-H, allowed us to determine that the axis of easy magnetization is parallel to the surface of the sample and that the anisotropy constant, K_u, is ~0.58 MJ/m^3, which is lower than the K_u of the carbon-free thin film ~0.78 MJ/m^3.

Keywords:

semiconductor spintronics, ferromagnetism, Mn5Ge3 thin films, epitaxy.

Reference:

1 M. Gajdzik, C. Sürgers, M.T. Kelemen, H.v. Löhneysen, Strongly enhanced Curie temperature in carbon-doped Mn5Ge3 films, J. Magn. Magn. Mater. 221 (2000) 248-254. https://doi.org/10.1016/S0304-8853(00)00494-7

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THIN FILMS / 143

Analysis of deposition parameters effects on ZnO properties by applying a Central Composite Design (CCD)

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Zinc oxide (ZnO) is one of the most outstanding semiconductors of the II-VI periodic table group, because of its wide band gap, transparency, n-type conductivity, environmental stability, and non-toxicity. These characteristics make it a promising material for various applications, including conversion, piezoelectric, gas sensors, light-emitting diodes, etc. Each of them requires specific properties for an optimal performance; therefore, it is necessary to know the material behavior when experimental conditions for obtaining are changed. Based on the above, in this work, a statistical analysis is applied to study the effects of substrate temperature (100-400 ℃), sputtering power (80-120 W), and oxygen partial pressure (20-60 %) on ZnO thin-films deposited by reactive RF-magnetron

sputtering with a deposition time of 30 min. The films were deposited on glass substrates using the experimental conditions resulting from a Central Composite Desing (CCD) of Experiment (20 samples). Thickness, optical transmittance, band gap, lattice parameters, and crystallite size were used as response variables. They were correlated by an ANOVA analysis. The Pareto chart analysis reveals that the film thickness variation is mainly influenced by the sputtering power increase. The samples have optical transmittance higher than 80 % and band gap values around 3.2 eV, which are not significantly affected by the experimental parameters. On the other hand, temperature and oxygen partial pressure, closely followed by sputtering power, modify the structural properties. The crystallite size tends to increase with temperature, indicating a crystallinity improvement. Additionally, the c-lattice parameter is affected by the oxygen partial pressure, as there is a trend to increase is observed as the oxygen partial pressure is increased.

Keywords:

DoE, thin films, RF-Sputtering, ZnO, characterization

Reference:

D.C. Montgomery, Design and analysis of experiments, eighth ed., John Wiley & Sons, Inc., Arizona, 2013.

This work was supported by:

To CONAHCYT for the postdoctoral scholarship to M. Loeza-Poot (CVU: 556332). Authors are grateful for the use of facilities of LANNBIO-CINVESTAV-Mérida ; supported by the grants: FOMIX-Yucatán 2008-108160, CONACYT LAB-2009-01-123913, 292692, 294643, 188345 and 204822.

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THIN FILMS / 171

SYNTHESIS AND CHARACTERIZATION OF Cu(In,Ga)Se2 THIN FILMS BY ELECTRODEPOSITION AND SUBSEQUENT SELENIZATION

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The literature reports conversion efficiency of solar cells greater than 23% for Cu(In,Ga)Se2 (CIGS) thin-film based solar cells, deposited by thermal evaporation technique. In this work, the use of electrodeposition (ED) was proposed as an alternative technique to thermal evaporation to prepare CIGS thin films because it is more accessible and low-cost technique. So, the synthesis, formation and growth of CuIn1-xGaxSe2 thin films obtained by ED is presented, as well as a systematic study on the band gap tuning. Such band gap tuning of CuIn1-xGaxSe2 thin films was achieved directly by performing variations of In3+ and Ga3+ concentrations into the electrolytic bath. CIGS band gap value was achieved by partial substitution of In by Ga into the grown film in a range from 1 to 1.4 eV, corresponding to a ratio of Ga from $0 \leq Ga/(In + Ga) \leq 0.64$. Cyclic voltammetry studies were performed on each Cu-In-Ga-Se electrolytic solution bath system to find out the deposition potential values for each different molar concentration. Electrodeposited CuIn1-xGaxSe2 thin films

were characterized by EDS/SEM, XRD, Raman spectroscopy and ellipsometry technique to determine chemical composition, morphology, crystal structure and study the dielectric function. Selenization of CuIn1-xGaxSe2 thin films was performed using a rapid thermal processing system in an over-pressure reactive atmosphere of N2/H2 (96 %:4 %) and elemental Se vapor at different treatment times.

Keywords:

Electrodeposition, Thin films, Band gap tunning, Cyclic voltammetry, Selenization.

Reference:

Contreras-Ruiz, M. A., Mendez-Blas, A., & Calixto, M. E. Band gap tuning of Cu(In,Ga)Se2 thin films by electrodeposition and their subsequent selenization using a rapid thermal annealing system. Journal of Solid State Electrochemistry, 25(2) (2021) 591–601. https://doi.org/10.1007/s10008-020-04832-7

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THIN FILMS / 147

ENHANCED SENSITIVITY IN NON-ENZYMATIC GLUCOSE SENSING USING METAL ELECTRODES MODIFIED WITH GRAPHENE OXIDE AND REDUCED GRAPHENE OXIDE

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The accurate and reliable monitoring of glucose levels in diabetic patients is crucial for effective disease management. This study investigates the potential of metal electrodes modified with nanomaterials for non-enzymatic glucose detection, focusing specifically on gold electrodes modified with graphene oxide (GO), reduced graphene oxide (rGO), and partially reduced graphene oxide (prGO). The objective is to compare the performance of these modified electrodes in glucose sensing. Various characterization techniques, including Raman spectroscopy, optical microscopy, cyclic voltammetry, amperometry, and UV-Vis absorbance spectroscopy, were employed to assess the properties and performance of the modified electrodes. The results indicate that GO-modified electrodes exhibit the highest sensitivity in glucose detection compared to their unmodified and rGO-modified counterparts. The findings demonstrate that non-reduced GO provides superior sensitivity in glucose sensing, highlighting its potential as a promising material for developing non-enzymatic glucose sensors. This relationship between the reduction level of graphene oxide and its sensitivity in glucose detection offers new insights into the design of effective glucose monitoring devices. These advances could significantly impact continuous glucose monitoring in diabetic patients, improving their quality of life and treatment. The study reveals the potential of nanomaterial-modified electrodes, particularly GO-based ones, as a new frontier in non-enzymatic glucose sensor development.

Keywords:

Glucose Sensing, GO, rGO,

Reference:

Phetsang, S., Kidkhunthod, P., Chanlek, N. et al. Copper/reduced graphene oxide film modified electrode for non-enzymatic glucose sensing application. Sci Rep 11, 9302 (2021).

This work was supported by:

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THIN FILMS / 157

SYNTHESIS OF ZINC OXIDE THIN FILMS BY THE SILAR METHOD ON POLYMERIC SUBSTRATES FOR FLEXIBLE ELECTRONIC APPLICATIONS

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During the last years the interest in studying metallic oxide thin films has increased, owing to potential applications as sensors, optical detectors, and photovoltaics. There exist several methods to obtain thin films, among them, the chemicals are economic and simpler using low temperatures without inert or vacuum atmosphere. Zinc oxide (ZnO) is a p-type semiconductor material with a hexagonal phase and a bandgap of 3.3 eV. In the present work, the ZnO thin films were deposited on glass substrates by using the Successive Ionic Layer Adsorption and Reaction (SILAR) method; it is by adjusting parameters to obtain optimal conditions and apply them on the thin films'deposition on polymeric substrates (polyethylene and polypropylene). The polymers, particularly the polyolefins, are flexible, light, and low-cost materials, features that can be used to process flexible electronics using ZnO thin films deposited on them. The ZnO thin films characterization by X-ray diffraction confirms a hexagonal phase formation with grain sizes between 30 and 48 nm, a bandgap energy around 3.03-3.28 eV determined by ultraviolet-visible spectroscopy, and Raman features confirms a bigger crystallinity at lower cationic concentration. Finally, the ZnO thin films features were influenced by the used substrate (glass or polymer), by adjusting the SILAR deposition parameters.

Keywords:

thin film, ZnO, polymer, semiconductor, SILAR

Reference:

P. Sreedev, M. Sunil, V. Rakhesh, N. S. Roshima, B. Shankar, and D. Krishnan, "Optical, structural and surface analysis of ZnO thin films prepared by SILAR method,"in AIP Conference Proceedings, American Institute of Physics Inc., Apr. 2020. doi: 10.1063/5.0004287.

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Departamento de Química Macromolecular y nanomateriales, Centro de Investigación en Química Aplicada. Enrique Reyna H. 140 San José de los Cerritos. Saltillo, Coahuila, México.

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THIN FILMS / 158

EFFECT OF ADDITION OF PRISTINE MONTMORILLONITE IN WATER-BORNE POLYMER USED AS COATING

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Composites water-borne epoxy/ pristine montmorillonite were prepared, and the composite was applied on carbon steel substrates as anticorrosive coating. Pristine montmorillonite were dispersed in the polymer at various concentrations. The specimens were immersed in a 3.5wt.% aqueous NaCl electrolyte to evaluate the effectiveness of their anticorrosive coating function. Scanning electron microscopy (SEM) analysis showed that the pristine montmorillonite were homogenously dispersed in the polymer matrix, resulting in flat and smooth surfaces. The X-ray diffraction (XRD) results showed that pristine montmorillonite was highly dispersed in the polymer matrix. The anticorrosive properties were evaluated by electrochemical impedance spectroscopy (EIS) at various exposure periods. Analysis results showed the optimal mixing ratio of water-borne epoxy and pristine montmorillonite. The obtained results indicate that polymer-pristine montmorillonite matrix composites provide improved corrosion protection properties even after various hours of exposure to the NaCl solution.

Keywords:

water-borne epoxy, montmorillonite, anticorrosive coating

Reference:

J. L. Varela Caselis, Et al, The use of montmorillonite organoclay in preparation of UV-cured DGBA epoxy anticorrosive coatings, Corrosion Engineering, Science and Technology, 53 (2018) 362-369. https://doi.org/10.1080/1478422X.2018.1

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THIN FILMS / 262

Magnetic and Electrical comparative of Amorphous Co-rich hybrid trilayers

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The study of electronic transport in magnetic multilayers structures have received significant attention since the discovery of giant magnetoresistance, leading to a new class of electronics based on electronic spin transport phenomena. We present an experimental comparative study of magnetic and electrical properties of amorphous Co-rich (VITROVAC6030) layer interaction with VITROVAC6030, Permalloy, and Niquel layers. Leica EM MED020 DC magnetron sputtering was employed to obtain VITROVAC/Au/Magnetic layer on a silica glass substratum, where we have varied the VITROVAC thickness on substratum for 30 nm, 62 nm, and 125 nm; a spacer Au layer with 5 nm of thickness; and 30 nm of ferromagnetic layer at the top. The X-ray diffraction study of the VITROVAC6030 mono layers, reveals that we preserve the amorphous state. Magnetic studies were measured using a vibrating sample magnetometer (VSM) and a ferromagnetic resonance (FMR). The hysteresis loops show three different coupling due to the interaction of magnetoelastic anisotropy and magneto crystalline anisotropy dependent on VITROVAC thickness on the substratum. The electrical measurements were carried out by four-probe method, where the resistivity as a function of VITROVAC thickness on substratum exhibit different behaviour as result of different magnetic coupling. This study suggests that magnetoelastic effects and magnetic shape anisotropy can be utilized for tunning magneto-electronic transport.

Keywords:

Amorphous thin film, magnetic anisotropy, magnetic coupling, magneto transport, sputtering.

Reference:

V. Drchal, J. Kudrnovský, P. Bruno, P. H. Dederichs, I. Turek, and P. Weinberger, Electron transport in magnetic multilayers: Effect of disorder, Phys. Rev. B 65, (2002) 214414. https://doi.org/10.1103/PhysRevB.65.214414.

This work was supported by:

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THIN FILMS / 339

Influence of Sodium Tripolyphosphate on Sb2S3 films obtained by chemical bath deposition: A new route

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Antimony sulfide (Sb2S3) films are usually obtained by Chemical Bath Deposition (CBD) at low temperatures (around of 2 ℃) and the concentrations of sulfur ions and antimony ions are very disproportioned respect to the compound (~ 1:10). In this work, the reactants were modulated to be near of the stoichiometry of the formula Sb2S3 (2:3), however, the deposition parameters were modified for the new route. Sodium tripolyphosphate (STPP) was added as a surfactant and therefore the temperature and time deposition were changed, 60 ℃ and 2 hours, respectively. The concentrations of sulfur, antimony and phosphorous were monitored in the films, x-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive x-ray analysis (EDS), Raman, and UV-Vis. Usually Sb2S3 exhibits an amorphous phase for the as deposited films and a thermal treatment it is necessary to its crystallization. Our results revealed that the crystallization was not possible for Sb2S3 films deposited with STPP, but a new effect was observed, the films exhibited a thermochromic effect. Our results about the influence of STTP on Sb2S3 films obtained by CBD may help to better understand the effect of the phosphate on the behavior of solar cells using a thermochromic absorber layer.

Keywords:

Sodium tripolyphosphate, thin films, Chemical Bath Deposition, thermochromic

Reference:

https://doi.org/10.1016/j.tsf.2014.08.024
https://doi.org/10.1016/j.tsf.2006.12.155
DOI: 10.5185/amlett.2010.8147
DOI: 10.22079/JMSR.2017.23346

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THIN FILMS / 196

Effect of PVA, complexing agent concentration and deposition time on morphological, optical, and photocatalytic properties of CdSe thin films by chemical bath deposition.

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In this study, a simple and cost-effective chemical bath deposition was employed to deposit CdSe thin films on glass substrates and PVA seeded substrates. The structure, morphology, and optical

properties of CdSe were manipulated by adjusting the experimental parameters, such as the deposition time, complexing agent concentration and type of substrates. With increase the complexing agent concentration from 2.02 M to 5.16 M, the CdSe particles growth decrease at the beginning of deposition, the PVA seeded substrates shown a better control in the thickness. The band gap increase with the use the PVA seeded substrates and when the ammonia concentration increases. The crystallinity was lightly better on PVA seeded substrates. The CdSe thin films deposited under PVA seeded substrates were evaluated on the photocatalytic degradation of Rhodamine B solution under visible light, the CdSe film with 75 nm of thickness shows better degradation percentage at 6 h of irradiation, reaching 60 % of decoloration.

Keywords:

CdSe, chemical bath deposition, seeded substrates, optical properties, photocatalysis, RhodamineB

Reference:

S. R. Devi et all, Chalcogenide Letters Vol. 19, No. 12, December 2022, p. 901 - 908

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THIN FILMS / 179

EVALUATION OF VANADIUM OXIDE THIN FILMS AS ELECTRO-CATALYST IN WATER SHIFT REACTIONS

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Recently, greenhouse emissions such as carbon dioxide, methane and nitrous oxide have contributed significantly to climate change, resulting in long term shifts in temperatures and weather patterns, putting humans and ecosystems at risk. This has lead researchers around the world to search and develop cleaner energy sources, in aims to join a set of more sustainable energies. It is in this context that hydrogen has positioned itself as an important energy vector, both in the transportation sector and in energy storage in photovoltaic and wind systems. Developing efficient hydrogen production systems is the first step in the large-scale implementation of this technology, where green hydrogen (hydrogen obtained by electrolysis using clean energy sources) has become the fundamental objective. An alternative to improve electrolysis processes is to look for catalysts that can improve the oxygen and hydrogen evolution reactions during electrolysis processes. In this work, it is proposed to synthesize and characterize nanostructured vanadium oxide thin films, evaluating their physical, chemical and electrochemical characteristics to identify their viability and potential application in hydrogen production. Vanadium oxide thin films were synthesize through the ultrasonic spray pyrolysis, an economic and scalable method, using vanadyl acetilacetonate as vanadium precursor. Obtained films are characterized by XRD and UV-vis to determine their structural and optical properties, were different phases of vanadium oxide were identified. Thin films obtained

were also electrochemically characterized and their application in water splitting reactions were evaluated.

Keywords:

Green hydrogen, hydrolysis, Vanadium Oxide Thin films, Clean energy

Reference:

Ehsan, M. A., et.al. (2024). International Journal of Hydrogen Energy, 52, 718–727.
Stanko Hocevar and William Summers (2008). Hydrogen Production, Hydrogen Technology.15-80

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THIN FILMS / 181

"SYNTHESIS AND CHARACTERIZATION OF A-FE2O3, ZNO AND A-FE2O3/ZNO THIN FILMS"

Authors: Eduardo Morales Ricárdez[1]; MARTIN GUADALUPE ZAPATA TORRES[1]; Jenniffer Katherine Olarte Villamizar[1]

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Zinc oxide (ZnO) requires an activation energy of 3.25 eV for photocatalytic processes, within the ultraviolet light spectrum. However, solar light comprises only 5% ultraviolet light, resulting in reduced efficiency when irradiating ZnO with sunlight.
Heterostructures offer the ability to modify the energy absorption ranges of materials. In this context, hematite (α-Fe2O3) has an activation energy of 2.02 eV and is employed in combination with ZnO, forming a type II heterostructure. This strategic combination extends the energy absorption range into the visible light spectrum making available the use of a big portion of the solar irradiance spectrum.
In this study, thin films of ZnO and α-Fe2O3 were prepared using the ultrasonic spray pyrolysis technique, exploring various deposition parameters to determine the optimal conditions for the material. Finally, the ZnO/α-Fe2O3 heterostructure was obtained through the combination of the precursor solutions, using the same technique.
Morphological, structural, and optical characterizations of the films were carried out. The results indicate that both materials have similar deposition conditions. The optimal concentration for the deposition is 0.05M, with a temperature of 450 ℃ and a deposition time of 30 minutes. Additionally, the heterostructure ZnO/α-Fe2O3 adheres to similar parameters as those previously mentioned, showing a significant band gap change.
The ultrasonic spray pyrolysis technique depends on various factors, such as the variation in the use of precursors, solvents, temperature changes, deposition times, carrier gas flow, and solution nebulization.

Keywords:

ZnO, Hematite, Ultrasonic spray pyrolysis, Thin films, UV-Vis Spectroscopy.

Reference:

Mariño-Otero, T., Oliver-Tolentino, M., Aguilar-Frutis, M., Contreras-Martínez, G., Pérez-Cappe, E., & Reguera, E. (2015). Effect of thickness in hematite films produced by spray pyrolysis towards water photo-oxidation in neutral media. International Journal Of Hydrogen Energy, 40(17), 5831-5836. https://doi.org/10.1016/j.ijhydene.2015.03.017

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THIN FILMS / 201

EFFECT OF LASER IRRADIATION ON STRUCTURAL, MORPHOLOGICAL, OPTICAL, AND ELECTRICAL PROPERTIES OF RF-SPUTTERED PURE AND AL-DOPED ZNO THIN FILMS

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Co-authors: Adolfo Hernández Collado [2]; Cristian Gómez Rodríguez [1]; Maria Isabel Mendivil Palma [3]; Rubén López Villegas [4]

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Zinc oxide (ZnO) thin films have grown interest in electronic devices, such as transistors and solar cells. For these applications, high quality ZnO thin films with enhanced structural, morphological, optical, and electrical properties are required. These can be obtained by different thermal treatments. Laser irradiation is a novel method that is selective, localized, and faster than traditional furnace annealing. In this work, ZnO and Al:ZnO (AZO) thin films were synthesized by RF magnetron sputtering and treated using a continuous CO2 laser source to enhance the thin films'properties. Laser treated ZnO thin films presented wurtzite structure with preferential orientation along the c-axis, whereas AZO thin films showed polycrystalline nature after laser treatment. Raman spectroscopy revealed the activation of anomalous B1high-B1low mode in irradiated ZnO and AZO thin films. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) detected morphology changes, which included the formation of bubbles at the surface of the treated samples and a reduction of surface rugosity. In addition, ZnO and AZO thin films showed high transmittance in the visible spectrum and band gap values in the range 3.25-3.28 eV and 3.36-3.38 eV, for ZnO and AZO thin films, respectively. An enhancement of the photoresponse for both ZnO and AZO thin films was achieved by the laser treatment using 4W, 266 W/cm2, and 2.5 mm/s. This work provides an essential insight for synthesizing high-quality ZnO and AZO thin films through the incorporation of continuous far-infrared laser irradiation as a heat treatment stage, for potential applications in solar cell devices.

Keywords:

ZnO thin films, RF magnetron sputtering, Laser processing

Reference:

1 K. Tian, B. Tudu, A. Tiwari, Growth and characterization of zinc oxide thin films on flexible substrates at low temperature using pulsed laser deposition. Vacuum 146 (2017) 483-491. https://doi.org/10.1016/j.vacuum.2017.01.018

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Universidad Veracruzana, Centro de Investigación en Materiales Avanzados, Universidad Autónoma de Nuevo León, Centro de Investigación Científica y de Educación Superior de Ensenada B.C Unidad Foránea Monterrey

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THIN FILMS / 251

Optimization of La0.7Ca0.3MnO3 thin films deposition for implementation in magnetoelectric heterostructures

Author: Maria de Lourdes Arreguin Hernandez[1]

Co-authors: Javier Alonso López [1]; Jesús M. Siqueiros Beltrones [1]; Luis Alejandro Arce Saldaña [1]; Noemí Abundiz Cisneros [1]; Oscar Raymond Herrera [1]; Subhash Sharma [1]

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Nowadays, the studies of lanthanum-based perovskites have great attention due to exhibit wide range of physical properties such ferromagnetic to paramagnetic phase transition, colossal magnetoresistance, magnetic anisotropies, high dielectric constant, and low dielectric loss; having high potential for diverse applications such a magnetic memory, magnetic sensor, detectors and spintronic devices [1-4]. In thin films, their physical properties like temperature transition and resistivity are strongly dependent on the thickness; moreover, previous studies have reported the modification of crystal structure generated at the interface with the substrate, and therefore the modification on their magnetoelectric properties. This work is focused on the optimization of the deposition parameters to obtain thin films of the half-metal La0.7Ca0.3MnO3 (LCMO) compound by sputtering, for the future implantation in devices based on magnetoelectric heterostructures. The LCMO thin films were grown by RF-magnetron sputtering with a commercially LCMO target (99.9%) on SiOx/Si (100) substrate. The optimal growth conditions on sputtering chamber were: an argon flow rate of 20 ml/min, a power of 150 W, at the substrate temperature of 600 ℃ with the deposit times of 5, 10, 15, 20, 25, and 30 minutes. Previously, the chamber was conditioned with a base pressure of 1.57 x 10-5 Torr. The thin films exhibit good crystalline growth showing a tetragonal structure with P4mm space group. The thickness increased with the increase of the deposition time from 60 nm at 5 minutes to 94 nm at 30 minutes. The bandgap values, obtained from ellipsometry, decrease from 3.0 to 1.9 eV with the increase of the deposition time from 5 to 30 minutes, respectively.

Keywords:

Thin Films, LCMO, Magnetoaleactric, Heterostrcutures, Sputtering

Reference:

B. Panda, et al., Phys. B. Condens. Matter 583 (2020)
X. T. Zeng and H. K. Wong, Appl. Phys. Lett. 66 (1995)
Y. L. Qin, et al., Philosophical Magazine 85:36 (2005)
J. Rubio-Zuazo, et al., Phys. B. 357 (2005)

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THIN FILMS / 252

INFLUENCE OF MIXED PHASES ON THE ELECTRICAL AND SUPERCONDUCTING PROPERTIES OF NBN THIN FILMS

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Niobium nitride (NbNx) thin films have been studied over the past few decades due to their unique properties, which include applications in RF cavities, microelectronic devices, infrared imaging photodetectors, superconducting magnets, and other non-superconducting-related properties such as corrosion resistance and high hardness. The Nb-N phase diagram has been extensively studied as a bulk material due to its many phases and complexity. However, the effects of these multiphases have not been thoroughly examined in the field of nanoscience.
The objective of this work is to study the influence of the presence of two or more phases on the electric and superconducting properties of NbNx thin films.
Thin films of NbNx were prepared using the pulsed laser deposition (PLD) technique on SiO_2/Si (100) substrates. Pure Nb (99.95%) targets were irradiated with an excimer laser ($\lambda = 248$ nm, 20 ns pulse width, and 10 Hz repetition rate) in a N_2 atmosphere, with varying deposition parameters such as substrate temperature, N_2 pressure, target-to-substrate distance, and laser energy (fluence). The films synthesized by PLD were analyzed using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), electric measurements of R vs. T at low temperatures (~10 K), and UV-Vis and Raman spectroscopies.
Films of NbNx were successfully prepared by the PLD method with mixed phases, including α-Nb(N), β-Nb_2N, and ε-NbN, among others. These phases significantly influence the electric properties of the materials. Films with fewer phases (one or two) exhibited better electronic and superconducting behaviors. Conversely, films with multiple phases demonstrated greater stability.

Keywords:

superconductor, niobium-nitride,thin, films, electric-devices

Reference:

N. Cansever, M. Danışman, K. Kazmanlı, The effect of nitrogen pressure on
cathodic arc deposited NbN thin film, Surf. Coat. Technol. 202 (2008) 5919–5923.

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THIN FILMS / 253

STRUCTURAL AND MAGNETIC PROPERTIES OF HIGH-ENTROPY $Sr(RuTiMnFeNb)O_3$ AND $Sr(RuTiMnFeSc)O_3$ THIN FILMS

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High entropy materials are those in which five or more elements, in equiatomic proportion, occupy a particular position of a crystal structure. In thin film form, these materials may exhibit unusual and interesting properties when comparing to bulk or to the parent material (the one with a single element in the referred position). In this work, we present two new high entropy ceramic systems, $Sr(RuTiMnFeNb)O_3$ and $Sr(RuTiMnFeSc)O_3$, that are based on the ferromagnetic ($T_c \sim 160K$ 1) $SrRuO_3$ perovskite with an orthorhombic deformation. Such systems were prepared in bulk, by solid the state reaction method, and in thin film form. Films were deposited by laser ablation, on Si substrates, using a 0.15 J/cm^2 fluency, pulse frequency of 2 Hz, oxygen pressure of 25 mT, a temperature of 650 ℃, of target-substrate distance and 20 min of deposition time. The morphology, crystalline structure and composition were obtained by the AFM, SEM, XRD, EDS and XPS techniques. Magnetization measurements (M(T) and M(H)) were carried out using a PPMS magnetometer. The XRD studies confirmed the single phase orthorhombic structure of both high entropy systems, in bulk as in films. The obtained films were homogeneous, determined by SEM, and they revealed in accord to the XPS analyses, a main 3+ oxidation state for the transition metal ions. Also, from the M(T, H = 500 Oe) and M(H, T around T_c) measurements, it was determined that the main magnetic role is played by the Fe^{3+} cations, with minor dependence on the $3d^0$, Sc^{3+} and $4d^2$, Nb^{3+} ions.

Keywords:

$SrRuO_3$, High entropy, Ceramics, Films, Ferromagnetic

Reference:

J.P.Corbett, K.-Y.Meng, J.J.Repicky, et al., Applied Surface Science, 153766 (2022).

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THIN FILMS / 255

A Simple Surface Modification of Glass Substrates to Promote Cadmium Sulfide Film Adhesion

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Abstract

In the context of chalcogenide semiconductor thin films, one of the most studied materials is cadmium sulfide (CdS) due to its interesting optical and electrical properties. Several deposition methods can be used, with chemical bath deposition (CBD) being one of the most important due to its simplicity and low cost. However, along with the widespread use of this technique, there exist insufficient studies and understanding of the underlying phenomena governing the growth of the films in different types of glass substrates, which lead to a well-known variability of adhesion strength through the wide variety of deposited materials. Surface modification processes are often employed to address this issue. In this work, we report the effect of temperature on the modification process of glass substrates by a SnCl2·2H2O aqueous solution to promote adhesion of CdS films synthesized by CBD. The higher temperatures in the modification solution resulted in greater surface modification. Moreover, further heat treatment of the modified surfaces enhanced the adhesion of CdS thin films. We suggest that this improvement can be attributed to the possible formation of SnO2 after heat treatment, a species known to promote adhesion. Overall, our results demonstrated an alternative surface modification method that can be conducted under simple conditions without the need for additional modifying agents. This research opens the possibility to study the deposition of other chalcogenide compounds to get a deep insight about the phenomena involved during the formation of the films on glass substrates.

Keywords:

Surface modification, Chemical bath deposition, Adhesion, Cadmium sulfide.

Reference:

García-Valenzuela, et al. (2019b). On the adherence of chemically deposited CdS films to common inorganic substrates: effect of Cd2+ concentration in solution, substrate surface chemistry, and reaction temperature. Chemistry select, 4(5), 1650-1665. https://doi.org/10.1002/slct.201803033

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THIN FILMS / 326

Study of chromium thin films by cathodic sputtering with rotating substrate holders

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Thin chromium films were synthesized by direct current magnetron sputtering on a rotating substrate holder that allows it to reach a speed of 6000 rpm. The magnetron sputtering direct current (DC) method is a film deposition technique that uses a direct current electric field to generate a plasma that bombards a target, detaching atoms of the target material that are deposited on the substrate to form a thin film, this method is also characterized by having a directly proportional relationship between the current and the deposition rate, while retaining the same parameters so that the thickness increases linearly with time.
The relationship between the rate of incidence of the atoms on the substrate surface and the lateral movement that occurs when the samples are rotated is expected to be something that modifies the characteristics of the deposited films. This is expected to produce structural changes induced by substrate rotation and to show effects on their surface morphology, microstructure and mechanical properties. The analysis of these samples is inspected tangentially by covering points on the surface to check if such changes were effected. During the deposition, values such as Argon gas flow, optimum chamber base pressure, and constant rotational speeds have to be kept fixed in order to maintain a stable deposit.
Chromium thin films were previously deposited with the stationary substrate and the same values to compare the deposition of the thin films showing different results when rotated at partial speed up to 6000 rpm.

Keywords:

sputtering deposition

Reference:

Starkov et al. (2017)

This work was supported by:

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THIN FILMS / 362

Memristive Behavior of YSZ ALD Devices

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This work investigates the memristive behavior of Yttria-Stabilized Zirconia (YSZ) capacitor devices, focusing on modeling the switching kinetics and their potential for various applications. We propose a model for incubation time in memristors where ion migration is the rate-limiting step. This model analytically correlates incubation time with electric field, diffusion coefficient, and temperature, enabling the determination of material properties for the low-resistance state. We further illustrate the model's application using YSZ thin films in parallel plate cells.

The investigation delves into the resistive switching properties of YSZ thin films. The devices exhibit excellent control over multilevel memory states and a transition from short- to long-term data retention, suggesting promise for neuromorphic applications. Interestingly, further analysis is required to understand how the switching process correlates with the observed increase in permittivity, which is different from traditional memristors.

Finally, future work is recommended to explore the influence of temperature on the electrical response of the films, investigating the potential for supercapacitor or pseudocapacitive behavior. These findings highlight the potential of YSZ devices for various applications, from memory to energy storage, and emphasize the need for further exploration of their unique characteristics.

Keywords:

memristor, ALD, thin film capacitor

Reference:

A Voltage-Driven Transport Model to Identify Ion Migration
as the Rate-Limiting Step in Memristive Switching
https://doi.org/10.1002/aelm.202300608

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THIN FILMS / 81

GROWTH OF HIGHLY TEXTURED NON-COLLINEAR ANTIFERROMAGNETIC D019-Mn3Ge/GaN (0001) THIN FILMS BY MAGNETRON SPUTTERING

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Non-collinear antiferromagnets have attracted much attention due to the possibility to exhibit anomalous and topological Hall effects. The D019-Mn3X (X = Ga, Ge and Sn) compounds, with hexagonal crystal structure (space group No. 194) and kagome spin structure in the (0001) plane, are candidates to show these effects, which could serve as the reading mechanism in future non-volatile magnetic data storage devices. In particular, D019-Mn3Ge (Mn3Ge) has an intrinsic weak in-plane ferromagnetic component due to the canting of Mn magnetic moments along its easy magnetization axis. In this work we report on the growth and magnetic properties of highly textured Mn3Ge thin films grown on GaN (0001) substrates by magnetron sputtering. The substrate temperature was fixed at 400 ℃, despite that Mn3Ge is a high temperature phase due to the influence of the hexagonal substrate. The lattice constants of Mn3Ge are a = 5.33 Å c = 4.31 Å and those of GaN (0001) substrate are a = 3.190 Å and c = 5.19 Å allowing a hexagon on hexagon growth between film and substrate within a GaN ($\sqrt{3}\times\sqrt{3}$)R30° surface unit cell with a lattice mismatch of 3.26%. This mismatch points out that Mn3Ge needs to be subjected to tensile strain to match the GaN lattice constant. Reflection high-energy electron diffraction and X-ray diffraction were used to confirm a hexagon on hexagon uniaxial texture. The antiferromagnetic phase of Mn3Ge needs Mn excess in order to stabilize the antiferromagnetic phase. We found precise conditions to grow antiferromagnetic Mn3Ge, which is well described by the magnetization vs. magnetic field, Néel temperature, coercivity and anisotropy upon the variation of Mn content.

Keywords:

Non-collinear antiferromagnet, thin film, magnetic properties

Reference:

T. Ogasawara, J.-y Kim, Y. Ando, A. Hirohata, Structural and antiferromagnetic characterization of noncollinear D019-Mn3Ge polycrystalline film, J. Magn. Magn. Mater. 473 (2019) 7–11, https://doi.org/10.1016/j.jmmm.2018.10.035

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THIN FILMS / 397

Effect of bath temperature in the formation of CdS related thin films and their evaluation as super-strate of CdTe films produced by RF sputtering

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Thin films were deposited by the Chemical Bath procedure employing bath temperatures of 30℃, 35℃, 40℃, 45℃, 50℃, 55℃, 60℃, 65℃, 70℃, 75℃, 80℃, 85℃ and 90℃ using reported precursors that produce CdS films. UV-Visible and Raman Spectroscopies were employed to evaluate film characteristics. It is observed a blue shift behavior in bandgap value as temperature decreased while Raman spectroscopy indicated CdS formation for films deposited above 60℃.

Films with CdS characteristics were employed to deposit on them CdTe films by RF sputtering. We report the results of the characterization of the chemical, optical and structural characteristics and their influence on the electrical transport properties of the as-grown and thermal annealed CdS/CdTe heterostructures.

Keywords:

sputttering, semiconductor heterostructures, thin films

Reference:

Vargas-Rueda, J. A., Alonso, A. R., Meléndez-Zamudio, M., & Meléndez-Lira, M. (2021). Chemical stability diagrams as a powerful tool to the synthesis of Cu2SnS3 thin films by chemical bath deposition. Materials Chemistry and Physics, 265, 124478.

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THIN FILMS / 237

AN ALTERNATIVE METHOD FOR SELECTIVE ETCHING OF SiO2 THIN FILMS

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Photolithography is an essential process manufacturing of integrated circuits, which involves the use of various materials with different properties. The silicon dioxide is widely used due to its optical and electrical properties; therefore, it is of utmost importance not only to have a method to synthesize it but also to have a method for the selective etching of silicon dioxide. We can mention two methods: chemical etching in hydrofluoric acid and plasma etching. This study aims to present an alternative method for silicon dioxide selective etching. This method consists of the sputtering deposition of a thin aluminum film pattern in the center of the surface of a substrate, for later deposit a silicon dioxide thin films all over the surface of the substrate including the thin aluminum film previously deposited. As a result, an A zone (SiO2/Al/substrate) and a B zone (SiO2/substate) will be obtained. Finally, the substrate is immersed in ferric chloride (FeCl3), with which after a few minutes the SiO2/Al system in the A zone will be detached from the substrate, while the system in the B zone remain intact. We can then deduce that silicon dioxide and aluminum seem to interact with each other through aluminum diffusion into the SiO2 thin film, resulting in a change in the SiO2 properties, so it can be detached from the substrate. This effect can be directly applied to photolithography technology.

Keywords:

Photolithography, silicon dioxide, SiO2, sputtering, etching, thin films

Reference:

P. J. Holmes, J. E. Snell, “A vapor etching technique for the photolithography of silicon dioxide”, Microelectronics Reliability Elsevier, Vol. 5, Issue 4, November 1966, pp. 337-341

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THIN FILMS / 366

AZO thin films obtention by atomic diffusion method in trilayer arrangements

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A series of AZO films were growm by using physical vapor deposited (PVD) in a DC Sputtering system (Intercovamex V3), varying the PpO2 (5, 10, 20, 30, 40, 50 y 75 mTorr), under power and argon flow constant. The selected aluminum contents (atomic ratio of Zn:Al) were 1:3, 1:7 and 1:12. The samples labeling as a function of partial pressure was made as follows: AZO1, AZO2, AZO3, AZO4, AZO5, AZO6 and AZO7, and their characteristics of percentage transmittance in the visible region, atomic ratio Zn:Al, band gap and thickness are summarized in Table 1. The thin films surfaces were characterized by scanning electron microscopy (SEM, JEOL JSM-7401F) and X-ray diffraction techniques (Panalytical X-Pro). The optical properties were made in a UV-Vis PERKIN-ELMER Lambda10. The electrical properties were obtained through the Hall Effect using the Van Der Paw method. An EGK equipment was used applying a magnetic field of 0.51T and a current of 50μA in order to determine the resistivity of the prepared thin films.

In this work we will focus on the deposition and characterization of thin films of ZnO, AZO and ZnO/Al/ZnO trilayer arrangements deposited by pulsed DC Magnetron Sputtering DCp-MS. It is widely used in the manufacture of hard, soft, anti-corrosion, decorative coatings and the manufacture of thin films with specific optical and electrical properties. In this process, the white or target functions as a cathode and is bombarded with positive ions of an inert gas accelerated due to a potential difference within a chamber, forming plasma, this causes the evaporation of the material atoms.

Keywords:

AZO, ZnO, XPS, Optical properties

Reference:

1 T Minami, Semicond. Sci, Technol. 20 (2005), p. S35.
[2] A Chen, K Zhu, H Zhong, Q Shao and G Ge, Sol. Energy Mater. Sol. Cells 120 (2014) p. 157.

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TRIBOLOGY, SURFACES AND INTERFACES / 67

CORROSION RESISTANCE AND HARDNESS EVALUATION ON AZ31B ALLOY BY ATMOSPHERIC PRESSURE PLASMA JET TiO2 COATING

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Magnesium (Mg)-based bio-alloys are used in biomedical applications such as bone fixation, cardiovascular stents, dental implants, etc. This research focuses on the mechanical and corrosion behaviour of substrates of AZ31B (Mg-Al-Zn) alloy. The thermal spray technique APPJ was used to deposit TiO2-based coating on the substrates. The microstructure, hardness and corrosion current of the material were all examined. This study demonstrates an improvement of the corrosion resistance of an AZ31B magnesium alloy achieved by the application of 2.5 μm-thin coatings generated by APPJ free of solvent process. This barrier layer protected substrate from 3.5 wt % NaCl and SBF solutions (Icorr = 130 & 125 mA, respectively) sustained by the existence of ceramic layer which is integrated (via physical anchoring) with the MgO inner particles. This corrosion resistance is due to its disordered structure, the creation of a passive coating and consistent material composition on the surface. Results reveal that, under the APPJ treatment, grain refinement and homogeneity can be improved meanwhile, pre-thermal treatment (500℃) tendency in the coating process significantly hold nearly substrate melting point. The TiO2-coated AZ31B alloy has improved its surface morphology and hardness (33% HRc increment). Furthermore, the difference in corrosion resistance of TiO2-based coatings was detected using their microstructures created during the coating deposition process. APPJ disintegrating melt deposition is a promising approach to develop Mg-based alloys for biomedical applications given that the corrosion resistance is related to the stability of the deposit and its chemical environment.

Keywords:

Microstructure, Adhesion, Corrosion behavior, Material composition, Hardness.

Reference:

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TRIBOLOGY, SURFACES AND INTERFACES / 148

MICROWAVE PLASMA ASISTED PLD DEPOSITION OF GaN THIN FILMS

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The hybrid plasma used in this work was created by combining a stationary microwave ECR (with magnetic field) discharge using nitrogen as the working gas, and the plasma formed during the pulsed laser ablation of a GaAs solid target. The pulsed plasma propagates perpendicularly through the microwave plasma flux. The hybrid plasma was created at a working pressure of 6 x 10-4 Torr. Plasma parameters such as density, electron temperature and mean kinetic ion energy were determined using Langmuir probes. The optical emission spectroscopy measurements showed a significant improvement of the excited species present in the hybrid plasma in comparison with the individual plasmas. The characteristics of the GaN thin films deposited at different experimental conditions, such as the proportion of nitrogen in the working gas, the mean kinetic energy of ions produced during the ablation process were studied by means of XPS, Raman spectroscopy and XRD.

Keywords:

: GaN thin films, microwave plasma, pulsed laser ablation

Reference:

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TRIBOLOGY, SURFACES AND INTERFACES / 83

Formation Laboratory of Surface Study, Modification and Application

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This work demonstrates the growth of the LEMAS laboratory of the Universidad Politécnica del Valle de México located in the state of Mexico. The Lemas laboratory allows the development and application of scientific knowledge, and strong support in the generation of high-quality human resources. It also aims to carry out research collaborations between different national and foreign universities, as well as offer scientific research services to the industry at a national level. With the purpose of developing and applying scientific knowledge in the areas of study, modification and application of surfaces, to propose and implement responses to technological problems present at the regional, state and/or national level. The LEMAS Laboratory seeks to contribute to the national development plan of Mexico and CONAHCYT 1

Keywords:

Surface Study, Modification, Application, Laboratory

Reference:

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TRIBOLOGY, SURFACES AND INTERFACES / 346

Characterization of hybrid plasma generated by combining microwave nitrogen plasma with láser ablation plasma of a molybdenum target.

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In the present work a nitrogen microwave ECR (electron cyclotron resonance) discharge was combined with the plasma created during the ablation of a molybdenum target to deposit MoN thin films. The deposit was formed on quartz substrates at a low deposition temperature (300 ℃). The hardness values of the MoN films show a specific dependence on the plasma parameters (mean kinetic energy (Ek) of the ions) that could be varied depending on the power density applied on the target. Plasma parameters were measured by Langmuir probe. The structural characterization of the films performed by X-ray diffraction showed the presence of the d-MoN (hexagonal) phase in all cases. The XPS analysis showed that the nitrogen content decreases as an effect of the increase of

the kinetic energy of the ions, which could explain the increase of hardness of the samples with the ion energy.

Keywords:

XPS analysis,X-ray diffraction,hardness,molybdenum,Plasma

Reference:

1 Z. N. Jaf, H. A. Miran, Z.-T. Jiang, M. Altarawneh, Rev. Chem. Eng. 3886, 1-33 (2021).
[2] F. Klimashin, N. Koutná, H. Euchner, D. Holec, P. H. Mayrhofer, J. Appl. Phys. 120, 185301 (2016).

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TRIBOLOGY, SURFACES AND INTERFACES / 79

TRIBOLOGICAL ANALYSIS OF TWO-LAYER CHROME COATING, NITRIDED, ELECTROLYTICALLY APPLIED ON TITANIUM

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The objective of this work is to tribologically characterize the two-layer hard coating applied electrolytically on pure titanium which was subsequently nitrided. A Plint TE 66® microabrasion machine was used to perform the wear test. A layer of zinc was initially deposited on the titanium. and later a layer of chrome was applied. Both layers were deposited using a novel electroplating technique that uses DTPA as an electrolyte, subsequently applying a nitriding process. Microabrasive wear resistance was determined using average 4 μm SiC diluted in distilled water. The lost volume (V) and wear coefficients (k) were obtained for the coating and for the uncoated metal. The results showed that pure titanium has a lower resistance to microabrasive wear compared to the coating (chrome/zinc), nitriding provides greater surface hardness, which influences and increases wear resistance. The wear trace was characterized by optical and electron microscopy (SEM), through which we identified the wear mechanisms of three-body rolling microabrasion.

Keywords:

Nitriding, microabrasion, electrolytically, Chrome, Zinc

Reference:

John Bibber, Sanchem Inc. Chicago, An Overview of Nonhexavalent Chromium Conversion Coatings – Part II: Zinc, Metal Finishing, Vol. 100, Issue 2 (2002) 98-102.

This work was supported by:

Instituto Politécnico Nacional and Escuela superior de Ingeniería Mecánica y Eléctrica, Unidad Zacatenco.

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TRIBOLOGY, SURFACES AND INTERFACES / 80

Techniques for determining the thickness of the lubricating oil film in refrigeration systems

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In refrigeration systems, the lubricating oil film plays a crucial role in reducing friction and wear between moving parts, thereby ensuring efficient and long-term operation. Accurately determining the thickness of this oil film is essential for optimizing system performance and preventing failures. This study aims to review various techniques used to measure the thickness of the lubricating oil film in refrigeration systems. The study concludes that the selection of the technique depends on specific system requirements, such as operational environment, desired accuracy, and available resources. Future research should focus on hybrid methods that combine the strengths of multiple techniques to achieve more comprehensive monitoring. This work highlights the importance of advanced measurement techniques in enhancing the reliability and efficiency of refrigeration systems.

Keywords:

Lubricating; Oil Film; Thickness; Refrigeration Systems; Tribology

Reference:

Wang, H., Zhao, L. (2019). Advances in Oil Film Thickness Measurement Techniques. Journal of Tribology, 141(5), 051601.

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TRIBOLOGY, SURFACES AND INTERFACES / 336

Deposition of Ti/Mg multilayer coatings on pyrex glass subjected to gamma radiation

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The study of effects and protection against gamma radiation on glass is the result of a need due to the boom of space missions focused on meteorological studies and observation of the earth and the universe, however, creating efficient shielding for certain components or systems and inhibiting damage caused by such radiation continues to generate great technological challenges to this day. The present work focuses on the study of changes of the transmittance of pyrex glasses coated with Ti/Mg nano multilayers of different periods, to determine the degree of protection that they can offer when the glasses are exposed to gamma radiation. The nanostructured multilayers were generated using the Pulsed Laser Ablation Deposition technique, where the Ti layer was deposited at low or high ion energies. The elemental composition and crystalline structure of the films is reported. Once the protective multilayers were obtained, 10x10 mm Pyrex glass samples were irradiated by exposing them in a controlled manner to a 60Co source at doses of: 1, 1.5, 8 and 9.5 kGy. The different multilayers were used as shields of the Pyrex against gamma irradiation and using a UV-Vis spectrophotometer, the transmittance of each of the irradiated samples was determined, reporting the variation between the protected samples and those not protected with the nanostructured multilayers.

Keywords:

Multilayers, Ti - Mg, PLD

Reference:

1 Nicolleta C. A. & A. G. Eubanks (1972). "Effect of simulated space radiation on selected optical materials". Applied Optics, Vol. 11, No. 6; 1365-1370.

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TRIBOLOGY, SURFACES AND INTERFACES / 199

STUDY OF THE OSCILLATIONS IN PIN-ON-DISK TRIBOLOGICAL TESTS

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In the searching of a better understanding of the tribological phenomena, in this work, the study of the oscillations in pin-on-disk tribological tests of three samples of steel at different lubrication conditions is addressed. One specimen was tested at dry condition, other was tested in water bath, and the last one was coated with a solid film coming from engine lubricant, later, it was also tested.

The friction coefficient data of the three tests were analyzed from statistical calculation of the mobile average and mobile standard deviation, the raw data of the friction profiles were taken as information signal, and the discrete Fourier transform method was used to identify the oscillation frequencies and its dynamic in the friction profiles. The results of the analysis yielded mobile average of the friction coefficients very similar to raw data and mobile standard deviation profiles indicating the transition of the friction profiles between high deviation and low deviation regions. The Fourier analysis revealed a non-oscillatory signal and some harmonic frequencies which intensities change along test time for the three specimens tested. From results, it is concluded that, while the high mobile standard deviation of the friction coefficient is related to oscillations, the low mobile standard deviation is related to the non-oscillatory signal, which is, in fact, a stochastic condition. The delay or advance of the changes in harmonic frequencies are associated with the lubrication media and the final friction coefficient. The understanding of the last relationship is useful to propose more efficient tribological systems.

Keywords:

Vibration spectra, elastic system, mechanical energy dissipation

Reference:

1. S. Domínguez-García, L. Béjar-Gómez, R. Maya -escas, J. Lara-Romero, B. Castro-Cedeño, and M. A. Espinos- Medina, "Friction Coefficient Dynamics of Tribological Coatings from Engine Lubricants: Analysis and Interpretation,"Coatings, vol. 13, no. 10, Oct. 2023, doi: 10.3390/coatings13101753.

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TRIBOLOGY, SURFACES AND INTERFACES / 86

Characterization of AISI 01 steel with surface treatment

Author: Ian Abisay Garcia Moreyra[1]

Co-authors: Ana Geraldin Espinoza Jusacamea [2]; Ernesto García [3]; Jorge Víctor Cortes Suarez [4]; Marco Antonio Doñu Ruiz [3]; Noé López Perrusquia [3]

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In this paper I will evaluate the hard surface formed on steel used in the manufacturing industry with a hard coating; with the boriding process with dehydrated pulp in a box at temperatures of 850, 900, 950 and 1000 ℃, with residence times of 1, 2, 3, 4 h. The morphological characterization of these phases obtained by the thermochemical boriding treatment will be performed by optical microscopy (OM). The FeB/Fe2B layers obtained on the surface of the material were determined

by X-ray diffraction (XRD); on the other hand, the microhardness will be evaluated by the Vickers microindentation technique. Finally, the adhesion of the FeB /Fe2B coating will be estimated by Rockwell testing with the VDI - 3198 standard. With the present work I will show the type of iron boride and its mechanical characteristics for possible applications in the manufacturing field.

Keywords:

coatings, surface, adhesion, FeB /Fe2B, borading

Reference:

Boriding kinetics and mechanical behaviour of AISI O1 steel
Friction and wear of borided AISI O1 steel with carbon nanomaterial deposit

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TRIBOLOGY, SURFACES AND INTERFACES / 87

Characterization of AISI P20 steel with surface treatment

Author: Jazmin Godinez Roa[1]

Co-authors: ERNESTO GARCIA [2]; JORGE VICTOR CORTES SUAREZ [3]; MARCO ANTONIO DOÑU RUIZ [1]; NOE LOPEZ PERRUSQUIA [1]

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In this work we will evaluate the hard surface formed on steel used in the plastics industry with a hard coating; with the boriding process with dehydrated pulp in the box at temperatures of 850, 900, 950 and 1000 ℃, with dwell times of 1, 3, 5, 7 hours. The morphological characterization of these phases obtained by the thermochemical boriding treatment will be carried out by optical microscopy (OM). The FeB /Fe2B layers obtained on the surface of the material were determined by X-ray diffraction (XRD); on the other hand, the microhardness will be evaluated by the Vickers microindentation technique. Finally, the adhesion of the FeB /Fe2B coating will be estimated by Rockwell testing with the VDI -3198 standard. This paper will show the type of iron boride and its mechanical characteristics for possible applications in the field of plastic injection molds.

Keywords:

Coatings, Surface, Adhesion, Boriding, Steel

Reference:

Pack-boriding of AISI P20 steel: estimation of boron diffusion coefficients in the Fe2B layers and tribological behaviour
Effect of Carbon Content and Boronizing Parameters on Growth Kinetics of Boride Layers Obtained on Carbon Steels

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TRIBOLOGY, SURFACES AND INTERFACES / 151

Hardness of MoxNy thin films deposited by microwave ECR assisted reactive pulsed laser deposition

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In the present work a nitrogen microwave ECR (electron cyclotron resonance) discharge was combined with the plasma created during the ablation of a molybdenum target to deposit MoN thin films. The deposit was formed on quartz substrates at a low deposition temperature (300 ℃). The hardness values of the MoN films show a specific dependence on the plasma parameters (mean kinetic energy (Ek) of the ions) that could be varied depending on the power density applied on the target. Plasma parameters were measured by Langmuir probe. The structural characterization of the films performed by X-ray diffraction showed the presence of the d-MoN (hexagonal) phase in all cases. The XPS analysis showed that the nitrogen content decreases as an effect of the increase of the kinetic energy of the ions, which could explain the increase of hardness of the samples with the ion energy.

Keywords:

mechanical properties, plasma, pulsed laser deposition, kinetic energy, molybdenum nitride

Reference:

1 Z. N. Jaf, H. A. Miran, Z.-T. Jiang, M. Altarawneh, Rev. Chem. Eng. 3886, 1-33 (2021).
[2] F. Klimashin, N. Koutná, H. Euchner, D. Holec, P. H. Mayrhofer, J. Appl. Phys. 120, 185301 (2016)

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TRIBOLOGY, SURFACES AND INTERFACES / 57

Tribological study of NbN coating on AISI 410 SS surfaces in different work environment.

Author: Ernesto David García Bustos[1]

Co-authors: Giovanni Ramirez [2]; Marco Atonio Figueroa-Guadarrama [3]; Sandra Rodil [2]; Stephen Muhl [2]

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The tribological performance is controlled by all the components involved in the system of contact, the work atmosphere, one of the most critical parameters that affect the chemical changes of the contact surfaces during the tribological operation [1-4]. This work presents the tribological results of AISI 410 SS surfaces coated and uncoated with NbN film produced by DC magnetron sputtering in argon, vacuum, and room atmosphere. The surfaces were structural, elemental, and morphology characterized using XRD, EDS-SEM, and SEM equipment, respectively. The tribological studies were carried out using equipment that was designed and constructed in the lab. The coefficient of friction (CoF) was registered in real time. At the same time, the wear rate produced by each work atmosphere was morphological, chemical, and elemental, characterized using SEM, Raman, and SEM-EDS, respectively. The average kinetic CoF value produced during the sliding-contact operation on the AISI 410 SS surfaces was similar for the tests in atmospheric and argon work environments, with a lower CoF value in vacuum. The wear rate produced on the steel surfaces was more significant in argon than in the other two work environments. The coated surfaces with NbN film showed a higher CoF value and wear rate in the atmospheric work environment than in the vacuum and argon work environment.

Keywords:

Tribology, Coating, Work environment, NbN, Raman spectroscopy

Reference:

1 Future perspectives on sustainable tribology, Renewable and Sustainable Energy Reviews.
2 Tribology in the space environment.

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TRIBOLOGY, SURFACES AND INTERFACES / 119

STUDY OF THE TRIBOLOGICAL PERFORMANCE OF BORIDED AISI M2 STEEL SUBSTRATES USING THE PIN-ON-DISC TEST

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Co-authors: Milton Carlos Elías-Espinosa ; Marco Antonio Doñu-Ruiz ; Miguel Ángel Camacho-Tapia ; Noé López-Perrusquia

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This study was carried out to characterize a boride layer obtained by thermochemical boriding treatment and to evaluate its tribological performance. AISI M2 steel substrates with an initial surface roughness Ra=0.2 μm were borided by powder packing technique, using the following combinations of temperature and exposure time: 1123 K for 2 h, 1123 K for 4 h, 1148 K for 3 h and 1173 K for 2 h. The phase type, microstructure, surface roughness and nanohardness of the boride layer formed on the surface of AISI M2 steel substrates were investigated by XRD, SEM, contact profilometer and instrumented indentation tests, respectively. Subsequently, tribological pairs formed by the resulting boride layer and an alumina sphere (static partner) were subjected to a wear test using the pin-on-disc test, under dry conditions and at room temperature. In addition, the curves of the friction coefficient as a function of distance were obtained. The results of this study showed that a single-phase Fe2B boride layer was formed on the surface of the borided substrates. At the surface of the Fe2B single-phase boride layer, the average depth of the valleys (0.95-1.49 μm) was greater than the average height of the peaks (0.81-1.26 μm). The coefficient of friction of the borided substrates was lower (0.51-0.75) compared to that of the unborided substrate (0.81). The average depth of the wear track formed on the borided substrates (1.63-3.31 μm) was less compared to that of an unborided substrate (22.58 μm). In the borided substrates there was a coexistence of a high coefficient of friction and high wear resistance, and vice versa; while in the unborided substrate there was a coexistence of a high coefficient of friction and low wear resistance.

Keywords:

boriding, pin-on-disc, friction, wear

Reference:

Holmberg K. and Matthews A. 2009 Coatings tribology: properties, mechanisms, techniques, and applications in surface engineering. Elsevier.

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TRIBOLOGY, SURFACES AND INTERFACES / 94

CHARACTERIZATION OF AGAR FILMS FUNCTIONALIZED WITH Ag AND TiO2 NPs AS AN ALTERNATIVE FOR SMART FOOD PACKAGING.

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Co-authors: ERIKA FABIOLA HERNANDEZ ELIZARRARAS [1]; ELVA GUADALUPE GUTIÉRREZ GARIBAY [1]; MAURO DONALDO SAUCEDO PLACENCIA [1]; ADALBERTO ZAMUDIO OJEDA [1]; SANTIAGO JOSÉ GUEVARA-MARTÍNEZ [1]; Ernesto David García Bustos [2]

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This study presents the characterization of food-grade agar films functionalized with 98 nm silver nanoparticles (Ag NPs) and 30 nm titanium dioxide nanoparticles (TiO2 NPs) at different concentrations, proposing each as an antibacterial packaging material and emphasizing their potential to preserve organic products during transportation, storage, and sale. The films were synthesized by microwave irradiation, which allows for uniform temperature distribution, assisting in the obtention of homogeneous films and reducing the process time. Nanoparticle characterization involves diverse techniques, including Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Dynamic Light Scattering (DLS), and UV-visible (UV-Vis) spectroscopy. Meanwhile, the agar films with different concentrations of NPs were characterized via Fourier Transform Infrared Attenuated Total Reflectance (FTIR-ATR) spectroscopy, UV-Vis, SEM, and antimicrobial assays. Grapes were coated with agar films with and without NPs to study the modification in food preservation, which exhibited significant preservation of water in the grapes and protection against oxidation of the grape membrane. The other results of these studies offer comprehensive insights into their physicochemical properties and potential applications within the food and perishable products industry. This research underscores the promising role of functionalized agar films in enhancing food safety and extending shelf life, contributing to advancements in intelligent packaging technologies.

Keywords:

Agar, Nanoparticles, Biopolymer, Smart-packing, Antibacterial.

Reference:

Bioactive agar-based functional composite film incorporated with copper sulfide nanoparticles.
Agar-based edible films for food packaging applications.
Antibacterial ability of immobilized silver nanoparticles in agar-agar films co-doped with magnesium ions.
Agar-based antioxidant composite films incorporated with melanin nanoparticles

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TRIBOLOGY, SURFACES AND INTERFACES / 168

CHARACTERISATION OF BORIDING ON 9254 STEEL WITH GREEN CHEMISTRY INTEGRATION

Author: Lizbeth Sanchez[1]

Co-authors: Dulce Viridiana Melo Máximo [2]; Marco Antonio Doñu Ruiz [1]; Milton Carlos Elías Espinosa [3]; Noé López Perrusquia [1]; Tomas de la Mora Ramírez [4]; Víctor Hugo Olmos Domínguez [4]

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[2] *Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Estado de México*

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Abstract

The automotive, maritime, aeronautical and agricultural industries need a series of innovative coatings on engineered that are submitted to high demand working conditions. For that, several research

projects are dedicated to improving the protective properties of the part surfaces in order to increase their useful life with the generation of a protective layer on the part´s surfaces. A good adhesion property between the a coating and surfaces of the part is one of the most important characteristic of a coated surfaces, being one good option, the generation of a coating by boriding process that can be the key to reducing wear and improve the useful life of engineering parts [3, 4]. In the same way, the reduction of waste is one of the main goal of the green chemistry, including the deposition process. This work shows the initial results of boriding processes allows to modify the surface properties of the material [5].In this study, ASI 9254 steel was. Specimens presented a square geometry with dimensions 2,54 cm x 2.54 cm and 1.5 cm of thickness. The boriding process was performed with reused boron paste of temperature at 1000℃for 4hrs,in a conventional muffleafter the thermochemical process, the box was removed to the cooling process at room temperature. The characterization of the type, morphology and thickness of the iron boride samples was obtained using optical microscopy (MO) using the equipment ZEISS Axio Vert.A1. The crystalline structure identified by X-Ray,with Bruker D8 Advance equipment, Cu Kα λ=1.5406 Å radiation. For the analysis of adhesion, the following standard was used VDI 3198 standard [8]. Cracks were also determined using the following Jeol JSM-6010LA (SEM) equipment, with ‘promising’ results .

Keywords:

Steel ,Boriding„characterisation,VDI3198

Reference:

Manufacturing, Engineering and Technology .
Thermochemical Surface Engineering of Steels, Elsevier Woodhead Publishing.
Optics & Laser Technology.
Defect and Diffusion Forum,
Microscopy and Microanalysis,
VDI. VDI 3198:

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TRIBOLOGY, SURFACES AND INTERFACES / 78

BEHAVIOR TO DRY ABRASIVE WEAR OF A BORIDING AND CARBONITRIDED AISI 8620 STEEL ANALYSIS

Author: MARTIN CASTILLO[1]

Co-authors: JESÚS GARCÍA [1]; MARÍA DE JESÚS VELÁZQUEZ VÁZQUEZ [1]

[1] *IPN ESIMEZ*

Corresponding Author: avinfer@hotmail.com

The objective of this article is to study the tribological behavior of an AISI 8620 steel, which was subjected to a boriding and carbonitriding process, analyzing the hardness and the relationship it has with respect to abrasion, as well as the formation of cracks generated. During the dry abrasive process, due to this phenomenon, it was observed that fracture wear occurs in the boride coating, as well as other types of wear, and a lower adhesion of the carbonitrided substrate is observed. The hardness obtained in the boriding steel was 57.8 HRC and its microhardness was 650 HV, while in the carbonitrided steel it is 58.3HRC and 660HV respectively. Although the hardness obtained in both treatments are very close, their behavior under the same conditions varies considerably, because this

difference directly influences the resistance presented by the abrasion phenomenon. The abrasion test carried out dry confirms that the carbonitriding coating allows less slippage of the abrasive particles compared to boring, in which the grooves generated are few and shallower, this is because there is less plastic deformation. The mass loss is lower compared to that obtained from carbonitrided steel. In general, boriding offers excellent resistance to wear, since there is a diffusion of boron in the crystalline network, altering the surface microstructure of the 8620 steel, which allows it to better resist abrasion, this is confirmed with a lower loss of mass.

Keywords:

tribological behavior, boriding, carbonitriding, plastic deformation

Reference:

T. Burakowski, J. Tacikowski, J. Senatorki (1990). Tribological properties in the diffusion layers of steel. Instytut Mechanike Precisvinei, Warzaw Poland.

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TRIBOLOGY, SURFACES AND INTERFACES / 393

AUTOMATION OF A WATER-CONDENSATION COLLECTION WATER SYSTEM USING VARIOUS COOPER SURFACES

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An automation system was designed and implemented, using ARDUINO, that allows us to continuously measure the environmental conditions and define the dew point to obtain condensed water in the collection system. With the object of explore the better surface to get condensation and precipitation of water we use various copper plates with different treatments, including pristine cooper, porous cooper (50μm pore size), and cooper with MWCNT in the surface, which were characterized using techniques such as contact angle, scanning electron microscope (SEM) and roughness analysis, each of these plates were put in a good thermal contact with a Peltier cell with its respective water-cooling system.

From the temperature and humidity obtained with a DHT11 sensor, and using a calibration curve that related the voltage and temperature of the surface of the Cu plate, the program determined the voltage needed to adjust the temperature to the dew point. The system regularly send to the power supply, or temperature controller, a signal to adjust the voltage on the board and thus maintain the optimal conditions to constantly condense the water under any external conditions.

Keywords:

Water, ARDUINO, dropwise condensation, Peltier cell, cooper, contact angle.

Reference:

Ankit Nagar, et al., ACS Nano 2020 14 (6), 6420-6435
Thanh X. Nguyen, et al., J. Phys. Chem. C 2011, 115

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TRIBOLOGY, SURFACES AND INTERFACES / 390

TRIBOLOGICAL PROPERTIES AND MICROSTRUCTURE OF (TiAlZrTaNb)Nx/TiAlZrTaNb MULTILAYERS GROWN ON HAYNES 282 SUPERALLOYS.

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Co-authors: Ingrid Johana Gonzalez Avila [1]; Jhon Jairo Olaya Florez [1]; Juan Pablo Gonzalez Lozano [1]; Oscar Edwin Piamba Tulcan

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TiAlZrTaNbNx/TiAlZrTaNb nano-multilayer films grown by High-Power Impulse Magnetron Sputtering (HiPIMS) on Haynes 282 superalloys, varying the bilayer period and a total thickness of about 1 μm. In this study, the influence of the bilayer period on the microstructure, tribological and mechanical properties of these films have been investigated. The microstructure, morphology and chemical composition of the coatings were analyzed by X-ray diffraction, Scanning Electron Microscopy and Energy Dispersive X-ray spectroscopy. The mechanical properties were evaluated by means of nanoindentation, and the tribological properties was studied with pin-on-disk technique. The performance of the (TiAlZrTaNb)Nx/ TiAlZrTaNb nanomultilayer was enhanced with the period increase, which can be attributed to the formation of a structure more dense . This multilayer architecture hinds columnar film growth resulting in better wear resistance.

Keywords:

Hipims , Haynes 282 , Multilayers , (TiAlZrTaNb)Nx, Wear.

Reference:

1. X. Chen.Y. Ding. y L.W. (2017). High-temperature oxidation. https://doi.org/10.16/j.ijrmhm2022.105937.

[2]. R. Larsson. y P. Hedenqvist. Coatings in motor vehicles, (2001). https://doi.org/10.1016/s0043-1648(01)00565-8.

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