## **XVII-ICSMV**



## **Report of Contributions**

Contribution ID: 14 Type: Oral

# IDENTIFICATION OF STRUCTURAL AND MECHANICAL PROPERTIES OF WILD CHIKUNGUNYA VIRUS (CHIKV) AND E2 N264Q MUTATED CHIKV.

Chikungunya fever is a zoonotic disease caused by the Chikungunya virus with a fatality rate of 1 death per 1,000 infected patients. The main symptoms of this disease are fever, muscle and joint pain, in most cases, these symptoms persist for two weeks; however, it is possible to develop a chronic form of Chikungunya disease where comorbidities that lead to death may develop. The introduction of mutations in the CHIKV virus has been observed to modify the way in which its surface glycoproteins interact, modifying the surface structure and decreasing the infectivity of the CHIKV. It is also known that this virus, in its infection process during its entry into the cell, crosses through mediums with different pH, so this work aims to study and characterize the stability and surface symmetry of CHIKV to contribute to the construction of a thermodynamic model of the assembly of this virus. The construction of this type of model for membrane-bound viruses, such as CHIKV, is very important since it is the basis of current methods for testing new destabilizing drugs or infection inhibitors. However, the most widely used methods today are based on the use of cell lines, which makes these tests very expensive and time-consuming. Raman spectroscopy is an analytical technique that provides information on the vibrational modes present in a sample and allows us to relate them to its structure and composition. It also has the advantage of being able to analyze samples in situ, modifying thermodynamic parameters in real-time, which is very useful for this work since it will facilitate the immediate observation of conformational changes in the glycoproteins of the surface of CHIKV by varying parameters such as temperature or pH and thus study the thermodynamic stability of the virus.

## **Keywords**

Chikungunya, AFM, Raman, SERS, Physical virology.

## Reference

Cardoso-Lima, R., Filho, J. F. S. D., de Araujo Dorneles, M. L., Gaspar, R. S., Souza, P. F. N., Costa dos Santos, C., ···Alencar, L. M. R. Nanomechanical and Vibrational Signature of Chikungunya Viral Particles. Viruses, 14(12). (2002) https://doi.org/10.3390/v14122821

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Track Classification: Characterization and Metrology

Contribution ID: 15 Type: Poster

## Nanoparticle formation in co-sputtered Cu-Ni films deposited by reactive RF-Sputtering\*

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 °C 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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XVII-ICSMV

/ Report of Contributions

Nanoparticle formation in co-  $\dots$ 

**Session Classification:** THIN FILMS

Track Classification: Thin Films

Contribution ID: 21 Type: Poster

## GROWTH OF SMFE1-XCOX THIN FILM BY MOCVD AND EXITU DIFFUSION PROCESSES

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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Session Classification: THIN FILMS

Track Classification: Thin Films

Contribution ID: 22 Type: Oral

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

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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Session Classification: SEMICONDUCTORS

Track Classification: Semiconductors

Contribution ID: 23 Type: Poster

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

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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Session Classification: PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 24 Type: Poster

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

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.

## This work was supported by

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Session Classification: PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 26 Type: Poster

## MULTILAYER MODEL SOFTWARE FOR CHEMICAL COMPOSITION ANALYSIS FROM XPS DATA

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  $[ZnO]_4$  (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 K $\alpha$  radiation: I: cobalt spinel. Surf. Interface Anal. 2016, 48, 252–256. https://doi.org/10.1002/sia.5933

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Session Classification: PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 27 Type: Oral

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

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  $1.5 \times 10$ -7 Torr and the pressure during sublimation was  $6.5 \times 10$  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  $1 \times 103$  L to  $1 \times 107$  L ( $1 \times 100$  L

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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**Session Classification:** PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 29 Type: Either

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

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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**Session Classification:** PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 34 Type: Poster

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

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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Session Classification: PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 47 Type: Oral

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

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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Session Classification: ATOMIC LAYER DEPOSITION

Track Classification: Atomic Layer Deposition

Contribution ID: 49 Type: Oral

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

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\(\times\) 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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**Session Classification:** PLASMA AND VACUUM

Track Classification: Plasma and Vacuum

Contribution ID: 50 Type: Oral

# EXPLORING THE IMPACT OF COUPLING SYNERGISTIC SEMICONDUCTORS α-Fe2O3 AND ZnO TO CONSTRUCT FEASIBLE BILAYER THIN FILM PHOTOCATALYSTS

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  $\alpha$ -Fe2O3/ZnO(5nm)/Glass and α-Fe<sub>2</sub>O<sub>3</sub>/ZnO(15nm)/Glass. The synthesis of ultrathin layers of ZnO was conducted using atomic layer deposition (ALD), whereas the deposition of the 200 nm  $\alpha$ -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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Session Classification: SEMICONDUCTORS

Track Classification: Semiconductors

Contribution ID: 55 Type: Poster

## A DIFFERENTIAL THERMAL LENS SPECTROMETRY METHOD FOR TRACE DETECTION

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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Track Classification: Characterization and Metrology

Contribution ID: 64 Type: Oral

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

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

N/A

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Session Classification: CHARACTERIZATION AND METROLOGY

Track Classification: Characterization and Metrology

Contribution ID: 67 Type: Oral

## CORROSION RESISTANCE AND HARDNESS EVALUATION ON AZ31B ALLOY BY ATMOSPHERIC PRESSURE PLASMA JET TiO2 COATING

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°C) 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. APPI 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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Session Classification: TRIBOLOGY, SURFACES AND INTERFACES

Track Classification: Tribology, Surfaces and Interfaces

Contribution ID: 81 Type: Oral

## GROWTH OF HIGHLY TEXTURED NON-COLLINEAR ANTIFERROMAGNETIC D019-Mn3Ge/GaN (0001) THIN FILMS BY MAGNETRON SPUTTERING

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 nonvolatile 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 °C, 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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Session Classification: MULTIFUNCTIONAL AND MAGNETIC MATERIALS

Track Classification: Thin Films