

## Functional Thin Films and Surfaces

### Room Palm 5-6 - Session MB2-1-MoM

#### Thin Films for Electronic Devices I

**Moderators:** Jiri Houska, University of West Bohemia, Czechia, Spyros Kassavetis, Aristotle University of Thessaloniki, Greece

10:20am **MB2-1-MoM-2 Enhanced Etching Resistance of Y2O3 Films Through Microstructure Control via Thermal Annealing**, *Shiao Wang, Qiuming Fu, Hongyang Zhao*, Wuhan Institute of Technology, China; **Tomasz Liskiewicz** [[t.liskiewicz@mmu.ac.uk](mailto:t.liskiewicz@mmu.ac.uk)], Manchester Metropolitan University, UK; *Ben Beake*, Micro Materials Ltd, UK; *Yanwen Zhou*, Wuhan Pudi Vacuum Technology Co., China

Yttrium oxide (Y2O3) is a promising material for etch-resistant coatings in semiconductor manufacturing due to its high hardness, high melting point, and excellent chemical stability. This study investigates the effect of thermal annealing on the microstructure and etching resistance of Y2O3 thin films, aiming to improve their performance without introducing additional phases. Current methods for improving Y2O3 etching resistance involve costly phase introductions, and the effect of annealing temperature on the etching resistance of Y2O3 thin films has been understudied.

Y2O3 films were deposited on P-type Si substrates using RF magnetron sputtering. The films were then annealed in a vacuum at 300°C, 600°C, and 900°C. The crystal structure was characterised using XRD, and surface morphology was observed with FESEM. Etching tests were conducted using inductively coupled plasma with two different environments, chemical etching (CF4 and O2) and mixed etching (CF4, Ar, and O2). The etching rates and surface roughness were determined using a step profiler and AFM respectively. Chemical bond analysis was performed using XPS.

XRD analysis revealed that the Y2O3 films exhibited a polycrystalline cubic structure. The sharpness of the diffraction peaks increased and then decreased with increasing annealing temperature, indicating grain size changes. FESEM images showed that the film annealed at 900°C had a dense, laminated structure with no pores or defects, while films annealed at 600°C and 300°C displayed rod-shaped grain structures with noticeable gaps. The etching rates of Y2O3 films were significantly lower than those of Al2O3, Si, and other materials. The 900°C annealed film exhibited the lowest etch rates. AFM analysis showed the roughness of Y2O3 thin films decreased after both chemical and mix etching. XPS analysis confirmed the formation of Y-F compounds during etching, with deeper F penetration in mix etching due to Ar+ sputtering.

The enhanced etching resistance of the 900°C annealed Y2O3 film is attributed to its high density and low surface roughness. In chemical etching, F radicals react with Y2O3, forming a Y-F protective layer, which reduces further etching. In mix etching, the additional Ar plasma facilitates the detachment of the formed Y-F compounds, increasing the etching rate compared to chemical etching.

This study demonstrates that thermal annealing is a cost-effective method to improve the etching resistance of Y2O3 films. The 900°C annealing resulted in a dense film with superior etching resistance, making it a promising material for protective coatings in semiconductor manufacturing.

10:40am **MB2-1-MoM-3 Integration of Pzt with Transparent Conductive Layers for Enhanced Piezoelectric Applications**, *Nicoleta Nedelcu* [[nnedelcu@mtroyal.ca](mailto:nnedelcu@mtroyal.ca)], *Fred Harford, Dylan Webb*, Mount Royal University, Canada; *Cristian Rugina, Ana Maria Mitu*, Institute of Solid Mechanics Romanian Academy, Romania; *Arcadie Sobetkii*, MGM Star Construct Ltd, Romania

Lead zirconate titanate (PZT, Pb(Zr,Ti)O<sub>3</sub>) is widely recognized for its superior piezoelectric properties, making it a key material in micro-actuator applications. PZT technology is extensively utilized in MEMS-based devices, including inkjet printheads, micro-speakers, and autofocus cameras. Quartz crystal resonators (QCRs), another essential component in communication systems, leverage the piezoelectric properties of quartz to generate stable oscillation frequencies. This study explores the integration of PZT with a transparent conductive layer to develop high-performance piezoelectric sensors and actuators. Specifically, we investigate the deposition of a conductive layer on PZT, QCRs, and quartz glass using DC sputtering. Optical characterization via UV-VIS spectrophotometry assesses transparency and optical properties, while dielectric constants are determined through mathematical modeling. X-ray diffraction (XRD) confirms the preservation of the pure perovskite phase in PZT, and surface morphology analysis using

SEM and AFM reveals a uniform superficial layer with dispersed indium tin oxide (ITO) particles (10–30 nm). The electromechanical impedance (EMI) method is employed to evaluate PZT/Ag, PZT/ITO, QCR/Ag, and QCR/ITO structures, with minor variations attributed to temperature fluctuations, electrode thickness, and device positioning.

The successful integration of PZT with a transparent conductive layer on ceramic substrates demonstrates promising applications in transparent piezoelectric sensors, interactive displays, and touch-sensitive interfaces. These findings provide a foundation for developing high-transparency, piezoelectric-based touch sensors with improved electrical and optical performance.

11:00am **MB2-1-MoM-4 High-Quality C-Textured Sc0.36Al0.67N Thin Films on 200 Mm Si Wafers for Piezoelectric Applications**, *Sanjay Nayak* [[sanjay.nayak@silicon-austria.com](mailto:sanjay.nayak@silicon-austria.com)], Silicon Austria Labs GmbH, Austria

Sc-alloyed AlN (ScAlN) has emerged as a promising candidate for next-generation piezoelectric materials, offering superior piezoelectric properties and thermal stability compared to traditional perovskite-based materials. However, the metastable nature of ScAlN and the challenges associated with achieving high-quality, phase-pure films, especially in multilayer stacks, have limited its practical applications. This work presents a significant advancement in ScAlN thin-film technology. By employing a carefully optimized process and a suitable buffer layer, we have successfully fabricated high-quality Sc<sub>0.36</sub>Al<sub>0.67</sub>N films with excellent piezoelectric properties. The bilayer films exhibit comparable crystalline quality to single-layer films, demonstrating the potential for scaling up the fabrication of complex ScAlN-based devices. We demonstrate the microstructural and stress tunability of ScAlN thin films by tuning the process parameters. The average piezoelectric coefficient ( $e_{31,f}$ ) measured over a 200 mm wafer was found to be  $-2.9$  C/m<sup>2</sup>, highlighting the exceptional performance of these films. This achievement opens new possibilities for the development of high-performance MEMS devices, including energy harvesters, resonators, sensors, and actuators, that leverage the unique properties of ScAlN.

11:20am **MB2-1-MoM-5 Patterned Silver Nanowire Network for CdSe@CdZnS/ZnS Green Quantum Dot Light-Emitting Diodes**, *Chia-Yu Lin, Tzu-Hsu Wen, Chun-Yuan Huang* [[cyhuang2004@gm.ntu.edu.tw](mailto:cyhuang2004@gm.ntu.edu.tw)], National Taitung University, Taiwan

Silver nanowire (AgNW) network possesses excellent conductivity and flexibility, making it an ideal material for electrodes of flexible optoelectronic devices. However, their high surface roughness can negatively impact device performance. To address this issue, the roughness of the patterned AgNW network electrode was reduced using a transparent photopolymer. To fabricate the patterned AgNW films, firstly, the polydimethylsiloxane (PDMS) substrates with proper size (18×18 mm<sup>2</sup>) were covered with the stainless-steel shadow mask and then treated with UV ozone for 30 minutes. A 2 wt % AgNWs-ethanol solution was spin-coated, annealed, and then covered with UV-curable polyurethane (Norland Optical Adhesive 63, Edmund Optics). After UV curing, the composite of AgNW/polyurethane was then peeled off from the PDMS, allowing the AgNWs/polyurethane composite conductive film to adhere to the poly(ethylene terephthalate)(PET) substrate. Accordingly, with high transparency of 77% and low sheet resistance of 7~9 Ω/sq, the patterned AgNW network embedded in the polyurethane matrix was obtained for the subsequent fabrication of quantum dot light-emitting diodes (QLEDs). The electrode was applied as the anode in green CdSe/CdZnS/ZnS QLEDs. With the device structure of AgNW network/PEDOT:PSS/TFB/QD/MgZnO/Al, the QLED emitting pure green light centered at 536 nm resulted in a turn-on voltage of 2.4 V, a maximum brightness of 72,922 cd/m<sup>2</sup>, and a current efficiency of 27.8 cd/A.

11:40am **MB2-1-MoM-6 Effects of Room Temperature Sputtered Nano-Interfaced WxMoyO3 Nanograins on Highly Responsive NO Sensing**, *Somdatta Singh* [[somdatta@ic.iitr.ac.in](mailto:somdatta@ic.iitr.ac.in)], Indian Institute of Technology Roorkee, India; *Ravikant Adalati*, University of Mons, Belgium, India; *Prachi Gurawal, Raman Devi*, Indian Institute of Technology Roorkee, India; *Gaurav Malik*, Jeonbuk National University, Republic of Korea, India; *Davinder Kaur, Ramesh Chandra*, Indian Institute of Technology Roorkee, India

This work demonstrates a heterostructure of monoclinic molybdenum trioxide (n-MoO<sub>3</sub>) and tungsten trioxide (n-WO<sub>3</sub>) with nano-interfaced (n-i@WxMoyO<sub>3</sub>) based NO gas sensing material. The nanocrystalline n-i@WxMoyO<sub>3</sub> thin film was coated using a single-step magnetron sputtering technique on an n-type (100) silicon substrate. Within the temperature range of approximately ambient temperature (50°C) to 350°C, this sensing material, WxMoyO<sub>3</sub> (where x = 0.71 and y = 0.29), detects NO gas and

investigates the impact of crystal structure and nanointerfaces on sensing performance. A heterostructure composed of several materials can enhance the interaction between the gas molecules and the sensor surface by producing interfaces that promote charge transfer. With a response/recovery time of around 300 seconds/125 seconds at 300°C, the n-i@W<sub>x</sub>Mo<sub>y</sub>O<sub>3</sub> has a low limit of detection (DL) of about 39 ppb and an excellent sensor response (SR = R<sub>g</sub>/R<sub>a</sub>) of about 44.15 for 50 ppm NO gas. Even at 50°C, the enhanced sensitivity of the sensing material with the nanointerface shows a strong affinity for NO molecules. It provides around 1.03 SR with response/recovery times of 53 and 71 seconds, respectively. The robustness of the n-i@W<sub>x</sub>Mo<sub>y</sub>O<sub>3</sub> thin film sensor was established by its excellent selectivity (SR = ~44.15) and long-term stability (60 days) towards 50 ppm NO at 300°C. The remarkable sensing properties of MoO<sub>3</sub> functionalized WO<sub>3</sub> nanograins indicate an exciting potential for NO gas sensors that operate close to ambient temperature (50°C).

12:00pm **MB2-1-MoM-7 Study on the Effect of Different Oxygen Flow Rates on Vanadium-Doped Zinc Oxide Thin Film Piezoelectric Pressure Sensors, Cheng Han Hsu [e204242271@gmail.com], National Cheng Kung University (NCKU), Taiwan**

The piezoelectric effect is a phenomenon where certain materials generate an electric charge when subjected to mechanical stress. This property is widely utilized in sensors, and energy-harvesting devices because it converts mechanical energy into electrical energy. ZnO is a promising material for energy-harvesting devices due to its piezoelectric and semiconductor properties, along with good biocompatibility and low environmental impact. However, its relatively low piezoelectric coefficient (12.4 pC/N) limits its potential in these applications. To enhance the piezoelectric coefficient, vanadium was doped into ZnO thin films. Vanadium ions have a higher valence than zinc ions, which improves electric polarization and increases the piezoelectric coefficient. Additionally, V<sup>5+</sup> ions, having a higher positive charge than V<sup>3+</sup> ions, create stronger polarity, further boosting the piezoelectric properties. By adjusting the oxygen flow rate during the sputtering process, the V<sup>5+</sup> content in the films is increased, enhancing the piezoelectric coefficient. In this study, we utilized an RF sputtering system with varying oxygen flow rates to prepare vanadium-doped zinc oxide thin films, which were then used to fabricate piezoelectric pressure sensor devices. The results show that as the oxygen flow rate increases, the grain shape of the thin films changes, and the grain size decreases. SEM reveals significant changes in the grain structure. XRD shows that the intensity of the 002 peak weakens as the oxygen flow rate increases, indicating structural changes in the thin films. XPS reveals that the content of pentavalent vanadium increases with higher oxygen flow rates, but decreases after reaching a critical value, which correlates with the trend observed in piezoelectric coefficient measurements. Further analysis of the O1s XPS shows that the lattice oxygen content in the films is higher than the surface adsorbed oxygen, with the lowest number of oxygen vacancies at a certain oxygen flow rate, which then increases as the oxygen flow rate rises. UV-visible spectra indicate that, due to the Burstein-Moss effect, the energy band structure of the thin films initially decreases and then increases with increasing oxygen flow rates. Finally, piezoelectric pressure sensors were fabricated from these thin films, and the stress sensitivity at different oxygen flow rates was measured. This study provides a comprehensive investigation of the structural, optical, piezoelectric properties of V-doped zinc oxide thin films at varying oxygen flow rates and explores their application as piezoelectric pressure sensors. The findings offer insights for optimizing thin film performance in piezoelectric sensing devices.

## Functional Thin Films and Surfaces

### Room Palm 5-6 - Session MB2-2-MoA

#### Thin Films for Electronic Devices II

**Moderators:** Spyros Kassavetis, Aristotle University of Thessaloniki, Greece, Tomas Kubart, Uppsala University, Sweden

2:40pm **MB2-2-MoA-4 Polycarbonate Transfer Techniques for the Fabrication of MoS<sub>2</sub> Based Field Effect Transistors**, Chih-Hao Chiang, Ruo-Yao Wang [tsubasaja@gmail.com], Meng-Lin Tsai, National Taiwan University of Science and Technology, Taiwan

In recent years, transition metal dichalcogenides (TMDs) have received significant attention due to their immense potential to extend Moore's Law, positioning them as promising semiconductor materials for next-generation electronic devices. The challenges of large-scale production and commercialization of TMDs remain key challenges for future development in practical applications. In the fabrication of TMD-based semiconductor devices, the interface between metal electrodes and TMD layers is critical. Traditional metal electrode deposition techniques facilitate the diffusion of metals in the TMD, potentially reducing the device performance or preventing proper operation. In this study, the metal electrode transfer technique using polycarbonate has been developed to significantly reduce such damage, ensuring the reliable operation of semiconductor devices. Gold electrodes initially deposited on silicon or SiO<sub>2</sub>/Si substrates via metal mask (channel length of 20 μm) and photolithography (channel lengths of 8 μm for photodetectors and 3 μm for field-effect transistors, FETs) have been successfully onto chemical vapor deposition (CVD)-grown MoS<sub>2</sub> nanosheets. The as-fabricated field effect transistors (FETs) have been characterized to exhibit switching current ratios of approximately 10<sup>4</sup>.

3:00pm **MB2-2-MoA-5 Advancing Piezo-Gated Transistor Performance by Bilayer of V-doped ZnO and Mesoporous PVDF-TrFE**, Yu Zhen Zhang [n56124650@gs.ncku.edu.tw], National Cheng Kung University (NCKU), Taiwan

In recent years, technology has rapidly advanced, enabling the development of flexible wearable electronics with great potential for applications such as nanogenerators and pressure sensors. Among flexible materials, β-phase PVDF-TrFE, which exhibits piezoelectric properties (d<sub>33</sub>=30–40pC/N), stands out as a promising composite. This polymer has a semicrystalline structure and displays excellent piezoelectric and ferroelectric properties while maintaining flexibility. However, VZO (d<sub>33</sub>=12–22pC/N) is also a piezoelectric material, and we aim to improve the device output by depositing it on PVDF-TrFE.

In this study, we aimed to enhance the flexibility and piezoelectric performance of PVDF-TrFE by blending it with zinc oxide nanoparticles and subjecting the mixture to thermal annealing at 120°C. We then applied 11,000 V through corona poling to align the dipole directions within the composite, followed by etching the ZnO to create a porous structure. Additionally, we used radio frequency magnetron co-sputtering that uses ZnO and V<sub>2</sub>O<sub>5</sub> as targets to deposit VZO thin film on both sides of the PVDF-TrFE to serve as conduction pathways. Finally, we deposited two Au electrodes to make a piezoelectric gate transistor device.

In the XRD analysis, we examined unpoled and corona-poled samples. The XRD patterns of the unpoled sample showed two peaks corresponding to the α phase which has negatively affects the piezoelectric properties. After poling, the pattern of the poled sample confirmed that the β phase completely dominates the PVDF-TrFE.

We investigated the current output of the piezoelectric gate transistor under various mechanical stresses at a 1V bias and 1Hz frequency. Devices with different dipole orientations exhibited opposite behaviors. Applying mechanical stress to the positively polarized surface generated negative charges at the VZO and PVDF-TrFE interface, creating a depletion region in the top surface channel and reducing current. Conversely, this led to an accumulation region, enhancing current. By applying a piezoelectric field to the gate, we could adjust the semiconductor channel's resistance and control current flow. This technique significantly advances the piezoelectric gate transistor device, paving the way for advanced applications in flexible and wearable electronics and sensing technologies.

3:20pm **MB2-2-MoA-6 Enhanced Synaptic Characteristics Under Applied Magnetic Field in V<sub>2</sub>O<sub>5</sub>/NiMnIn Based Switching Device for Neuromorphic Computing**, Kumar Kaushlendra [kumar\_k@ph.iitr.ac.in], Indian Institute of Technology Roorkee, India; Davinder Kaur, Indian Institute of Technology Roorkee, India

The present study reports a memory structure Al/V<sub>2</sub>O<sub>5</sub>/NiMnIn on a flexible stainless-steel (SS) substrate for neuromorphic applications. The fabricated device exhibits gradual SET and RESET switching characteristics with an OFF/ON resistance ratio of ~100, good consistency of 4500, and excellent data retention capability up to 3000 s. The current-voltage (I-V) study supports an Ohmic conduction mechanism in the low resistance state (LRS). In contrast, the trap-controlled modified space charge conduction mechanism demonstrated the high resistance state (HRS). The resistance versus temperature measurement (R-T) in the LRS and HRS of the device signifies that oxygen vacancies form the conduction filament. We further analyze the synaptic functioning by applying identical consecutive voltage pulses, and the device's conductance change has been observed. These characteristics show a good representation of the biological memory synapse in terms of the artificial memory device. Long-term potentiation (LTP) and long-term depression (LTD) show nonlinear and asymmetry behavior, which is substantial for neuromorphic applications. A considerable shift in LTP and LTD was detected by applying external temperature and magnetic field. This is explained via temperature and magnetic field strain in the functional NiMnIn bottom electrode of the fabricated device. The mechanical flexibility of the memory structure was tested by exploring the switching characteristics with various bending angles and bending cycles. Therefore, the present study offers new avenues for flexible devices with high data storage capability for futuristic neuromorphic applications.

4:00pm **MB2-2-MoA-8 Fabrication and Characterization of Iron Titanate Thin Films as a Potential Tunnel Barrier for Magnetic Tunnel Junction (MTJ's)**, Adnan Kareem [adnankareem94@gmail.com], Jozef Stefan Institute, Slovenia, Pakistan

Spintronics addresses rising power dissipation in electronic circuits by offering advantages such as 0% standby leakage, low power consumption, unlimited durability, non-volatility, and compatibility with CMOS technology [1]. In this research work focuses on magnetic tunnel junctions (MTJs) in spintronics, investigating the barrier layer for efficient electron spin transfer, crucial for Magnetic Random Access Memory (MRAM). Iron titanate thin films have attracted research interest due to their potential applications in spintronic devices [2]. An application-oriented electrodeposition technique was used to prepare iron titanate thin films with varying electrolyte molarities [1,2]. XRD results reveals the amorphous behavior of As-deposited thin films. Magnetic field (MF) annealing improved the structural and magnetic properties, the Fe<sub>2</sub>TiO<sub>4</sub> phase was observed, confirming a spinel structure with increased crystallite size and strengthened phase as molarity increased. Magnetic analysis using a vibrating sample magnetometer (VSM) showed soft ferromagnetic behavior in annealed thin films, while the as deposited thin films show para-ferromagnetic mixed behavior. As-deposited films had lower saturation magnetization compared to annealed films.

In conclusion, Fe<sub>2</sub>TiO<sub>4</sub> thin films fabricated via electrodeposition demonstrate significant potential for future spintronic devices specifically in the advancements of MRAM technology.

References:

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4:20pm **MB2-2-MoA-9 Fabrication of IZO/IGZO-Based Vertical Thin-Film Transistor and Its Integration with OLEDs for High-Density Display**, Nahyun Kim [knhangle0215@naver.com], Seok Hee Hong, Jun Hyeok Lee, Ho Jin Lee, Tae Geun Kim, Korea University, Republic of Korea

The rising demand for next-generation applications, such as augmented reality (AR), virtual reality (VR), and wearable devices, has made ultra-high-resolution displays with pixel densities reaching thousands of pixels per inch (PPI) essential. Achieving such high resolutions requires innovative driving circuits and advanced structures for the driving units. Conventional planar thin-film transistors (TFTs) face significant challenges at nanoscale

# Monday Afternoon, May 12, 2025

channel lengths, including short-channel effects and threshold voltage ( $V_{th}$ ) instability, which reduce reliability and performance [1]. Therefore, planar TFTs are inadequate as drivers for high-resolution displays, positioning vertical channel TFTs (VTFTs) as a promising alternative [2]. Conventional VTFTs feature spacers between the top and bottom electrodes, with a channel layer formed along the spacer sidewalls. However, sidewall interface conditions can result in unstable channel characteristics and lower carrier mobility compared to planar TFTs [3],[4].

Herein, we propose a novel VTFT architecture utilizing a dual-layer metal oxide channel structure, as depicted in Figure 1(a). To further enhance integration, the top electrode of the VTFT is employed as the reflective electrode in OLED devices, enabling a VTFT-based top-emitting OLED integration. We address channel stability by implementing an  $HfO_x$ -based dual-layer oxide spacer, which generates a quasi-2D electron gas at the oxide interfaces with high electron density, as shown in Figure 1(b). This concentrated electron layer facilitates main channel formation at the interface while optimizing the dual-layer thickness maximizes carrier mobility along the channel path. Additionally, pulsed Joule heating enables localized activation of the active layer without external thermal processing, allowing low-temperature processing by avoiding direct substrate heating. This supports flexible display applications compatible with various substrate materials. Experimental results indicate high performance with a mobility of  $16.34 \text{ cm}^2/\text{Vs}$ ,  $V_{th}$  of 0.2 V, subthreshold swing of 0.4 V/dec, and an on/off ratio exceeding  $10^5$  (Figure 1(c)).

Finally, based on these results, we propose an integrated VTFT/OLED structure, realizing a high-integration display component. The integrated VTFT/OLED solution not only offers superior mobility and stability but also supports low-temperature processing for diverse substrates, contributing significantly to advancements in next-generation display technologies. This approach shows substantial potential for applications in AR/VR, wearable devices, and high-resolution monitors, advancing new possibilities in display technology.

**4:40pm MB2-2-MoA-10 Preventing Native Oxide Formation in Niobium Thin Films Through Platinum Encapsulation, Anya Chatteraj [achattara@bnl.gov], Aswin Anbalagan, Brookhaven National Laboratory, USA; Jinhyun Cho, Stony Brook University, USA; Mingzhao Liu, Brookhaven National Laboratory, USA**

This study investigates the impact of encapsulating niobium (Nb) thin films with platinum (Pt) to enhance the performance and stability of qubits in quantum computing, focusing on the role of thin film technology. Niobium-based qubits hold significant promise for quantum computing, but their performance is often compromised by oxide formation and dielectric losses, which contribute to decoherence and limit their coherence times. To address these challenges, a Pt capping layer was applied to Nb thin films with the goal of preventing oxide formation, reducing dielectric loss, and maintaining the superconducting properties of Nb. The Nb thin films were optimized using sputtered deposition, ensuring high-quality film growth, and Pt was subsequently deposited in a controlled, oxygen-free environment to minimize exposure to the atmosphere and reduce the risk of oxidation. To evaluate the effectiveness of the Pt encapsulation, a series of structural and chemical analyses were conducted, including Grazing Incidence X-ray Diffraction, and Hard X-ray Photoelectron Spectroscopy. These techniques confirmed that the Pt capping layer effectively prevented the formation of significant oxide layers at the Nb/Pt interface, an essential factor in improving qubit stability and mitigating decoherence. While some alloying between Nb and Pt was observed, it did not negatively impact the superconducting properties of the Nb films, which maintained a critical transition temperature ( $T_c$ ) of approximately 9 K. This indicates that the superconductivity of Nb was preserved despite the Pt encapsulation, highlighting the potential of this approach to enhance qubit stability without compromising performance. The results demonstrate that encapsulating Nb with Pt in thin film form significantly improves qubit stability by mitigating dielectric loss and oxide formation, crucial factors for maintaining coherence in quantum computing. This method offers a promising pathway for improving the performance of Nb-based qubits, particularly in applications such as quantum communication, where long coherence times and stable qubits are vital for efficient data processing and analysis. While the results are promising, further research is needed to refine deposition techniques, explore alternative capping materials, and optimize the fabrication process to achieve even longer coherence times. These efforts are essential to realizing the full potential of Nb-based qubits in practical quantum computing applications.

## References

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2. Wang *et al.* 2015. *Applied Physics Letters*, 107(16).

**5:00pm MB2-2-MoA-11 Multicomponent Doping for Suppressing Resistivity Scaling of RuAl Intermetallic Compound for Next-Generation Interconnects, Yi-Ying Fang [ian6325508428@gmail.com], Yung-Hsuan Tsai, Yu-Lin Chen, Shou-Yi Chang, National Tsing Hua University, Taiwan**

Ruthenium (Ru) and molybdenum (Mo) with a low product of resistivity ( $\rho_0$ ) and electron mean free path ( $\lambda$ ) have been considered as potential interconnect materials to replace copper (Cu) [1]. However, as the size of interconnects shrinks, metallic materials with an even shorter  $\lambda$  are needed to suppress resistivity scaling. Intermetallic compounds (IMCs) with strong bonding, a low diffusivity and a short  $\lambda$ , are promising candidates [2]. Previously, we investigated RuAl IMC, which has a low bulk resistivity ( $14 \mu\Omega\text{-cm}$ ), a short  $\lambda$  (about 4 nm) and an excellent thermal stability, but its  $\rho_0 \times \lambda$  value ( $5.6 \times 10^{-16} \Omega\text{m}^2$ ) is still high, causing a sharp increase in resistivity below 5 nm [3]. This study further added 10% one-to-multicomponent alloys (denoted as 1B-5B) into RuAl B2 IMC using co-sputtering, as a strategy to further reduce  $\lambda$  through lattice distortion and enhanced orbital overlap. Experimental results indicated that the  $\text{Al}_5\text{Ru}_4(\text{Nb})_1$  films retained an ordered B2 structure. Electrical measurements revealed that the bulk resistivity was influenced by both the lattice distortion of the IMCs and the electronegativity of the doped elements, which increased the electronic disorder and broadened the band structure [4], leading to a stronger impurity scattering. Although the  $\text{Al}_5\text{Ru}_4(\text{Nb})_1$  IMCs had a higher intrinsic resistivity than RuAl, the multicomponent doping effectively reduced the electron mean free path from about 3 nm to only about 1 nm. Consequently, compared to RuAl, the 4B- and 5B-doped  $\text{Al}_5\text{Ru}_4(\text{Nb})_1$  IMCs demonstrated a lower  $\rho_0 \times \lambda$  value of  $4.5 \times 10^{-16} \Omega\text{m}^2$  that is expected to mitigate the sharp resistivity increase at a reduced thickness. Furthermore, the thermal coefficients of resistivity (TCR) of the  $\text{Al}_5\text{Ru}_4(\text{Nb})_1$  IMCs of only 0.03/°C were comparable to that of RuAl and lower than that of pure metals, effectively minimizing the resistivity fluctuations with temperature. Additionally, with a large negative formation enthalpy of about -45 kJ/mol, the  $\text{Al}_5\text{Ru}_4(\text{Nb})_1$  IMCs exhibited exceptional thermal stability even at an extreme temperature of 800°C, demonstrating its strong potential as a reliable interconnect metallization material without the need of diffusion barrier.

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## Functional Thin Films and Surfaces

### Room Palm 5-6 - Session MB2-3-TuM

#### Thin Films for Electronic Devices III

**Moderators:** Jiri Houska, University of West Bohemia, Czechia, **Ufuk Kilic**, University of Nebraska - Lincoln, USA

8:00am **MB2-3-TuM-1 Morphological Effects and Impurity Levels on the High-Temperature Electrical Insulation of reactively sputtered AlN**, **Norma Salvadores Farran** [[norma.salvadores@tuwien.ac.at](mailto:norma.salvadores@tuwien.ac.at)], Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria; **Tomasz Wojcik**, Christian Doppler Laboratory for Surface Engineering of high-performance Components, Austria; **Carmen Jerg**, Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein; **Astrid Gies**, Oerlikon Balzers, Oerlikon Surface Solutions, Liechtenstein; **Jürgen Ramm**, Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein; **Szilard Kolozsvári**, **Peter Polcik**, Plansee Composite Materials GmbH, Germany; **Jürgen Fleig**, **Tobias Huber**, Institute of Chemical Technologies and Analytics, TU Wien, Austria; **Eleni Ntemou**, **Daniel Primetzhofer**, Department of Physics and Astronomy, Uppsala University, Sweden; **Helmut Riedl**, Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria

Aluminum nitride-based ceramics are renowned for their insulating properties and high thermal conductivity. Consequently, these materials have been employed for various applications across a range of temperature conditions, with a particular focus on insulating purposes. Nevertheless, as the electrical conductivity is a thermally activated process, the mobility of charge carriers at elevated temperatures presents a significant challenge for insulating thin film materials.

The aim of this study is to explore the effect of morphological features (i.e. grain size or porosities) and impurities on hexagonal structured AlN thin films using different physical vapor deposition techniques. Given the difficulties associated with maintaining process stability during the deposition of insulating coatings, various reactive PVD techniques have been explored, including magnetron sputtering (DCMS), high-power pulsed magnetron sputtering (HIPIMS), and pulsed magnetron sputtering (PMS). All films were grown in an in-house developed magnetron sputter system using 3" Al targets in a mixed Ar/N<sub>2</sub> atmospheres. Phase formation has been examined using X-ray diffractometry (XRD), while the morphology was investigated in detail through scanning and transmission electron microscopy (SEM and TEM). The insulating behaviour of all films grown on metallic substrates was analysed using in-situ impedance spectroscopy across a temperature range from 400°C to 750°C – utilizing differently sized Ti/Pt lithography pads. The concentration of impurities, especially oxygen, was determined through the use of electron-induced X-ray emission spectroscopy (ERDA).

The results of the impedance measurements demonstrated a correlation between the electrical properties of the films and their morphological characteristics. The films grown via HIPIMS exhibited the highest morphological density and the greatest resistance over temperature. The samples deposited via PMS also demonstrated high electrical resistivity, although the values decreased at a certain level. It was not possible to determine the insulating properties of the films grown via DCMS, due to the presence of pinholes in the samples which also signifies a less dense morphology. Moreover, the influence of impurities as O<sub>2</sub> has a significant effect on reducing the electrical resistivity of the films.

8:20am **MB2-3-TuM-2 Pulsed Laser Deposition of Epitaxial Ti<sub>3</sub>AlC<sub>2</sub> MXene Thin Films on Al<sub>2</sub>O<sub>3</sub>(0001) Substrate**, **Pramod Kumar** [[pramod.kumar@surrey.ac.uk](mailto:pramod.kumar@surrey.ac.uk)], Indian Institute of Technology Roorkee, India, University of Surrey, UK; **Ananya Bansal**, Indian Institute of Technology Roorkee, India; **Satheesh Krishnamurthy**, University of Surrey, UK; **Ramesh Chandra**, Indian Institute of Technology Roorkee, India

The newly explored two-dimensional transition metal carbides/nitrides, popularly known as MXene, are a new family of 2D materials with diverse applications. The coexistence of both ceramic and metallic nature, giving rise to exceptional mechanical, thermal, electrical, chemical properties and wide range of applications. Although several solution process techniques are there to deposit the MXene on substrate, but there is a need of high-quality epitaxial thin films for the above stated applications. In this work, Ti<sub>3</sub>C<sub>2</sub>X<sub>n</sub> MXene powder was synthesized using acid etching method. Epitaxial thin films were deposited on sapphire substrate (Al<sub>2</sub>O<sub>3</sub>, 0001) for the first time using pulse laser deposition (PLD) with Ti<sub>3</sub>C<sub>2</sub>X<sub>n</sub> pellet as the source. The

X-ray diffractometer and morphology studies showed the epitaxial nature of the film with columnar growth. The electrical conductivity of the film was found to be ~9421 S/cm. Resistance-temperature graph showed semiconductor-like behaviour for all the thickness tested. The thin film was also highly corrosive resistant in nature when tested with standard acidic, alkaline and saline solutions, which makes it ideal for anticorrosive coatings. Moreover, the p-n and n<sup>+</sup>-n devices on silicon substrate also resulted in a high switching ratio compared to other 2D materials. Our results demonstrate the potential of PLD as a novel method for the growth of epitaxial MXene thin films.

**Keywords:** MXene; pulsed laser deposition, epitaxial growth, corrosion resistance, switching diode

8:40am **MB2-3-TuM-3 Sputter Epitaxy of Predicted Dirac Semimetal MgTa<sub>2</sub>N<sub>3</sub>**, **Julien Baptiste** [[baptiste.julien@nrel.gov](mailto:baptiste.julien@nrel.gov)], **Sage Bauers**, National Renewable Energy Laboratory, USA

Ternary nitrides exhibit a wide range of functional properties, including superconductivity, magnetism, thermoelectricity, as well as topological properties. Among these, MgTa<sub>2</sub>N<sub>3</sub> (MTN) has been predicted to be a Dirac semimetal with an interesting potential for topological phases tunability. These unique electronic properties tied to its layered crystal structure. In this work, we synthesized epitaxial MTN thin films using reactive RF sputtering on c-cut sapphire substrates. The as-deposited films exhibit a (111)-oriented disordered rocksalt structure (rs-MTN), with a high-quality epitaxy, confirmed by X-ray diffraction (XRD) and rocking curve analysis. To transform the disordered rocksalt phase into the targeted layered phase (P6<sub>3</sub>/mcm), we annealed the precursor films in NH<sub>3</sub>. This method showed significant promise, successfully inducing the phase transformation at lower temperatures while maintaining film integrity, decent epitaxy and mitigating secondary phase formation. Structural analysis revealed that annealing the epi-film precursor under NH<sub>3</sub> yields to a phase transformation from the (111)-oriented rs-MTN into a c-axis textured layered MTN. Whereas the precursor rocksalt shows weak thermally activated conduction, preliminary electro and magneto-transport measurements on the layered MTN films reveal promising properties for a Dirac semimetal.

9:00am **MB2-3-TuM-4 Stabilization of Cubic or Orthorhombic Structure in Sputtered Tin Sulfide Thin Films for Thermoelectric Applications**, **Rémy Juliac**, **David Pilloud**, **Sylvie Migot**, **Axel Tahir**, **Jaafar Ghanbaja**, **Brigitte Vigolo**, **Nicolas Stein**, **Jean-François Pierson** [[jean-francois.pierson@univ-lorraine.fr](mailto:jean-francois.pierson@univ-lorraine.fr)], IJL / CNRS / Univ. Lorraine, France

Tin sulfide (SnS) is a p-type semiconducting material with a band gap of approx. 1.3 eV. This compound is a promising material for thermoelectric applications, as an alternative to SnSe with the same crystallographic phase Pbnm but with no critical chemical elements [1]. Indeed SnS may crystallize in various structures, the orthorhombic phase (Hertzenbergite, α-SnS), being the most stable one. Other structures are also reported in the literature, such as the π-SnS one that crystallizes in a cubic structure (P2<sub>1</sub>3) [2].

In the present work, SnS thin films have been deposited using pulsed-DC magnetron sputtering of a tin sulfide target. The effect of the experimental deposition conditions (total pressure and substrate temperature) to the structure, the microstructure, the composition and the functional properties has been studied.

The deposition total pressure strongly influences the structure of SnS thin films. The use of low pressure (0.5 Pa) favors the growth of the metastable cubic phase. A columnar microstructure with stacking faults has been evidenced by high resolution transmission electron microscopy for the films deposited at low pressure. Deposition at high pressure (1.5 Pa) induces the synthesis of the orthorhombic phase, the most stable phase. At intermediate pressure, the films are biphased: cubic + orthorhombic. The electrical properties of the films are strongly influenced by their structure. On one hand, the orthorhombic phase exhibits a high electrical resistivity that strongly decreases the transport properties. On the other hand, the cubic phase shows a low electrical resistivity that improves the film properties.

The cubic structure being a metastable one, this phase is not obtained anymore when the films are deposited on a heated substrate. For temperature lower than 100 °C, the orthorhombic phase is the only one detected by X-ray diffraction and Raman spectroscopy. The film microstructure becomes porous when the SnS films are deposited at a temperature higher than the ambient one. Such a porous microstructure

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has a negative impact on the electrical properties and therefore the thermoelectric properties.

[1] Tan *et al.*, Thermoelectrics with earth abundant elements: low thermal conductivity and high thermopower in doped SnS, *J. Mater. Chem. A* 2 (2012) 17302

[2] Guc *et al.*, Structural and vibrational properties of  $\alpha$ - and  $\pi$ -SnS polymorphs for photovoltaic applications, *Acta Mater.* 183 (2020) 1

9:20am **MB2-3-TuM-5 Governing Metal-Insulator Transition in Ultra-Thin VO<sub>2</sub> Films by Surface Engineering**, **Andres Hofer [juhofer@ucsd.edu]**, UC San Diego, USA; **Ali Basaran**, General Atomics, USA; **Alexandre Pofelski**, Brookhaven National Laboratory, USA; **Tianxing Damir Wang**, **Victor Palin**, UC San Diego, USA; **Yimei Zhu**, Brookhaven National Laboratory, USA; **Ivan Schuller**, UC San Diego, USA

The metal-insulator transition (MIT) in vanadium dioxide (VO<sub>2</sub>) thin films is strongly affected by grain size, thickness, and interfacial properties. Typically, the MIT is substantially suppressed for thickness below 50 nm when substrates like sapphire and silicon are used. While some studies have shown that films below 20 nm thickness can be achieved without compromising the integrity of the MIT, complex pre or post-growth processing is required. We show that engineering the substrate surface before the deposition facilitates the direct deposition of ultra-thin 15 nm thick films, exhibiting over four orders of resistance change across the MIT, which is comparable to its bulk counterpart. Our findings indicate that the interface between the thin film and the substrate is crucial to the structural evolution during the initial growth layer. With the appropriate surface preparation, the desired VO<sub>2</sub> MIT transition can be obtained independently of the substrate's crystalline orientation. Furthermore, we propose a novel approach to obtain high-quality MIT in ultra-thin VO<sub>2</sub> films by magnetron sputtering. Unlike traditional film depositions, we incorporate a pre-deposited 1.5 nm thick vanadium oxide buffer layer, thereby eliminating the need of different materials besides vanadium oxide or complex pre- and post-growth processing. We also demonstrate that our unique growth methodology improves the MIT of 25 nm VO<sub>2</sub> thin films on standard silicon substrates. This study reveals a compelling approach for the direct growth of ultrathin VO<sub>2</sub> films exhibiting a high-quality MIT, which is commonly accepted as unattainable on technologically essential substrates such as sapphire and silicon.

9:40am **MB2-3-TuM-6 Probing the Metal-Insulator Transition at YTiO<sub>3</sub>/LaTiO<sub>3</sub> Interfaces via Soft Chemical Synthesis**, **Alexandre Simoes [zirpoli.simoese@unesp.br]**, Rua Souza Oliveira, Brazil

In this study, we present optimized growth conditions for the fabrication of YTO/LTO heterostructured thin films using the polymeric precursor method combined with spin coating. The films were deposited on (100) Pt/TiO<sub>2</sub>/SiO<sub>2</sub>/Si substrates at 850 °C, resulting in films with a mean grain size of approximately 20.0 nm and a surface roughness of 5.50 nm. X-ray diffraction (XRD) analysis reveals that the YTO/LTO heterostructured films, synthesized via the polymeric precursor method, are free of secondary phases and exhibit a highly homogeneous morphology with no evidence of interaction between the sublayers. The piezoelectric and magnetic properties of the YTO/LTO heterostructures are attributed to modifications in the Ti-O-Ti bond lengths and tilting of the oxygen octahedra, which in turn affect the electrons in the eg orbitals of the Ti atoms in both layers. This hypothesis is further supported by Rietveld refinement and X-ray photoelectron spectroscopy (XPS) results, which suggest that the magnetic behavior of the films is not only due to the non-integer 3d occupancy of Ti ions at the surface but also the structural distortion of the YTO/LTO interface, influenced by the underlying silicon-coated platinum substrates. The films exhibit a high intrinsic dielectric constant ( $\epsilon_r \approx 70$ ) and a loss tangent ( $\tan \delta$ ) of approximately 0.41 at 1 kHz, indicating structural distortions along the TiO<sub>6</sub> octahedra in the basal plane of the film. A metal-to-insulator transition observed in the heterostructured films supports the idea of a competing mechanism, where strong electron orbital dynamics and multi-orbital electronic correlations govern the switching behavior between SET and RESET states. Additionally, the electrode area and switching cycles influence the film's properties, making it suitable for use as a correlated random access memory (CeRAM). In conclusion, we demonstrate that this simple, low-cost chemical process yields high-quality heterostructured films with promising potential for applications in non-volatile resistive memories.

10:00am **MB2-3-TuM-7 the Influence of Substrate Bias on Properties and Microstructure of High-Density Nanotwinned Ag Thin Films for High Power Device**, **Pinning-Chun Kuo [icanfire93@gmail.com]**, **Fan-Yi Ouyang**, Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan

In response to the increasing demands for advanced technologies, including autonomous vehicles, self-driving systems, and artificial intelligence computing (AIPC), the concept of 3D-IC has emerged. Advanced packaging techniques that exhibit high reliability, superior properties, and the capacity to endure elevated operating temperatures are necessary to address these demands. The predominant technique employed is Cu-to-Cu direct bonding; however, this method necessitates high-temperature processing (>350°C), during which Cu tends to oxidation, thus requiring a high vacuum environment for execution. In contrast, Ag has demonstrated superior electrical and thermal conductivity, and great oxidation resistance, making it a promising candidate for metal-to-metal direct bonding techniques in atmospheric conditions.

This study successfully fabricated high-density nanotwinned Ag thin films on SiC substrates utilizing magnetron sputtering and investigated the impact of substrate bias on the microstructure and properties of the films. The results show that nanotwinned structures were found on all samples, characterized by a high density of nanotwins with an average twin spacing of 7 nm. The grain size remained relatively consistent as the substrate bias was increased from 0 V to -80 V; however, grain growth was observed when the substrate bias was further increased from -80 V to -120 V. In addition, the samples deposited without bias exhibit a resistivity of 2.17  $\mu\Omega \cdot \text{cm}$  and a hardness of 1.9 GPa, significantly surpassing that of bulk Ag (0.58GPa). When the substrate bias increases to -60 V, the resistivity further decreases to 1.96  $\mu\Omega \cdot \text{cm}$  and hardness reduce to 1.55 GPa. Moreover, a comparative analysis was also conducted on the microstructure and properties of nanotwinned Ag thin films deposited on Si and SiC substrates. The influence of the substrate bias on nanotwin formation of Ag thin films for both substrates is discussed and compared.

Key word : nanotwin, metal-to-metal direct bonding, advanced packaging techniques

10:20am **MB2-3-TuM-8 Electrodeposited Zirconium Titanate Thin Films: Structural, Magnetic, and Dielectric Properties for Spintronic Applications**, **Ibra Saeed [ifrasaeed1998@gmail.com]**, University of Milano Bicocca, Milan, Italy, Pakistan

Zirconium titanate (ZrTiO<sub>4</sub>) thin films have emerged as a cornerstone material in the advancement of spintronic devices, owing to their exceptional structural, magnetic, and dielectric properties [1,2]. This study harnesses a precise electrodeposition technique to fabricate ZrTiO<sub>4</sub> thin films, meticulously varying the molarity of electrolytes from 0.01M to 0.05M. X-ray diffraction (XRD) analysis reveals a transition from amorphous behavior at 0.01M to the formation of phase-pure, orthorhombic ZrTiO<sub>4</sub> at higher molarities, with a notable increase in crystallite size, indicative of enhanced phase stability. Vibrating Sample Magnetometer (VSM) measurements demonstrate a pronounced soft ferromagnetic behavior, with an impressive saturation magnetization peaking at 29 emu/cm<sup>3</sup> at 0.05M. Dielectric studies reveal a significant dielectric constant of 180 at log f=2 and a minimal tangent loss of 0.02 at 0.05M, showcasing superior dielectric performance. Cole-Cole plots further elucidate the dielectric properties, indicating dominant grain boundary resistance. The comprehensive analysis underscores the potential of ZrTiO<sub>4</sub> thin films as pivotal components in next-generation spintronic devices, offering unparalleled structural integrity, magnetic prowess, and dielectric efficiency [2].

These findings pave the way for the integration of ZrTiO<sub>4</sub> thin films in high-performance, energy-efficient spintronic applications, marking a significant leap forward in material science and device engineering.

## References:

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Juma, A., Acik, I.O., Oluwabi, A.T., Mere, A., Mikli, V., Danilson, M., & Krunks, M., (2016). Zirconium doped TiO<sub>2</sub> thin films by chemical spray pyrolysis. *Applied surface science*, 387, 539-54.

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10:40am **MB2-3-TuM-9 Enhancing High-Entropy MEMS with Superior Thermal Stability and Scalability**, *Li-Hui Tsao [nthu031239@gmail.com]*, National Tsing Hua University, Taiwan; *Ying-Hao Chu*, National Tsing Hua University, Taiwan

Microelectromechanical Systems (MEMS) are essential in modern technology due to the increasing demand for multi-functional devices and Internet-of-Things (IoT) applications. In typical cases, the piezoelectric layers in MEMS serve as the main component for actuation, sensing, and transduction, which lead zirconate titanate (PZT) is widely used with high piezoelectricity. However, challenges, including poor thermal stability and degradation after long-term usage, have hindered its further development. Thus, it is crucial to introduce new material designs to solve these problems. In this work, a high-entropy material,  $\text{Pb}(\text{Mg}_a\text{Nb}_b\text{Ti}_c\text{Hf}_d\text{Zr}_e)\text{O}_3$  (PMNTHZO), is developed with colossal piezo-response and superior thermal stability. The sluggish diffusion effect diminishes the critical phase transformation and contributes to the robust properties at 523 K. Meanwhile, the integration with an 8-inch silicon substrate further suggests the massive potential for practical usage. In conclusion, this work demonstrates a novel high-entropy material with several intriguing physical properties, paving the way for next-generation electronic devices.

## Functional Thin Films and Surfaces

### Room Palm 1-2 - Session MB1-WeA

#### Thin Films and Surfaces for Optical Applications

**Moderators:** Rajiv Pethe, Vital Chemicals, USA, Juan Antonio Zapien, City University of Hong Kong

2:00pm **MB1-WeA-1 Experimental and Theoretical Insights into UV-Active Chirality in Glancing Angle Deposited Zirconia Nano-Helical Metamaterial Platforms**, *Ufuk Kilic [ufukkilic@unl.edu]*, Matthew Hilfiker, University of Nebraska-Lincoln, USA; Shawn Wimer, Raymond Smith, University of Nebraska - Lincoln, USA; Christos Argyropoulos, Pennsylvania State University, USA; Eva Schubert, Mathias Schubert, University of Nebraska - Lincoln, USA

**INVITED**

Chirality, the property of handedness in molecules or objects that prevents them from being superimposed on their mirror images, is optically manifested as circular dichroism (CD)—the differential absorption of left- and right-handed circularly polarized light. However, chirality found in nature is inherently weak, challenging to spectrally control, and primarily active in the ultraviolet (UV) region of the spectrum [1-3]. Enhancing UV-active chirality, crafting UV-active photonic wave-guide systems and also detecting chiral molecules through metamaterial platforms remains a challenge, as most designs are optimized for the infrared (IR) to visible spectral ranges [3].

In this study, we fabricated ultra-wide bandgap (~5 eV) zirconia (ZrO<sub>2</sub>) thin films using the glancing angle deposition (GLAD) method with electron beam evaporation. When the particle flux was directed at normal incidence (0°), uniform coating of flat ZrO<sub>2</sub> thin films were successfully fabricated. In contrast, directing the flux at an oblique angle (85.5°) with continuous substrate rotation (24 seconds per revolution) yielded spatially coherent, super-lattice nano-helices. Generalized spectroscopic ellipsometry (GSE) technique was used to extract frequency-dependent complex dielectric functions and identify band-to-band transitions spanning the near-IR to vacuum-UV (VUV) spectrum. Strong VUV-active CD responses were experimentally observed in ZrO<sub>2</sub> nano-helical metamaterials using Mueller matrix GSE. Additionally, visualization of both near- and far-field characteristics induced by circularly polarized illumination, along with the theoretical validation of the VUV-active chiroptical response, were investigated using finite element modeling (FEM) based full wave simulations. The systematic FEM calculations also revealed that the chiral properties could be tuned by (i) adjusting the structural parameters of the nano-helices and (ii) incorporating plasmonic subsegments into the helical structure.

Our research outputs suggest that the proposed metamaterial design holds significant potential for applications such as high-power chiro-optic photonic and electronic circuits, quantum information systems, UV-active topological insulators, and chiral sensing technologies.

[1] Kilic, U., *et al.*, *Nat. Commun.* 15, 3757 (2024).

[2] Kilic, U. *et al.*, *Adv. Funct. Mater.* 31.20: 2010329,(2021).

[3] Sarkar, S. *et al.*, *Nano letters* 19.11: 8089-8096,(2019).

2:40pm **MB1-WeA-3 Optical and Electrical Properties of Thermochromic W-Doped VO<sub>2</sub> Films Prepared at a Reduced Temperature (350 °C) on Glass Substrates with YSZ Interlayers**, *Sadoon Farrukh [sadoon@kfy.zcu.cz]*, Jaroslav Vlček, Jiří Rezek, Radomír Čerstvý, Jiří Houška, Tomáš Kozák, University of West Bohemia - NTIS, Czechia

Vanadium dioxide (VO<sub>2</sub>) is an extremely interesting and increasingly investigated coating material due to its reversible first-order transition between a low-temperature monoclinic VO<sub>2</sub>(M1) semiconducting phase and a high-temperature tetragonal VO<sub>2</sub>(R) metallic phase relatively near room temperature (approximately 68 °C for the bulk material). High modulation of the infrared transmittance, and electrical and thermal conductivity makes VO<sub>2</sub>-based films a suitable candidate for numerous applications, such as electronic and optical switches, thermal sensors, smart thermal radiator devices for spacecraft, adaptive thermal camouflage, and energy-saving smart windows with automatically varied solar energy transmittance.

The application potential of these films depends on the ability to achieve not only the VO<sub>2</sub> stoichiometry but also the crystallization of the VO<sub>2</sub>(M1/R) phase under as industry-friendly process conditions as possible, i.e., at a deposition temperature close to 300 °C (usually used temperatures are higher than 450 °C) and without any substrate bias voltage in case of

usually used magnetron sputter techniques. Moreover, the transition temperature needs to be reduced down to 25 °C for many applications (e.g., smart windows). Besides the optical transmittance in the visible range, the characteristics of the semiconductor-metal transition, such as phase-transition amplitude, hysteresis width, and phase-transition sharpness, are of key importance.

The paper deals with crystal structure, optical and electrical properties, and semiconductor-metal transition characteristics of strongly thermochromic W-doped VO<sub>2</sub> films with a reduced transition temperature (24-33 °C). They were deposited at a reduced temperature(350 °C) onto glass substrates with two versions of Y-stabilized ZrO<sub>2</sub> (YSZ) interlayers (serving also as a highly optically transparent bottom antireflection layer) possessing different crystal orientations, and onto bare glass and monocrystalline YSZ and Al<sub>2</sub>O<sub>3</sub> substrates for comparison. The W-doped VO<sub>2</sub> films were deposited using a controlled reactive deep oscillation magnetron sputtering (DOMS) of a single V-W (3.0 wt.%) target. The DOMS is a modified version of HiPIMS with packages (macropulses) of short high-power micropulses.

3:00pm **MB1-WeA-4 Enhancing Optical Properties and Photocatalytic Performance with Nanopatterned Anodized Aluminum Oxide on transparent substrate**, *Fu-Gi Zhong [fugi.en12@nycu.edu.tw]*, Shih-Hsun Chen, National Yang Ming Chiao Tung University (NYCU), Taiwan

In recent years, the rapid advancement of nanotechnology has driven an increasing demand for high-performance nanostructured materials. Among various fabrication techniques, anodic aluminum oxide (AAO) films have attracted significant attention due to their excellent chemical and thermal stability, transparency, and tunable nanoporous structure. AAO features highly ordered nanopore arrays, making it an ideal template for functional thin films, especially in applications requiring high surface area and aspect ratios. By integrating functional ceramic or semiconductor coatings, materials deposited on AAO can self-assemble into nanostructures, further enhancing their optical and chemical reactivity and making them highly suitable for applications in sensors, photocatalysis, and other fields requiring heightened sensitivity and resolution.

This study focuses on the fabrication of AAO structures on transparent substrates, followed using Atomic Layer Deposition (ALD) to coat these structures with ZnO thin films, aiming to produce transparent, nanostructured porous films on both sides of the substrate. By integrating ZnO coatings with AAO structures, we plan to investigate light transmission and surface interaction properties, thereby enhancing optical performance and photocatalytic efficiency and making the films more suitable for high-sensitivity, multifunctional sensor and photocatalytic applications.

3:20pm **MB1-WeA-5 A Comparative Study: The Structural and Optoelectronic Properties of Al- and Ga-Doped ZnO Films Deposited by Atmospheric Pressure Plasma Jet**, *Chih-Yun Chou [f10k45003@ntu.edu.tw]*, National Taiwan University, Taiwan

Aluminum-doped zinc oxide (AZO) and gallium-doped zinc oxide (GZO) are leading transparent conductive oxides (TCOs) for optoelectronic applications, valued for high transparency and conductivity. GZO provides superior carrier mobility and lower resistivity, while AZO is more cost-effective and less toxic. This study compares AZO and GZO films prepared via atmospheric pressure plasma jet (APPJ) deposition, allowing for precise parameter control to evaluate Al and Ga's effects on ZnO film properties and their suitability in advanced optoelectronics.

Structural analysis using X-ray diffraction (XRD) and scanning electron microscopy (SEM) reveals both AZO and GZO films exhibit a hexagonal wurtzite structure with a *c*-axis orientation. The broader full-width at half maximum (FWHM) at (002) peak and higher strain in GZO films suggest more pronounced lattice distortion, likely due to Ga's higher doping efficiency. Further, reducing the working distance, thereby increasing processing temperature, effectively eliminates surface particles in GZO films but not in AZO films. This temperature-driven improvement enhances the mobility of Ga atoms on the substrate surface, leading to a more cohesive and uniform film morphology in GZO.

Optoelectronic properties assessed via UV-Vis spectroscopy and Hall effect measurements indicate that GZO films maintain high visible-range transparency (>80%) compared to AZO films (>70%). In the near-infrared range, GZO transparency decreases significantly (<40% at 1400 nm) due to its higher carrier concentration. Overall, AZO films show lower electronic performance, likely due to complex defect formation and increased impurity scattering, evidenced by higher Urbach energy (*E<sub>u</sub>*) values (0.28-0.29 eV for AZO films and 0.26 eV for GZO). Decreased APPJ working distance enhances carrier mobility, improving the figure of merit at 550 nm



for GZO from  $11 \times 10^{-3} \Omega^{-1}$  to  $26.4 \times 10^{-3} \Omega^{-1}$  and for AZO films from  $0.4 \times 10^{-3} \Omega^{-1}$  to  $0.8 \times 10^{-3} \Omega^{-1}$ .

In conclusion, while AZO and GZO films both possess favorable characteristics for TCOs, their electronic behaviors diverge markedly under APPI processing. Al doping tends to introduce complex defects that limit carrier mobility and concentration, making AZO less suitable where high conductivity is essential. In contrast, GZO films achieve higher carrier concentration and mobility, making them more appropriate for applications where efficient charge transport is critical. The findings also emphasize the significance of the APPI working distance parameter and underscore the importance of selecting appropriate dopants and understanding defect dynamics to optimize ZnO-based TCO performance.

**3:40pm MB1-WeA-6 Unveiling the Interplay of Structural, Optical, and Hydrophobic Properties of Sputtered Grown PTFE@AISiN Thin Films, Raman Devi, Somdatta Singh, Ramesh Chandra [ramesh.chandra@ic.iitr.ac.in], IIT Roorkee, India**

Radio frequency (RF) magnetron sputtering technique was used to develop PTFE@AISiN thin films on glass substrates at temperatures ranging from 250°C to 450°C. Methods like X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), UV-Vis Spectroscopy, water contact angle (CA) measurements, and nanoindentation were used to examine the structural, morphological, optical, hydrophobic, and mechanical properties of PTFE@AISiN at various substrate temperatures (250°C-450°C). XRD studies showed that the coating deposited with an Ar:N<sub>2</sub> ratio of 20:6 at various substrate temperatures formed a hexagonal phase, demonstrating its polycrystalline nature. A nanocomposite with microstructure has been formed by embedding AlN nanocrystallites in a soft amorphous matrix of Si<sub>3</sub>N<sub>4</sub> provides better mechanical properties. The contact angle measurement method displayed an excellent contact angle of around ~118° (good hydrophobicity). According to optical transparency measurements, all coatings exhibited > 90% transparency in the visible spectrum. The PTFE@AISiN coated at 450°C had the highest hardness value greater than 25 GPa.

**Keywords:** optical transparency, magnetron sputtering, thin film, hydrophobicity; nanoindentation, hardness

**4:00pm MB1-WeA-7 High-Entropy Oxide Thin Film as Absorber Layer for Near Infrared Photodetectors, Shao-Chun Chao [sc0705chao@gmail.com], Tai-An Chen, Jyh-Ming Ting, National Cheng Kung University (NCKU), Taiwan**  
A novel light-absorbing material of high-entropy oxide (HEO) was synthesized using the sol-gel method. The sol-gel method offers advantages such as low cost, high uniformity, flexible material preparation, and suitability for large-scale production. In this study, a streamlined process was used to produce uniform, controllable nanostructured thin films. By leveraging the properties of HEO, the film properties were adjusted, making it an excellent absorber layer in photodetectors. The HEO material demonstrated an unparalleled ability to absorb a broad spectrum of light, ranging from 300 to 1400 nm. We measured the performance of a photodetector with an Ag/HEO/n-Si structure. Under near-infrared illumination, this photodetector exhibited an impressive high photoresponse, generating a high photocurrent density of approximately 10 mA/cm<sup>2</sup> at an incident light wavelength of 1050 nm, with a peak responsivity of 1.545 A/W, and an external quantum efficiency (EQE) exceeding 182%, surpassing most oxide-based photodetectors reported in the literature. The outstanding performance of this device is attributed to the high concentration of oxygen vacancies in the HEO compound, resulting in significant light absorption and high EQE. Furthermore, this study is the first to use the sol-gel method to prepare HEO thin-film absorber layers, demonstrating the material's excellent potential in the field of photodetectors.

**4:20pm MB1-WeA-8 Effective Ways to Enhance the Performance of N-MoS<sub>2</sub>/P-CuO Heterojunction Based Self-Powered Photodetectors, Davinder Kaur [davinder.kaur@ph.iitr.ac.in], Indian Institute of Technology Roorkee, India**

The present study investigated two effective routes to improve the response time and the detection range for the n-MoS<sub>2</sub>/p-CuO heterostructure (a conventional p-n heterojunction). In the first rectification, an insulating aluminium nitride (AlN) layer was inserted in between the molybdenum disulfide (MoS<sub>2</sub>) and cupric oxide (CuO) layer, which eventually converted the conventional p-n heterojunction to Semiconductor-Insulator-Semiconductor (SIS) with a superior carrier tunneling mechanism. Interestingly, the fabricated heterostructure exhibits self-powered and broad-range photoresponse. The response time (rise time

and fall time) of the fabricated n-MoS<sub>2</sub>/p-CuO heterojunction decreases from 93.35 ms and 102.68 ms to 11.31 ms and 12.73 ms with the insertion of ultrathin insulating AlN layer. The higher responsivity and ultrafast photoresponse in n-MoS<sub>2</sub>/AlN/p-CuO (SIS) heterojunction can be ascribed to the carrier tunneling mechanism through the ultrathin-insulating AlN layer. Moreover, the detection range can be enhanced up to the UV region by adding a layer of MoS<sub>2</sub> quantum dots (QDs) on the surface of the MoS<sub>2</sub> layer in the fabricated heterostructure. The fabricated n-MoS<sub>2</sub> QDs/n-MoS<sub>2</sub>/AlN/p-CuO heterostructure shows photoresponse in a broad range from UV to NIR radiations. The obtained results demonstrate the n-MoS<sub>2</sub>/AlN/p-CuO (SIS) heterostructure with the addition of MoS<sub>2</sub> QDs shows excellent potential for next-generation ultrafast optoelectronics applications.

**4:40pm MB1-WeA-9 Influence of SHI irradiation on the Photoluminescence and Dielectric properties of bilayer structured Au/GeO<sub>2</sub> thin films for Optoelectronics applications, Mahendra Singh Rathore [mahendra.rathore8944@paruluniversity.ac.in], Anand Y. Joshi, Parul University, India; Srinivasa Rao N., MNIT Jaipur, India**  
**Abstract**

In the present work, the effects of swift heavy ion beam irradiation on the engineering the physical, optical, photoluminescence and dielectric properties of bilayer structured Au/GeO<sub>2</sub> thin films have been investigated. GeO<sub>2</sub> and Au thin films have been grown onto silicon substrate using electron beam evaporation. Eventually the prepared Au/GeO<sub>2</sub>/Si thin films were irradiated with 100 MeV Ag ions at different ion fluences ranging from  $1 \times 10^{12}$  to  $1 \times 10^{13}$  ions/cm<sup>2</sup>. The pristine and irradiated samples were characterized using XRD, RBS, SEM, AFM, UV-Vis reflectance and photoluminescence Spectroscopy. The dielectric properties, AC conductivity, dielectric and tangent loss were analyzed of the pristine and irradiated samples. The results reveal that the nucleation of Au NCs was observed with increase in fluence. The elemental composition and film thickness observed using RBS measurements. The surface morphology and topography results reveal that the nucleation of particles with increase in ion fluences. Broad PL band observed in visible region which corresponding to the green light emission due to the presence of Au NCs. The CIE curve plotted from the PL data. The oxygen vacancy related defect states as well as surface Plasmon resonance (SPR) induced absorption and subsequent electron injection from Au NPs to conduction band of GeO<sub>2</sub>. The dielectric properties varied with irradiation. The variation in electronic transition of wide band gap GeO<sub>2</sub> NC's by nucleation of gold NP's are considered to practical application in optoelectronics devices such as wavelength detection and optical switching devices and have been discussed in details.

**Keywords:** Au/GeO<sub>2</sub> thin films, ion beam irradiation, XRD, RBS, Photoluminescence, Dielectric properties.

**5:00pm MB1-WeA-10 Diffusion of Ni Within Polycrystalline Zinc Oxide Layer: An Approach Combining Different Techniques for a Nanoscale Analytical Response, Hervé Montigaud [herve.montigaud@saint-gobain.com], SVI, Joint Unit CNRS/ Saint Gobain, 41 quai Lucien Lefranc, Aubervilliers, France; Justine Voronkoff, Saint Gobain Research Paris, 41 quai Lucien Lefranc, Aubervilliers, France; Ludovic Largeau, C2N-CNRS/Université Paris-Saclay, France; Jacques Perrin - Toinin, RWTH Aachen University, Germany; Thierry Cretin, Saint Gobain Research Paris, 41 quai Lucien Lefranc, Aubervilliers, France; Ekaterina Burov, SVI Joint Unit CNRS / Saint Gobain Aubervilliers, France**

In the context of global climate change, the low emissivity glazing developed by glass makers contributes to tackle the thermal losses of the buildings. Within these systems for windows, the radiative part is reduced by a thin metallic silver layer included in a stack that reflects especially far-infrared. This 12nm-thick Ag layer is embedded between other nanometric layers such as nitride (SiNx), oxide (ZnO, SiOx, SnZnOx) and sub-nanometric metallic layer (NiCr), all deposited by magnetron sputtering. The structure and mainly the composition of each layer are influenced by the deposition conditions and also post-annealing step in the case of tempered glasses. Different interactions occurred at the interface between the substrate and the stack and between the layers such as inter-diffusion phenomena<sup>1,2,3</sup>. It is crucial to follow the consequences onto the local composition of the layers to control the final performances of the glazing.

The present work focuses on the system composed by nickel chromium and zinc oxide layers, from its deposition to its annealing until 600°C. NiCr/ZnO layer stack was deposited on an Si wafer by magnetron sputtering and then annealed<sup>4</sup>. The diffusion of the nickel from the nanometric NiCr layer within the polycrystalline zinc oxide layer and Ni precipitation at the interfaces had been characterized. The local composition within the polycrystalline zinc

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oxide was addressed until the nanometer scale thanks to the combination of techniques such as Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS), AtomProbe Tomography (APT), Scanning Transmission Electron Microscopy (STEM), and by exploiting the added value of each one. For instance, we have studied the contribution of grain boundaries compared to nanocrystals on the Ni diffusion.

## keywords

NiCr, ZnO, sputtering, diffusion, polycrystalline layer, ToF-SIMS, APT, STEM

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5:20pm **MB1-WeA-11 Fabrication of High Quality Titanium Nitride Nanostructures for Plasmonics, Spyros Kassavetis [skasa@physics.auth.gr], Stavros Panos, Nikos Pliatsikas, Despina Tselekidou, Panos Patsalas, Aristotle University of Thessaloniki, Greece**

Transition metals nitrides (TMNs) emerge as alternative plasmonic nanomaterials suitable for a wide range of applications from photovoltaics to photonics and medicine. The TMNs are conductive ceramics that combine exceptional properties such as substantial electronic conductivity, high melting point (>3000 K) and tunable work function, while they are particularly stable in hostile chemical environments, high temperature, and strong electric fields. Among them, Titanium Nitride (TiN) emerges as significant candidate material for practical plasmonic applications (biosensors, catalysis and photochemistry, solar energy harvesting, photo-detection, and optical storage of information).

In this work, we focus on novel and cost-efficient fabrication techniques of alternative plasmonic nanostructures. TiN nanostructures with controlled spacing and tunable dimensions (thickness and lateral dimensions) were fabricated using a combination of Nanosphere Lithography (NSL) and several reactive magnetron sputtering (MS) deposition techniques such as DC, Closed-Field Unbalanced MS or Highly Power Impulse MS (HIPMS) with the aim to study the fundamentals that will unlock the fabrication of high quality TMNs nanostructures for plasmonic applications.

NSL appears as a very promising approach, due to its rapid implementation and compatibility with wafer-scale processes, combines the advantages of both top-down and bottom-up approaches and includes: (a) development of the nanospheres monolayer colloidal mask, (b) deposition of the desired material in the empty space between the nanospheres and (c) removal/lift-off of the nanosphere colloidal mask to “reveal” the deposited material. Specifically, a suspension of monodisperse polystyrene nanospheres (diameter,  $d=552$  nm or  $d=175$  nm) was spin coated on a substrate such as Si (001), glass, flexible or PET to form the colloidal mask. A UV ozone process was used to confine the triple-junction vias of the polystyrene mask. Subsequently, the selective growth of TiN was made by the above mentioned MS in Ar/N atmosphere by varying the TiN thickness from 10 to 30 nm, while the MS process parameters were also fine-tuned to increase the directionality of deposited species such as the negative bias voltage during the growth of the TiN.

The arrays of ordered TiN nanostructures appear after the lift-off of the mask. Atomic Force Microscopy characterization of the samples showed the fabrication of TiN nanostructures, with low concentration of point defects, similar structure with the continuous TiN films of high electrical conductivity and plasmonic performance, and durability at least up to 400° C.

## Functional Thin Films and Surfaces Room Palm 3-4 - Session MB3-ThM

### Low-dimensional Materials and Structures

Moderators: Tomas Kubart, Uppsala University, Sweden, Vladimir Popok, FOM Technologies, Denmark

8:00am **MB3-ThM-1 A Novel Platform for Topologically Protected Quantum Computation: Massively Parallel Self-Assembled Pentasilicene Nanoribbons**, *Guy Le Lay* [guy.lelay@univ-amu.fr], Aix-Marseille University, France

The novel platform, which we propose for the emergence of Majorana Zero Modes (MZMs), i.e., non-abelian anyons, which could be possibly braided for realizing topologically protected quantum computation, is based on massively parallel, high aspect ratio, spontaneously self-organized epitaxial nanoribbons (NRs) proximitized by a standard s-wave superconductor [1,2]. These highly perfect NRs are atom-thin pentasilicene nanoribbons (SiNRs) [3,4]. They could host distant MZMs at their extremities allowing for the creation of highly stable qubits preserved against external disturbances and environmental noise, hence, protected from decoherence. Clearly, the self-assembly of these defect-free SiNRs could be a distinct advantage over presently engineered or atom-by-atom constructed nanowires.

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8:20am **MB3-ThM-2 Multilayers of Two-Dimensional (2d) Ti<sub>2</sub>B<sub>2</sub>CiX, Obtained from Selective Etching of 3DTiInB<sub>2</sub>**, *Rodrigo Ronchi* [rodrigo.ronchi@liu.se], *Johanna Rosen*, Linköping University, IFM, Sweden  
Authors: Rodrigo M. Ronchi <sup>1</sup>, Emile Defoy <sup>3</sup>, Andrejs Petruhins <sup>1</sup>, Justinas Palisaitis <sup>2</sup>, David Portehault <sup>3</sup>, Jonas Björk <sup>1</sup>, P.O. Å. Persson <sup>2</sup>, Johanna Rosen <sup>1</sup>

With the rapid expansion of two-dimensional (2D) MXenes <sup>1</sup> efforts have been made to find other families of nanolaminated materials in both 3D and 2D. One such group is boron-containing compounds, known as MAB phases, where metal (M) and boron (B) layers are separated by layers of A-elements (A=Al, In, etc.). Due to their similarities with MAX phases, experimental attempts to etch these 3D materials into its 2D counterpart have primarily involved selective etching of the A-layers using hydrochloric <sup>2-5</sup> and hydrofluoric acids <sup>6,7</sup> and, more recently, Lewis acids/molten salts <sup>7-10</sup>.

Despite, the 2D Mo<sub>4/3</sub>B<sub>2-x</sub> boridene <sup>6</sup>, the subsequent experimental research has demonstrated that 2D metal borides are significantly more challenging to obtain than MXenes (metal carbides/nitrides) <sup>11</sup>. For instance, MoAlB phase was only partially etched to Mo<sub>2</sub>AlB<sub>2</sub><sup>2,4,8</sup>. Molten salt etching of Hf<sub>2</sub>InB<sub>2</sub> has resulted in complete oxidation to HfBO <sup>7</sup>, rather than forming a halogenated MBene. Additionally, unsuccessful acid etching trials have been reported for Fe<sub>2</sub>AlB<sub>2</sub> <sup>6</sup>, Mo<sub>5</sub>SiB<sub>2</sub> <sup>6</sup>, Ti<sub>2</sub>InB<sub>2</sub> <sup>12</sup> and Hf<sub>2</sub>InB<sub>2</sub> <sup>7</sup>. Further, while In atoms from Ti<sub>2</sub>InB<sub>2</sub> have been removed through a dealloying reaction <sup>12</sup>, TEM images and the *Cmcm* space group found suggests that the resulting TiB is a 3D material, instead of a 2D counterpart.

Here, we present the synthesis of 2D multilayer Ti<sub>2</sub>B<sub>2</sub>Cl<sub>x</sub>, obtained from molten salt (ZnCl<sub>2</sub>) etching of Ti<sub>2</sub>InB<sub>2</sub>. Energy Dispersive (EDS) and Electron Energy Loss Spectroscopies (EELS) confirm that indium is fully removed and replaced by chlorine atoms from the salt, leading to an increased c-lattice parameter and a corresponding shift in X-ray diffraction (XRD) peaks to lower angles. Furthermore, transmission electron microscopy (TEM) shows the laminated atomic structure, with chlorine terminations of the stacked 2D sheets. These XRD and TEM results are consistent with density functional theory (DFT) calculations. *In situ* XRD experiments further reveal that the 3D to multilayer (ml) 2D transformation occurs without any intermediate phase. Furthermore, our DFT results provide insights into the reaction mechanism governing this transformation.

This work not only establishes the 3D MAB phases as 2D MBene precursors but also unlocks new possibilities for engineering of 2D multilayer metal borides using molten salt etching, facilitating controlled surface chemistry. This work paves the way for a new class of functional nanomaterials with

Figure, references and authors information: supplemental document

8:40am **MB3-ThM-3 Conformal Multifunctional Polymeric and Inorganic Aerogel-Like Oxide Thin Films for Optical and Energy Applications by Plasma Technology**, *Gloria P. Moreno, Triana Czermak, Jose Obrero, Francisco J. Aparicio, Juan Ramón Sánchez-Valencia, Ana Borrás, Angel Barranco* [angelbar@icmse.csic.es], Institute of Materials Science, CSIC, Spain **INVITED**

The Remote Plasma Assisted Vacuum Deposition (RPAVD) process is a versatile methodology for fabricating functional nanocomposites from non-chemically polymerizable organic functional molecules and functional metal coordination compounds. This approach combines the physicochemical reactions inherent to plasma polymerization processes with the vapor deposition of functional molecules tailored to the specific demands of target applications. The resultant cross-linked polymer films exhibit insolubility and exceptional thermal stability. These films can incorporate a precise concentration of nearly any thermally stable, photo-functional molecule. The method exhibits scalability at the wafer level and complete compatibility with solvent sensitive and delicate substrates. Initially, this process was applied to developing thin optical films and photonic devices, encompassing optical filters, photonic sensing chips, and lasing media. Nevertheless, the film properties can be fine-tuned for various other functional applications, such as creating controlled wetting and ice-retarding surfaces, antimicrobial coatings, and high performance dielectric ultrathin films. We will also showcase very recent results about the encapsulation of nanostructures on surfaces and its role in encapsulating and modifying perovskite solar cells. Additionally, we will present recent results about the development of conformal aerogel-like oxide nanostructures by combining RPAVD and plasma processing of metal-containing plasma polymers. These aerogel-like oxide films have straightforward applications in photonics, omniphobic surfaces, solar cells, and smart coatings.

#### References

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9:20am **MB3-ThM-5 Cluster-assembled Computers**, *Paolo Milani* [paolo.milani@mi.infn.it], University of Milan, Italy **INVITED**

Self-assembled nanoparticle or nanowire networks have recently come under the spotlight as systems able to obtain brain-like data processing performances by exploiting the memristive character and the wiring of the junctions connecting the nanostructured network building blocks [1]. Recently it has been demonstrated that nanostructured Au films, fabricated by the assembling of gold clusters produced in the gas phase, have non-linear and non-local electric conduction properties caused by the extremely high density of grain boundaries and the resulting complex arrangement of nanojunctions [2,3]. Starting from the characterization of this system, it has been proposed and formalized a generalization of the Perceptron model to describe a classification device based on a network of interacting units where the input weights are non-linearly dependent. This model, called "Receptron", provides substantial advantages compared to the Perceptron as, for example, the solution of non-linearly separable Boolean functions with a single device [4]. Here I will present and discuss the relevant aspects concerning the characterization and implementation of nanostructured networks fabricated by supersonic cluster beam deposition of gold and platinum clusters for neuromorphic computing and data processing applications [5,6].

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10:20am **MB3-ThM-8 Analysis and 3D Modelling of Percolated Conductive Networks in Nanoparticle-Based Thin Films**, *Stanislav Haviar [haviar@kfy.zcu.cz]*, University of West Bohemia, Czechia; *Benedikt Prifling*, Ulm University, Germany; *Tomáš Kozák, Kalyani Shaji*, University of West Bohemia, Czechia; *Tereza Košutová*, Charles University, Czechia; *Šimon Kos*, University of West Bohemia, Czechia; *Volker Schmidt*, Ulm University, Germany; *Jiří Čapek*, University of West Bohemia, Czechia

Thin films composed of copper oxide nanoparticles (NP) were synthesized using a magnetron-based gas aggregation source (MGA), with nanoparticle sizes controlled by varying the exit orifice diameter. The 3D model of the synthesized NP-based was constructed and assessed.

(i) Comprehensive characterization of the nanoparticle-based thin films was performed using SEM, TEM, SAXS, and XRD to determine particle morphology, size distribution, porosity and others.

(ii) The obtained experimental data served as inputs for generating virtual 3D microstructure models through a data-driven stochastic hard sphere packing algorithm, incorporating factors such as particle size distribution, porosity, and vertical density profiles.

(iii) These virtual structures were refined to account for oxidation-induced swelling and film roughness, enabling the simulation of realistic conductive networks.

(iv) A computational model incorporating a simplified adsorption mechanism was developed to simulate oxygen adsorption effects on surface conductivity, and finite element method (FEM) simulations were conducted to calculate the electrical resistivity of the modelled networks under varying oxygen partial pressures.

(v) The simulated resistivity values were validated against experimental measurements obtained via four-point probe resistivity techniques at 150°C under different oxygen concentrations, demonstrating both qualitative and quantitative agreement.

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10:40am **MB3-ThM-9 Tailoring of Nanoparticle Deposition Rate and Film Structure Through Substrate Biasing: Enabling Sputtering-Based Synthesis of Novel Catalyst Materials**, *Dominik Gutnik [dominik.gutnik@unileoben.ac.at]*, *Florian Theodor Knabl*, Montanuniversität Leoben, Austria; *Prathamesh Patil*, CEST GmbH, Austria; *Christine Bandl*, Montanuniversität Leoben, Austria; *Tijmen Vermeij*, *Daniele Casari*, Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland; *Michael Burtscher*, *Christian Mitterer*, Montanuniversität Leoben, Austria; *Christian M Pichler*, CEST GmbH, Austria; *Barbara Putz*, Montanuniversität Leoben, Austria

Metallic nanoparticles (NPs) exhibit intriguing properties as a consequence of their spatial confinement and their high surface-to-volume ratio. A topic rising in importance is the utilization of NPs as catalysts for energy conversion and storage. To facilitate more advanced use of NPs, a thorough understanding of their synthesis-structure-property relations is crucial.

In this study, the effect of different substrate biases on the deposition of size-selected Cu NPs, fabricated via Magnetron Sputtering Inert Gas Condensation (MS-IGC) in a so-called Haberland system, is analyzed. NPs nucleate and grow within the aggregation zone (usually pressures of 10 to 100 Pa), collect charge through plasma interactions and are accelerated by adiabatic expansion upon exiting the aggregation zone through an orifice. The charge they collect enables analysis and manipulation of nanoparticles through a Quadrupole Mass Spectrometer (QMS) before deposition on the substrate.

With this approach, Cu NPs with a diameter of 1.8 nm and 8 nm were filtered and accelerated towards the substrate with positive bias voltages of 0, 300 and 1000 V. In-situ QMS data reveals a significant increase of the NP-flux with higher biases, especially for smaller NP-diameters. Furthermore, changes in the morphology of the resulting thin films which were deposited for up to 45 minutes are observed with Scanning Electron Microscopy and changes in surface coverage and porosity are studied with X-ray Photoelectron Spectroscopy and Low-Energy Ion Scattering Spectroscopy.

Our results show that with rising bias voltages, the NP deposition rate estimated through QMS increases by 32% for the 8 nm diameter NPs, and the morphology of the resulting thin film shifts towards more densely packed structures, attributed to the higher energy of the NPs on impact [1]. An alternative method of NP synthesis in the form of hollow cathode sputtering will also be presented as a high throughput technique. With this technique, orders of magnitude higher NP deposition rates with position-dependent morphology can be obtained. These findings could facilitate the deposition of NP-based films with higher efficiency and with tailored morphology, making this technique more attractive for e.g. the synthesis of catalysts.

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11:00am **MB3-ThM-10 Tailoring Microstructure and Composition of Composite CuO/WO<sub>3</sub> Nanoparticle-Based Thin Films for Enhanced H<sub>2</sub> Gas Sensing**, *Kalyani Shaji [kalyanis@kfy.zcu.cz]*, *Stanislav Haviar*, *Petr Zeman*, *Michal Procházka*, *Radomír Čerstvý*, *Jiří Čapek*, University of West Bohemia - NTIS, Czechia

The conductometric gas sensors operate by modulating the electrical conductivity of the sensing material through adsorption-desorption reactions between the target gas and the sensor surface. Metal oxide semiconductors (MOS) are conductometric materials highly sensitive to oxidizing and reducing gases. In addition, composite MOS-based materials may further benefit from formed heterojunctions potentially significantly improving the sensitivity. Our focus is to develop advanced hydrogen-gas sensing materials composed of a mixture of p-type CuO and n-type WO<sub>3</sub> nanoparticles (NPs) with optimized microstructure of the film and volumetric ratio of CuO to WO<sub>3</sub> NPs in the film for enhanced H<sub>2</sub> gas sensing.

The NP-based thin films were synthesized using a magnetron-based gas aggregation source in Ar+O<sub>2</sub> gas mixture. First, effect of thermal annealing on the microstructure (i.e., NPs diameter, formed necks, porosity) of the films was studied since gas sensing materials are usually operated at elevated temperatures (up to 400°C). The CuO, WO<sub>3</sub> and their composite (1:1 volumetric ratio) samples were annealed at temperatures in the range 200 - 400°C in synthetic air and subsequently thoroughly investigated using various characterisation techniques such as SEM, XRD, XPS, and Raman spectroscopy. Significant changes in particle size were observed in the case of CuO-based material, while WO<sub>3</sub>-based and composite materials exhibited minor microstructural changes, even at elevated temperatures. Notably, at 400°C, the composite crystallized into a novel phase. Second, the volumetric ratio of CuO to WO<sub>3</sub> NPs in the films was optimized to maximize the response of the material. We demonstrate that a synergetic effect is reached when an optimum number of p-n heterojunctions is established in the material providing enhanced response of the composite film compared to the films formed by single-material NPs.

This study highlights the crucial role of thermal treatment in influencing NP microstructure, offering insights into stabilizing and tuning NP-based thin films for enhanced gas sensing. Additionally, the optimized ratio of CuO and WO<sub>3</sub> NPs within the composite improved H<sub>2</sub> sensing performance by promoting optimal p-n heterojunction formation, demonstrating that precise compositional control can significantly boost the sensitivity of nanostructured systems.

11:20am **MB3-ThM-11 Influence of Pretreatment and Deposition Parameters on Carbon Nanotubes Synthesized Directly on Oxidized Steel Substrates via Pulsed DC PACVD**, *Manuel C. J. Schachinger [manuel.schachinger@fh-wels.at]*, *Francisco A. Delfin*, University of Applied Sciences Upper Austria; *Bernhard Fickl*, *Bernhard C. Bayer*, Vienna University of Technology, Austria; *Andreas Karner*, *Johannes Preiner*, *Christian Forsich*, *Daniel Heim*, University of Applied Sciences Upper Austria; *Bernd Rübige*, *Christian Dipolt*, *Thomas Müller*, RÜBIG GmbH & Co KG, Austria

Carbon nanotubes have recently attracted considerable attention due to their distinct qualities such as elevated strength-to-weight ratio, excellent thermal conductivity, high aspect ratio and special electronic and optical properties. However, the widespread use of CNTs is limited by their costly production, partly due to the laborious substrate-catalyst preparation involving expensive transition metals like Ni or Co, which must be sputtered and sintered to form sufficient growth sites on the substrate material. To avoid the costly and time-consuming pretreatment, it was shown that direct growth of carbon nanotubes on steel substrates is possible by

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application of a simple surface oxidation step prior to the synthesis process. The aim of this work is to optimize the oxidation pretreatment of the steel in a way that specific tailoring of the nanotube properties such as diameter, length and morphology becomes possible. To achieve this, cylindrical EN 1.4301 (AISI 304) steel samples were subjected to an oxidation step in air at atmospheric pressure for 15 s, 3 minutes and 15 minutes at 300, 400 and 500 °C, respectively. Subsequently, the synthesis process was carried out in the PACVD 40/60 system (RÜBIG, Austria) utilizing a unipolar pulsed DC discharge. Power density was varied between 50 and 100 W/m<sup>2</sup>. Ar, H<sub>2</sub> and C<sub>2</sub>H<sub>2</sub> gas concentrations were 67 vol.-% 32 vol.-% and 1 vol.-%, respectively. The pressure was 200 Pa and synthesis time was 1 h. The obtained CNTs as well as the oxidized steel surfaces after pretreatment were then analysed using SEM, EDS, TEM, AFM, XPS and Raman spectroscopy. SEM images showed the formation of a high-density forest of CNTs fully covering the steel surface for substrate-oxidation times greater than 15 s. Tube diameter increased with increasing oxidation times and temperatures from 20 to 200 nm. TEM revealed the formation of bamboo-like CNTs involving a tip growth-mechanism. Raman spectroscopy showed the characteristic D, G and D' peaks, with a large I(D)/I(G) ratio, indicating an elevated degree of disorder. AFM revealed significant RMS roughness and morphology variations of the oxidized steel surfaces dependent upon oxidation time and temperature, which were correlated with the nanotube length and diameter. In summary, it was possible to achieve CNTs with tailored properties only via the variation of the surface oxidation step prior to the synthesis, achieving a cost-effective production process that can easily be adapted to the specific requirements of the applicator.

11:40am **MB3-ThM-12 The Influence of Magnetic Field on the Cluster Growth in a Magnetron Sputtering Gas Aggregation Source**, *Joao Coroa*, Teer Coatings Ltd, UK; **Giuseppe Sanzone** [[giuseppe.sanzone@teercoatings.co.uk](mailto:giuseppe.sanzone@teercoatings.co.uk)], Teer Coatings Ltd., UK; *Tibor Höltzl*, Furukawa Electric Institute of Technology, Hungary; *Hailin Sun*, Teer Coatings Ltd., UK; *Ewald Janssens*, KU Leuven, Belgium; *Jinlong Yin*, Teer Coatings Ltd., UK

Clusters produced by physical methods in gas phase have yet to see widespread adoption due to low deposition rates, despite the benefits that they could bring to many applications. It's demonstrated in this study that unbalancing the magnetic field configuration of a magnetron within a sputtering gas aggregation source significantly enhances dimer formation and subsequent cluster growth. Based on experimental results obtained with four magnetic field configurations, along with ab initio simulations, we discussed various scenarios for dimer formation and proposed that the contribution of ArPd<sup>+</sup> is essential for an increase in cluster throughput. We analysed the resulting plasma spatial distribution and demonstrated that the selected magnetic field configuration significantly influences the lifetime of ArPd<sup>+</sup> particles. When their lifetime is long, more ArPd<sup>+</sup> can react with another metal atom (Pd) and form other stable complexes (Pd<sub>2</sub>, Pd<sub>2</sub><sup>+</sup> or ArPd<sub>2</sub><sup>+</sup>), a critical first step in cluster growth, increasing cluster throughput by a factor of 150-fold. The proposed mechanism might be material-independent as other metal-argon dimers (ArCu<sup>+</sup>, ArTi<sup>+</sup> and ArCo<sup>+</sup>) have also been reported in the literature.

12:00pm **MB3-ThM-13 Tracking the Evolution of Ag Nanoparticle Solutions Upon Atmospheric Exposure Using a Combined Spectroscopic Approach**, *Héloïse Lasfargues* [[lasfargues@mch.rwth-aachen.de](mailto:lasfargues@mch.rwth-aachen.de)], *Lilli Charlotte Freymann*, *Jochen M. Schneider*, *Clio Azina*, RWTH Aachen University, Germany

With nanoparticles (NPs) finding increasing use in various fields such as the biomedical industry or catalysis, sputtering onto liquids (SoL) has attracted interest over the last decade as a single step method for NP production, requiring only a target and a host liquid. Beyond NP properties like size and shape, colloidal stability is of high importance and is primarily determined by the combination of NP material and liquid. The current understanding of NP stability in solutions produced by SoL being limited, further research is needed to thoroughly describe the complex interactions occurring between NP and liquid host. In this context, silver (Ag) NP solutions were produced by magnetron sputtering onto canola oil and their stability under atmospheric exposure was investigated by combining infrared (IR), UV-visible (UV-vis) and X-Ray photoelectron spectroscopy (XPS) measurements, with transmission electron microscopy observations (TEM). A color change from dark brown to light orange was observed within 35 days of atmospheric exposure of the as-synthesized solutions. This color change was accompanied by the formation of hydroperoxides, as revealed by IR spectroscopy and XPS. The observation of peroxides signals oil oxidation, suggesting that the latter was promoted by the presence of Ag NPs upon oxygen incorporation. In terms of size, more than 90% of the NPs were < 5

nm in diameter in the as-synthesized solutions, with an average size of 2.9 ± 2.3 nm. Upon atmospheric exposure the proportion of NPs > 5 nm in diameter increased by ~100% after 35 days, indicating that the NPs continue to grow in the solution. In addition to size variations, TEM analysis suggests the formation of Ag-Ag<sub>x</sub>O Janus-type NPs in large proportion and therefore partial oxidation of the produced NPs upon atmospheric exposure. These observations were correlated with UV-vis measurements, where a red shift of ~ 15 nm of the localized surface plasmon resonance and an absorbance decay of the solutions after 35 days was detected. Finally, the comparison of XPS spectra of the pure oil with as-synthesized and aged NP solutions revealed the formation of carboxylate groups (-COO<sup>-</sup>) and their interaction with Ag in the near-surface volume probed.

## Functional Thin Films and Surfaces

### Room Golden State Ballroom - Session MB-ThP

#### Functional Thin Films and Surfaces Poster Session

##### **MB-ThP-1 Two-Dimensional Vacancy Confinement in Anatase TiO<sub>2</sub> Thin Films for Enhanced Photocatalytic Activities, Junwoo Son [junuson@snu.ac.kr], Seoul National University, Republic of Korea**

Light-driven energy conversion devices call for the atomic-level manipulation of defects associated with electronic states in solids. However, previous approaches to producing oxygen vacancy ( $V_O$ ) as a source of sub-bandgap energy levels have hampered the precise control of distribution and concentration in  $V_O$ .

Here, a new strategy to spatially confine  $V_O$  at the homo-interfaces is presented by exploiting the sequential growth of anatase TiO<sub>2</sub> under dissimilar thermodynamic conditions. Remarkably, metallic behavior with high carrier density and electron mobility is observed after sequential growth of the TiO<sub>2</sub> films under low pressure and temperature (L-TiO<sub>2</sub>) on top of high-quality anatase TiO<sub>2</sub> epitaxial films (H-TiO<sub>2</sub>), despite the insulating properties of L-TiO<sub>2</sub> and H-TiO<sub>2</sub> single layers. Multiple characterizations elucidate that the  $V_O$  layer is geometrically confined within 4 unit cells at the interface, along with low-temperature crystallization of upper L-TiO<sub>2</sub> films; this two-dimensional  $V_O$  layer is responsible for the formation of in-gap state, promoting photocarrier lifetime (~ 300 %) and light absorption. These results suggest a synthetic strategy to locally confine functional defects and emphasize how sub-bandgap energy levels in the confined imperfections influence the kinetics of light-driven catalytic reactions.

This work is performed by the collaboration with Mr. Minwook Yoon, Dr. Yunky Park, Ms. Hyeji Sim, Ms. Hee Ryeung Kwon, Dr. Yujeong Lee, Prof. Ho Won Jang, Prof. Si-Young Choi.

##### **MB-ThP-2 Fabrication of Metal-Based Superhydrophilic and Underwater Superoleophobic Surfaces by Laser Ablation and Magnetron Sputtering, Adham Al-Akhali [alakhali.adham@gmail.com], Guizhou University, China**

Fabricating underwater superoleophobic surfaces is an advanced technique for controlling undesirable oil and wax adhesion on engineering structures and household appliances. This article presented a facile method based on the combination of laser ablation of stainless steel substrates followed by magnetron sputtering of a metallic tungsten target to fabricate superhydrophilic and underwater superoleophobic surfaces. The results showed that the laser-ablated stainless steel substrate without coatings exhibited hydrophilicity and underwater oleophobicity. However, its transition to superhydrophilicity and underwater superoleophobicity with a 0° water contact angle and higher than 156° underwater oil contact angles occurred after the deposition of a thin tungsten film followed by annealing at 300 °C. In addition, the prepared surface maintained its wetting behavior for more than 4 weeks, even in corrosive aqueous HCl and NaOH solutions. According to the data from SEM and XPS, this distinguished wetting behavior resulted from the presence of the regular microscale texture patterns, abundant hydroxyl content, and low carbon content on the tungsten layer after annealing at 300 °C. Thus, laser ablation combined with magnetron sputtering of tungsten demonstrated effective results in fabricating superhydrophilic and underwater superoleophobic surfaces that are independent of the initial wetting of the substrates.

##### **MB-ThP-3 Synthesis and Characterization of Zn Doped CsPbI<sub>3</sub> Perovskite Quantum Dots, Ya-Fen Wu [yfwu@mail.mcut.edu.tw], Hao-Yu Jhai, Ming Chi University of Technology, Taiwan**

The increasing focus on sustainable energy has driven advancements in renewable technologies, with quantum dot solar cells gaining particular interest in photovoltaics for their ability to efficiently convert sunlight into electricity. Early cells used II-VI semiconductors with high crystallinity and luminescence but were limited by toxicity and complex synthesis. In contrast, all-inorganic perovskite quantum dots such as CsPbX<sub>3</sub> (X=Cl, Br, I) have gained prominence due to their excellent photoelectric properties, low cost, and easy to be manufactured. Moreover, compared to organic-inorganic perovskites, all-inorganic perovskites are more stable under high temperature and with extremely high quantum yield. Consequently, they are gradually becoming mainstream in research and development.

Metal ion doping is widely recognized as one of the most effective strategies to enhance the efficiency of perovskite light-emitting devices. In this study, CsPbI<sub>3</sub> all-inorganic perovskite QD thin films were prepared with

various concentrations of zinc acetate (0%, 3%, 5%, and 7.5%) added as dopants. Temperature-dependent photoluminescence was carried out from 20 K to 300 K. To investigate the thermal behaviors of peak energy, full width at half maximum, and intensity of the PL spectra measured from our samples, the carrier emission mechanism, electron-phonon scattering, electron-phonon interaction and thermal expansion effect on the band-gap are discussed. As the increasing of the Zn doping concentration from 0% to 7.5%, the PL peaks were shifted from 1.74 eV to 1.73 eV at 20 K. In addition, a noticeable blueshift of emission peaks was observed with increasing temperature for all the samples, which attributed to the effects of lattice thermal expansion and electron-phonon interactions. The PL intensity increases as the Zn doping concentration increases from 0% to 5% and then decreases as the doping concentration is 7.5%. It implies that Zn doping lowers the defect density in QDs by reducing lattice distortion and enhancing crystal quality; but under higher doping concentration, the dopants may not have enough time to move into the right positions of the structure, result in the degradation the thin film quality. Furthermore, the PL intensity decreases with increasing temperature for all the samples; however, the sample with 5% Zn doping concentration exhibited the highest intensity at 300 K. It reveals that the optical properties of CsPbI<sub>3</sub> QD thin films was improved by an appropriately increasing Zn doping.

##### **MB-ThP-4 Improved Photovoltaic Performance of Si-Based Hybrid Solar Cells via Mo<sub>2</sub>C Bridging in 2D MoS<sub>2</sub> nanosheets @ 0D Carbon Colloid Dots, Ta-Cheng Wei [dvt8756713@gmail.com], Chia-Yun Chen, National Cheng Kung University (NCKU), Taiwan; Chih-Chiang Yang, National Yunlin University of Science and Technology, Taiwan**

Recent advances in silicon-based hybrid solar cells, distinguished by high photovoltaic efficiency, low production costs, and strong environmental resilience, position them as promising candidates for solar energy conversion. [1] Solution-processed few-layer MoS<sub>2</sub> sheets enhance solar capture, but improved charge separation is essential, and their moisture sensitivity limits stability by attracting electrons. [2] This study introduces MoS<sub>2</sub>/Mo<sub>2</sub>C/carbon colloid dots (CCDs) heterostructures within a PEDOT:PSS matrix, utilizing Mo<sub>2</sub>C electron-transport channels to facilitate the transfer of photoexcited electrons from MoS<sub>2</sub>. This configuration fosters positive trion formation via interactions with defect-bound excitons on CCD surfaces, reducing recombination rates and enhancing photovoltaic performance. [3, 4] To elucidate carrier transfer mechanisms in these heterostructures, MoS<sub>2</sub>@CCD heterojunctions with Mo<sub>2</sub>C bridging interfaces facilitate efficient electron transfer. Photoluminescence (PL) enhancement factors ( $\beta$ ) were used to characterize trion emissions across HT interfaces compared to intrinsic trion emissions in CCDs, by analyzing three distinct MoS<sub>2</sub>@CCD blends within a PEDOT:PSS matrix, grounded in fundamental transport phenomena. [5] This design achieves a 16.1% efficiency, 1.6 times higher than conventional hybrid solar cells, with outstanding long-term stability, advancing photophysical bound-carrier research in photovoltaics.

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##### **MB-ThP-5 Top-Emitting QLEDs with a Thin Stabilizing Layer to Prevent Agglomeration, Jaehyung Park [parkja0404@kyonggi.ac.kr], Kangsuk Yun, Jaehwi Choi, Jiwan Kim, Kyonggi University, Republic of Korea**

Colloidal quantum dots (QDs) are semiconductor nanoparticles composed of a core, shell, and organic ligands. They have unique optical and electrical properties due to quantum confinement effects, which enable the bandgap to vary with particle size. This characteristic allows easy modification of emission wavelengths, producing various colors of light. QDs are compatible with solution process and notable for their narrow full-width at half-maximum for the high color purity. Due to these advantages, quantum dot light emitting diodes (QLEDs) that use QDs as light emitting layers are being recognized as a promising next-generation display technology. In the field of AR/VR devices, Organic Light Emitting Diode on Silicon (OLEDOs) has received significant attention recently. This technology uses silicon as a substrate and emits light from the top with micropatterned structure, thus

research on top-emitting devices is essential. However, there is still limited research on QLEDs in this area.

In top-emitting quantum dot light emitting diodes (TQLEDs), a transparent metal such as Ag is commonly used as the top electrode due to its high transparency and electrical conductivity. However, the deposition of thin Ag layer to achieve high transparency leads to agglomeration, which prevents the formation of a uniform layer, and results decreased conductivity. In this study, we used 2,2',2''-(1,3,5-Benzotriazolyl)-tris(1-phenyl-1-H-benzimidazole) (TPBi) as a stabilizing layer to suppress the agglomeration of Ag in TQLEDs. TPBi has high electron affinity, which makes it effective in interacting with Ag to inhibit agglomeration. Various thickness of TPBi was applied to investigate the change of Ag agglomeration. As a result, the transmittance of transparent top electrode was over 50%, and TQLEDs incorporating TPBi as a stabilizing layer successfully achieved a maximum luminance exceeding 100,000 cd/m<sup>2</sup>. Enhanced top electrode can provide another approach to improve the performance of top-emitting devices.

**MB-ThP-6 Impact of Chlorine Incorporation on the Electrical and Structural Properties of Solution-Processed a-IGZO TFTs, Gyoong Chung [qu3xing29@gmail.com], Dae Woong Kim, Yong-Sang Kim, Sungkyunkwan University (SKKU), Republic of Korea**

We investigated the influence of chlorine incorporation on solution-processed amorphous indium-gallium-zinc oxide (a-IGZO) thin-film transistors (TFTs). During the TFT fabrication process, materials inevitably interact with unintended elements. Notably, chlorine is an essential component in various stages of TFT fabrication, including as a precursor for metal oxide deposition and as a dry etching gas, making exposure to chlorine nearly unavoidable. Therefore, understanding chlorine's role in affecting the electrical and material properties of TFT devices is crucial.

In this study, we immersed a-IGZO films in NaCl solution to incorporate chlorine into the films. X-ray Photoelectron Spectroscopy (XPS) analysis revealed that chlorine formed bonds with metals and increased oxygen vacancies (Vo). The area ratio of M-O was lower in the IGZO thin film soaked in NaCl, reaching 46.5%, compared to 52.8% in the unsoaked film. Additionally, the concentration of oxygen vacancies, which can act as trap sites in the oxide channel layer, increased from 38.0% in the unsoaked sample to 44.4% in the NaCl-soaked sample. This structural change led to a degradation in IGZO's electrical performance. Compared to pristine TFTs, the saturation mobility of a-IGZO TFTs soaked in NaCl solution decreased from 1.46 to 0.20 cm<sup>2</sup>/V·s, while the subthreshold slope increased from 0.38 to 0.99 V/dec, indicating higher defect density. XRD analysis showed that soaking in NaCl solution did not alter the film's crystallinity. Furthermore, we compared the impact of chlorine diffusion on IGZO films deposited via the sputtering process. These findings suggest that chlorine exposure during fabrication must be carefully controlled to achieve the desired electrical performance targets for a-IGZO TFTs.

**MB-ThP-7 Electrochemical Insights into All-Solid-State Symmetric Supercapacitors Based on Sputter-Grown WSe<sub>2</sub>, Akshay Tomar [atomar@ic.iitr.ac.in], Somdatta Singh, Ananya Bansal, Prachi Gurawal, Ramesh Chandra, IIT Roorkee, India**

All-solid-state supercapacitors represent a promising advancement in energy storage technology, providing superior energy density, enhanced safety, and a compact design compared to conventional supercapacitors and batteries. Their potential as flexible, bendable, and wearable energy storage solutions have garnered significant interest. The capacitance and energy density of supercapacitors can be improved through the introduction of novel electrode materials or by utilizing electrolytes with high potential windows. In this study, we successfully fabricated a high-quality porous thin film of tungsten diselenide (WSe<sub>2</sub>) on a flexible graphite substrate using an environmentally friendly DC magnetron sputtering technique, without the need for additives or binders, under optimized conditions. The resulting thin film exhibited a nanoflake morphology with an increased surface area, which provided a greater number of active sites for ion adsorption and desorption, thereby enhancing both capacitance and energy density. The WSe<sub>2</sub>@graphite composite demonstrated a remarkable specific capacitance of 310 F/g at a scan rate of 10 mV/s, with 95% capacitance retention after 5000 charge-discharge cycles in a three-electrode configuration. An all-solid-state flexible symmetric supercapacitor (FSS) device was subsequently constructed, utilizing WSe<sub>2</sub> as both the cathode and anode, separated by a highly flexible 6M KOH/PVA solid-state gel electrolyte. This device achieved a high cell voltage of 1.4 V and an excellent specific capacitance of 38.932 F/g at a scan rate of 50 mV/s. Comprehensive electrochemical performance analyses, including charge-discharge measurements at varying current densities, revealed a specific

capacitance of 17 F/g, an energy density of 4.62 mWh/g, and a power density of 3457 mW/g, along with outstanding electrochemical stability of 92% after 5000 cycles at a current density of 5 mA/g. The exceptional electrochemical performance, combined with the flexible characteristics of the WSe<sub>2</sub>@graphite thin-film-based symmetric supercapacitor, positions this device as a promising candidate for the development of next-generation flexible, bendable, and wearable energy storage systems.

**MB-ThP-8 Highly efficient of QLEDs Using SnO<sub>2</sub> Electron Transport Layers Deposited by RF Sputtering, Jaehwi Choi [jksix@kyonggi.ac.kr], Jaehyung Park, Kangsuk Yun, Jiwan Kim, Kyonggi University, Republic of Korea**

Colloidal quantum dots (QDs) are semiconductor nanoparticles with unique optical and electrical properties. By controlling particle size, QDs can exhibit various colors and provide excellent color reproducibility. Due to these advantages, quantum dot light-emitting diodes (QLEDs) using QDs as the emissive layer are studied actively. In QLEDs, the electron transport layer (ETL) is essential for electron transport and charge balance, and optimizing ETL can enhance device stability and efficiency. In general, ZnO nanoparticles (NPs) are commonly used as ETL for their high electron mobility and transmittance. However, ZnO NPs aggregate easily at room temperature, leading to reduce stability. Therefore, SnO<sub>2</sub>, which offers high electron mobility, transmittance, and excellent stability, is gaining attention as an ETL material. Typically, the ETL is deposited via solution processes like spin coating, but this method has challenges such as difficulty in thickness control, poor crystallinity and uniformity of the thin films. In this study, we deposited SnO<sub>2</sub> as the ETL using RF sputtering process for high reproducibility and excellent crystallinity. It is well known that crystallinity of inorganic materials are directly related to their electrical properties. To adjust the physical and chemical properties of SnO<sub>2</sub> thin film, we controlled the substrate temperature and Ar/O<sub>2</sub> ratio during RF sputtering while fabricating inverted devices with the structure of ITO/SnO<sub>2</sub>/QDs/CBP/MoO<sub>3</sub>/Al. As the substrate temperature increased, the crystallinity of sputtered SnO<sub>2</sub> thin film improved, which led the enhancement of electron mobility and improvement of electrical properties of devices. QLEDs employing the optimized SnO<sub>2</sub> ETL exhibited more than 120,000 cd/m<sup>2</sup> and a current efficiency of 15 cd/A which showed comparative performance with QLEDs using soluble SnO<sub>2</sub>NPs as an ETL. Additionally QLEDs with sputtered ETL showed better stability due to the uniform SnO<sub>2</sub> layer, which is advantage for practical display mass production.

**MB-ThP-9 Optimizing Y<sub>2</sub>O<sub>3</sub> Coating for Improving Plasma Resistance in Dry Etching Process, Sunil Kim [sunil725.kim@semes.com], Sunghwan CHO, Ja Myung Gu, Seungpil Chung, Gil Heyun Choi, SEMES Co., Ltd., Republic of Korea**

Plasma-resistant Y<sub>2</sub>O<sub>3</sub> coating is essential for extending the durability and replacement cycles of semiconductor components that face intense etching conditions. Plasma etching typically involves both physical ion bombardment and chemical reactions with surface. To counter these effects, recent advancements in Y<sub>2</sub>O<sub>3</sub> coating focus on enhancing etch resistance and film density through physical vapor deposition (PVD) methods. While several studies have aimed to further improve the plasma resistance of PVD Y<sub>2</sub>O<sub>3</sub> coatings by increasing hardness, our observations suggest that beyond a certain hardness threshold (>900 HV), the relationship between hardness and plasma resistance became weak. Consequently, this study focuses on the characteristics of residual surface stress as a primary factor influencing plasma resistance. The residual stress in the coating was measured using X-ray diffraction (XRD) equipment and calculated based on the peak shift observed with varying psi angles. Comparing residual stress and plasma resistance in PVD Y<sub>2</sub>O<sub>3</sub> coatings manufactured under identical conditions, we found that coatings with tensile surface stress exhibited approximately 25% better plasma etch resistance than those with compressive stress. Although both coatings displayed similar grain size and hardness, the superior plasma-resistant coating demonstrated a tensile surface stress of around 600 MPa, whereas the less resistant sample had a compressive stress of approximately 300 MPa. This enhanced resistance in tensile-stressed coatings can be attributed to channeling effects, where the increased atomic spacing prevents accelerated plasma ions from interacting directly with atoms, allowing them to pass through specific crystallographic directions without obstruction. This study aims to establish a better understanding of the correlation between surface residual stress and plasma etch resistance in PVD Y<sub>2</sub>O<sub>3</sub> coatings and to propose new criteria for evaluating such coatings, ultimately contributing to enhanced performance in etching equipment.

**MB-ThP-10 Electrical and Morphological Properties of Alloyed Al<sub>2</sub>O<sub>3</sub> Thin Films at High Temperatures, Norma Salvadores Farran** [[norma.salvadores@tuwien.ac.at](mailto:norma.salvadores@tuwien.ac.at)], Florentine Scholz, Tomasz Wojcik, Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria; Carmen Jerg, Astrid Gies, Jürgen Ramm, Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein; Szilard Kolozsvári, Peter Polcik, Plansee Composite Materials GmbH, Germany; Jürgen Fleig, Tobias Huber, Institute of Chemical Technologies and Analytics, TU Wien, Austria; Balint Hajas, Institute of Materials Science and Technology, TU Wien, Austria; Helmut Riedl, Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria

Aluminium oxide (Al<sub>2</sub>O<sub>3</sub>) is a well-known insulating material employed in a wide range of applications, both as structural component as well as in thin film form. Al<sub>2</sub>O<sub>3</sub> can be stabilized in several polymorphs, in addition to an amorphous modification. Especially the amorphous state of Al<sub>2</sub>O<sub>3</sub> exhibits interesting features, considering the absence of crystalline defects for diffusion of charge carriers paired with the difficulties in stabilizing crystalline Al<sub>2</sub>O<sub>3</sub> during physical vapor deposition (PVD). Furthermore, amorphous materials are free of pinholes, which is favourable for a number of applications. Consequently, it is crucial to investigate economically and sustainably viable deposition techniques to grow insulating Al<sub>2</sub>O<sub>3</sub> thin films.

Therefore, this study focuses on the effect of alloying elements such as silicon and yttrium-zirconium (YZr) on the thermal stability of amorphous Al<sub>2</sub>O<sub>3</sub> based thin film materials up to 1200°C. The amorphous Al<sub>2</sub>O<sub>3</sub> thin films have been synthesised via a reactive Modulate Pulse Power (MPP) sputtering processes. In all depositions, an in-house developed sputter system, equipped with a 3" Al target, was used in a mixed Ar/O<sub>2</sub> atmosphere. To this end, two types of targets were employed: an Al-Si target and Al-YZr target. The impact of the deposition parameters on the structure, morphology, and electrical resistivity at high temperatures was investigated using high-resolution characterization methods such as XRD, SEM, HR-TEM or in-situ set-ups for annealing treatments. The insulating behaviour of the coatings was analysed using in-situ impedance spectroscopy across a temperature range. Ti/Pt electrode pads were deposited on the thin films using a lithography process for the purpose of electrical characterization. In addition, the bonding type was investigated via XPS, which was also employed to determine the chemical composition across the thickness of the coating.

**MB-ThP-11 Analysis of Four-Point Bending Test for Nb, Ta, and V-Doped CrYN Thin Films Deposited by Closed-Field Unbalanced Magnetron Sputtering, Banu YAYLALI, Gokhan Gulten, Mustafa YESILYURT, Yasar TOTIK,** Atatürk University, Turkey; Justyna Kulczyk Malecka, Peter Kelly, Manchester Metropolitan University, U.K.; Ihsan Efeoglu [[ifeoglu@atauni.edu.tr](mailto:ifeoglu@atauni.edu.tr)], Atatürk University, Turkey

The increasing expectations and requirements for engineering materials are steadily compelling researchers to evolve and innovate further. Adding transition metals to coating architectures is becoming increasingly attractive as it improves structural and mechanical properties. In this work, CrYN thin films incorporating transition metals Nb, Ta, and V were deposited on a 316L stainless steel substrate using Closed Field Unbalanced Magnetron Sputtering (CFUBMS) with a DC and pulsed-DC power supply. The microstructural properties of the thin films were analyzed using scanning electron microscopy (SEM), while X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) provided a comprehensive understanding of the coating structure by providing information on crystallographic and surface chemical properties. Mechanical properties were evaluated using nanoindentation testing, which provided accurate measurements of hardness and elasticity, while scratch testing assessed critical load values. In addition, four-point bending tests were performed at room temperature to characterize the CrYN:Nb/Ta/V transition metal nitrides (TMNs), providing a more comprehensive analysis of the mechanical behavior (flexural strength and elastic modulus) and adhesion properties of the coating. The mechanisms of coating damage (crack formation and density, spalling, flaking, and separated coating particles) were analyzed as a result of four-point bending tests. The Taguchi approach was employed to investigate how deposition parameters—such as target current, duty cycle, and pulse frequency—affect elastic modulus and bending strength. Superior structural (homogeneous and dense film) and mechanical properties (CrYN:Nb/Ta/V high hardness values of 21.4, 18.2, 16.1 GPa, and bending strengths of 707, 711, and 697 MPa, respectively) were obtained. The positive correlation between hardness and bending strength points to an enhancement in the overall durability of the thin film.

**MB-ThP-12 Halide-Treated ZnMgO Nanoparticles for Improving Stability of InP Based Quantum-Dot Light-Emitting Diodes, Kangsuk Yun** [[riverstone@kyonggi.ac.kr](mailto:riverstone@kyonggi.ac.kr)], Jaehyung Park, Jaehwi Choi, Jiwan Kim, Kyonggi University, Republic of Korea

Quantum dots (QDs) are nanometer-sized semiconductor particles, and Quantum Dot Light Emitting Diodes (QLEDs) are electroluminescent devices that use QDs as an emitting layer. As QD size decreases, the quantum confinement effect enhances the discreteness of energy levels, leading to an increased bandgap. Consequently, by manipulating the size of QDs, it is possible to produce various colors of light and enhance color purity by narrow full width at half maximum. ZnMgO NPs, which are currently used as the electron transport layer (ETL) in QLEDs, are actively researched due to their high electron mobility and chemical stability. However, there are inevitable oxygen vacancies in thin films using ZnMgO NPs, which reduce the performance of QLEDs by exciton quenching. In this study, we used ZnMgO NPs as the ETL to fabricate InP QD-based QLEDs, which consisted of multilayers: ITO/ZnMgO/red InP QDs/CBP/MoO<sub>3</sub>/Al. First, we formed ZnMgO NPs film on ITO glass and passivate halides on ZnMgO NPs to reduce oxygen vacancies. New Zn-halide and Mg-halide peaks were observed in the x-ray photoelectron spectroscopy. Additionally, photoluminescence (PL) measurements showed that halide-treated ZnMgO NPs exhibited a higher PL intensity compared to untreated ZnMgO NPs. These results indicate that the halide treatment effectively reduces oxygen vacancies in ZnMgO NPs, and its effect was verified with the inverted structured QLEDs. The maximum luminance of QLEDs with halide-treated ZnMgO NPs (h-QLEDs) showed 1,134 cd/m<sup>2</sup>, compared to 696 cd/m<sup>2</sup> for the QLEDs with pristine ZnMgO NPs (p-QLEDs). After aging for 48 hours in a nitrogen atmosphere, h-QLEDs showed 1,290 cd/m<sup>2</sup>, but the performance of p-QLEDs decreased dramatically to 64.67 cd/m<sup>2</sup>. The experimental results indicated that the halide-treated ZnMgO NPs enhance the optical properties and stability of QLEDs, which can contribute QDs display commercialization.

**MB-ThP-13 Inkjet Printing of Silver Film on Polydimethylsiloxane for Soft Electronics, Hsuan-Ling Kao** [[snoopy@mail.cgu.edu.tw](mailto:snoopy@mail.cgu.edu.tw)], Chang Gung University, Taiwan; Li-Chun Chang, Mingchi University of Technology, Taiwan; Min-Hsuan Lu, Chang Gung University, Taiwan

As the development of fifth-generation mobile communication technology expands into medical intelligence, the demand for flexible and wearable devices has increased significantly. The flexible polymer substrates are very promising for expansion into millimeter wave band applications. Among these polymers, Polydimethylsiloxane (PDMS) has recently gained much attention for the development of wearable antennas, sensors, and RF switch. PDMS is a transparent and colorless high molecular polymer with biocompatibility. Its mechanical properties are similar to human skin (elastic modulus ~2 MPa) and can be smoothly attached to the surface of object. Therefore, PDMS is like human skin and can be attached to various parts of the human body, making it an electronic skin for biological monitoring. In order to fabricate electronic devices on these flexible plastic materials, the interconnection using metal layers are essential. However, PDMS is softer than other flexible substrates, and its surface has poor wettability, making it difficult for the metal layer to adhere. Therefore, traditional production methods such as transfer printing or screen printing cannot be used to produce electrodes. Inkjet printing technology is used to deposit metal films on PDMS using non-contact material deposition and digital patterning. The inkjet printing technology can produce highly conductive films at a lower process temperature, without the need for etching steps and the process is simple. In this work, inkjet-printed silver thin film on PDMS substrate process was established. First, the PDMS surface uses plasma technology to control its energy and time to convert hydrophobicity into hydrophilicity. Then, silver films were printed onto PDMS substrate, followed by curing in an oven to remove excess solvent and material impurities. Multi-pass printing is required to achieve good conductivity and enough thickness. The conditions for plasma treatment of PDMS were examined by water contact angle to optimize surface wettability. The conductivity, thickness and surface morphology of the printed metal film depend on the printing thickness and sintering temperature. The conductivity and surface morphology were measured using the four-probe method and SEM photos. The optimization of inkjet printing process and surface treatment study of inkjet-printed silver film were presented with details. Based on optimal conditions, inkjet-printed silver lines on PDMS substrate were implemented to study the RF performance. The results demonstrate that inkjet printing of metals on PDMS substrates offers the feasibility of soft electronics.



# Thursday Afternoon, May 15, 2025

**MB-ThP-14 Magnetolectric Sensors for Flexible MEMS Applications, Davinder Kaur [davinder.kaur@ph.iitr.ac.in]**, Indian Institute of Technology Roorkee, India

**Magnetolectric Sensors (ME)** have the potential to contribute to sustainable development because of their peculiar features such as lower power requirement, enhance energy efficiency, reduced environmental impact, applications in renewable energy, enable precision agriculture, infrastructure monitoring, health monitoring, optimize waste management, and contribution to overall resource conservation. The present study reports the fabrication of highly flexible, cost-effective, nano-structured magnetic field sensor comprising AlN/Ni-Mn-In ME heterostructure fabricated over magnetostrictive Ni foil. The ultra-low magnetic field up to or less than  $\sim 1$   $\mu$ T has been easily detected from the fabricated sensor. Further the surface acoustic wave (SAW) delay line-based piezo resonator has been fabricated over highly flexible AlN/Ni-Mn-In/Kapton for flexible MEMS application. The fabricated device resonates at  $\sim 1.40$  GHz. The effect of the external magnetic field on the resonance frequency (fR) of the device has been investigated and tunability ( $\Delta fR/fR$ )  $\sim 9\%$  was observed. The device displays high sensitivity of  $\sim 0.94$  Hz/nT at room temperature. The alteration in the fR can be attributed to the  $\Delta E$ -effect in the AlN/Ni-Mn-In heterostructure. The flexibility of the fabricated magnetic field sensors has been investigated in terms of the bending cycles and bending angle. The sensor characteristics remain unchanged up to  $\sim 2500$  bending cycles. The integration of these novel ferromagnetic shape memory alloy (FSMA, i.e., Ni-Mn-In) based flexible piezo-resonator into various systems can enhance efficiency, reduces environmental impact, and contributes significantly to the overarching goal of sustainable development.

**Keywords:** Ferromagnetic shape memory alloys, flexible magnetic sensor, lead-free piezoelectric, magnetostrictive effect, surface acoustic waves (SAW).

**MB-ThP-15 Flexible UV-Vis photodetectors based on NiO<sub>x</sub> thin film obtained by magnetron r.f. sputtering, Eddue Osuna-Escalante [eddue.osuna@uabc.edu.mx]**, David Mateos-Anzaldo, Oscar Pérez-Landeros, Roumen Nedev, Ivan Cardoza-Navarro, Esteban Osorio-Urquiza, Mario Curriel-Álvarez, Nicola Nedev, Universidad Autónoma de Baja California, Mexico

Flexible optoelectronic devices based on transparent substrates are attracting interest for potential applications in wearable sensors, flexible displays and transparent electronic devices. Among various fabrication techniques, magnetron r.f. sputtering stands out for preparation of high-quality films. The principal advantages of this technique are high adhesion, low density of defects, high compatibility with flexible substrates, and control over the deposited material composition.

Flexible photodetectors based on NiO<sub>x</sub> deposited by magnetron r.f. sputtering at room temperature and 50°C, using powers in the range of 40-80W over ITO-PET and ITO-PEN substrates were fabricated. The obtained films were evaluated using ellipsometry to determine their thicknesses and optical constants. Thermal evaporation was used to deposit Au as top electrodes.

To assess the performance as photodetectors in the UV-visible spectrum, the fabricated devices were electrical characterized by current-voltage measurements in dark and under the incidence of different light emitting diodes. In addition, the fabricated flexible photodetectors were tested for mechanical and electrical stability after cyclic bending stress.

**MB-ThP-16 Large Area Synthesis of Hexagonal Boron Nitride Layers on SiO<sub>2</sub>/Si Substrates, Diego Lundquist Lundquist [dlundquist7949@sdsu.edu]**, Abinash Bhuyan, Mary Becker, Jennifer Brumley, Sanjay Behura, San Diego State University, USA

**Diego Lundquist**, C. Abinash Bhuyan, Mary Becker, Jennifer Brumley, Sanjay K. Behura\*

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Hexagonal boron nitride (h-BN) is a two-dimensional material that has recently been the focus of research for hosting single photon emitters at room temperature. Its spin-optical properties make an ideal candidate for quantum technologies. Existing research relies on exfoliated hBN for its application which restricts its scalability for various practical applications. Also, the current synthesis of chemical vapor deposition grown hBN is on catalytic substrates such as Cu, Al, Ni, and Co. As a result, hBN film is transferred onto desired substrates for photonics applications. This study focuses on synthesizing large-scale hBN film on dielectric substrates, which allows for direct characterization of its high optical properties. Through the

optimization of a two-zone, low-pressure chemical vapor deposition (LPCVD), hBN grown directly on SiO<sub>2</sub>/Si substrates using the sublimation of ammonia borane complex as precursor and ultra-high pure H<sub>2</sub> as carrier gas. CVD-grown hBN films were characterized to confirm the large-area growth. Typical optical and scanning electron microscopic images reveal the uniform growth of hBN on SiO<sub>2</sub>/Si substrate. Raman spectroscopic measurement reveals the signature peaks at 1368 cm<sup>-1</sup> which corresponding to E<sub>2g</sub> in-plane B-N vibrational modes in hBN.

**MB-ThP-17 Influence of partial pressure of argon/oxygen and temperature on photosensors based on n-Si/NiO<sub>x</sub>, Esteban Osorio [esteban.osorio@uabc.edu.mx]**, Autonomous University of Baja California, Mexico; David Mateos-Anzaldo, Mario Curriel-Alvarez, Eddue Osuna Escalante,, Oscar Perez-Landeros, Ivan Cardoza-Navarro, Roumen Nedev, Benjamin Valdez-Salas, Nicola Nedev, Autonomous University of Baja California, Mexico

This work reports photosensors based on non-stoichiometric nickel oxide obtained by radio-frequency magnetron sputtering on n-Si substrates in a mixed atmosphere of argon/oxygen. The amount of oxygen was varied from 0-4% of the total atmosphere. Also the deposition temperature was varied in the range of 0-100°C. Corning glass substrates were also used to determine the band gap and transparency of the obtained film. The photosensors were characterized by ellipsometry in a 350 to 1000 nm range. Au ( $\sim 400$ nm) deposited by thermal evaporation was used as top and back contact for electrical characterization. Current-voltage measurements were performed in a dark chamber under red, green, blue and UV illumination.

**MB-ThP-18 Topological Insulator, Reduced Graphene Oxide/Silicon Nanowire Arrays for Ultra-Broadband Photodetectors, Hsu Hsun-Feng [hfsu@dragon.nchu.edu.tw]**, Huang Tzu-Yun, National Chung Hsing University, Taiwan

Topological insulator, such as bismuth telluride (Bi<sub>2</sub>Te<sub>3</sub>), has narrow bulk band gap and has a Dirac-type surface stat. Thus, it can absorb middle or long-wavelength infrared light and has low resistivity. Graphene, which is a 2D material, exhibits broadband light adsorption and a rapid response due to its Dirac cone structure. Therefore, graphene is an expected material for broadband photodetectors. Its drawbacks are the properties of a high electron-hole recombination rate and a low photoresponse. However, reduced graphene oxide (rGO) has lower electron-hole recombination rate comparing with graphene due to its functional group and edge defects. Silicon has become very popular for many applications because of the unique advantages of CMOS compatibility and high integrated density. Silicon nanowire (SiNW) array has low reflectivity that can raise light harvesting efficiency. Thus, in this study an ultra-broadband photodetector was fabricated by combining with the Bi<sub>2</sub>Te<sub>3</sub>, rGO and SiNW array.

The silicon substrate is etched using metal-assisted chemical etching to an obtain SiNW array. Then, Bi<sub>2</sub>Te<sub>3</sub> was deposited on SiNW array by chemical vapor deposition (CVD). Using photocatalytic reduction to reduce graphene oxide on a SiNW array to form a thin film. Finally, silver electrodes are deposited on both sides of the specimen to create a device. Optical sensing is performed using 940 nm near-infrared light and 5500 nm mid-infrared light.

The results show that, under suitable process conditions using by CVD, Bi<sub>2</sub>Te<sub>3</sub> and tellurium (Te) precipitates with a size of approximately 500 nm can be formed on the SiNW array. It can reduce the reflectance of the device in the near- to mid-infrared range (1200–2500 nm). For sensing 940 nm near-infrared light, the light is primarily absorbed by the SiNW array, generating electron-hole pairs that increase carrier concentration and produce photocurrent. The rGO coating can reduce the contact resistance between the electrode and the silicon nanowires, enhancing the responsivity and sensitivity of the photodetector. When irradiated with mid-wavelength infrared light at 5500 nm, the Bi<sub>2</sub>Te<sub>3</sub>/SiNW array device also exhibits a rapid response characteristic. The reason is that, upon illumination, electron-hole pairs are generated in the Bi<sub>2</sub>Te<sub>3</sub> particles. Electrons are conducted through the SiNW to the electrodes, producing a photocurrent in the external circuit. Notably, the rGO/Bi<sub>2</sub>Te<sub>3</sub>/SiNW device with a mesh-like rGO film, compared to a fully covered rGO film, demonstrates superior responsivity and faster response times in sensing both 940 nm near-infrared light and 5500 nm mid-infrared light.

**MB-ThP-19 Microstructural Evolution of Co-Sputtered Nanocrystalline Cu-Ag Alloy Thin Films During Annealing Process, Yu-Lin Liao [20193eileen@gmail.com],** College of Semiconductor Research, National Tsing Hua University, Taiwan; Tsai-Shuan Kuo, Fan-Yi Ouyang, Department of Engineering and System Science, National Tsing Hua University, Taiwan

Copper and silver films, known for excellent conductivity, are widely used as conductive layers in semiconductors. In 3D IC technology, direct bonding replaces solder balls to reduce RC delay and power consumption. To understand the potential of copper-silver alloys for direct bonding, it is very important to understand the properties and structure of copper-silver films. In the study, we investigate the microstructural evolution of the two-phase Cu-Ag alloy films during the annealing process with different doping concentrations and annealing temperatures for 1, 24 and 48 hours respectively. Oversaturated fine crystalline Cu-Ag alloy films with doping levels of 20 at.% and 40 at.% of Ag were fabricated using a magnetron sputtering system. The films were then annealed at four temperatures, i.e. 200°C, 250°C, 300°C, and 400°C to understand their thermal stability and property evolution. The results show that Cu concentration on the surface slightly increases with rising annealing temperature after annealing for 1 and 24 hours. But when the annealing temperature increased to 400°C, the rich Ag, instead of Cu, was accumulated to the surface of the films. In addition, Oversaturated solid solution films were annealed at 3 different vacuum levels ( $1 \times 10^{-6}$  torr,  $5 \times 10^{-3}$  torr, and 760 torr). The microstructural and property evolution during annealing and the corresponding mechanism will be discussed in detail.

**MB-ThP-20 Multifunctionality in Frequency Tuning of PMN-PT/Ni-Mn-In Integrated Film Bulk Acoustic Wave Resonator for Flexible MEMS Applications, Diksha Arora [diksha@ph.iitr.ac.in], Davinder Kaur,** Indian Institute of Technology Roorkee, India

Flexible and tunable bulk acoustic wave (BAW) resonators are opening new possibilities in flexible MEMS, wireless devices, and wearable magnetic sensors. This work presents a highly adaptable thin-film BAW resonator constructed with a PMN-PT piezoelectric layer positioned between magnetostrictive Ni-Mn-In electrodes on a flexible Ni substrate. This device, operating at a resonance frequency ( $f_R$ ) of 5.31 GHz, demonstrates significant tunability via both magnetic and electric fields. A magnetic field of 1200 Oe produces an  $f_R$  shift of approximately 450 MHz, achieving a sensitivity of around 3.75 Hz/nT and an impressive 9.6% tunability. Similarly, a 10 V DC bias yields an  $f_R$  downshift of roughly 360 MHz, with electric field sensitivity and tunability measured at about 36 Hz/ $\mu$ V and 6.8%, respectively. The device's resonance performance aligns with the modified Butterworth-Van Dyke model, and its quality and reliability remain intact through 3,000 bending cycles, underscoring its potential in advanced flexible electronics, tunable MEMS, and magnetic sensors.

**MB-ThP-21 Fabrication and Properties of Zinc Oxide Thin Film Prepared by Thermal Evaporation Method, Bassel Abdel Samad [bassel.abdel.samad@umoncton.ca], Zackaria Kabore,** Université de Moncton, Canada

Thin films of ZnO were deposited with a thickness of 50 nm using the thermal evaporation technique at different substrate temperatures during the deposition process. Optical measurements of transmittance and reflectance were performed using a spectrophotometer, and the film thickness was characterized using spectroscopic ellipsometry. Based on these measurements, the bandgap was calculated: it is 3.68 eV for the sample at room temperature and 4 eV for the other temperatures. Additionally, the electrical properties were characterized using an electrometer and a four-point probe. The resistivity values for the sample were found to be in the order of gighohms ( $G\Omega$ ), and conductivity increased with rising temperature. Finally, the activation energy was calculated for a metallic sample with a Zn phase.

**MB-ThP-22 High-Performance Methyl Mercaptan Gas Sensor based on Tellurene Nanowires for Breath Analysis Application, Yeonjin Je [jejinjin7@gmail.com], Sang-Soo Chee,** Korea Institute of Ceramic Engineering & Technology, Republic of Korea

Tellurene, 2D semimetallic material composed of tellurium atoms, exhibits exceptional sulfur compound gas sensing capabilities due to its strong affinity and a high hole mobility of  $2000 \text{ cm}^2/\text{Vs}$ . These distinct properties enable a rapid gas response time even at room temperature, in contrast to metal oxide-based gas sensors operating above  $300 \text{ }^\circ\text{C}$ . Among sulfur compound gas molecules, methyl mercaptan ( $\text{CH}_3\text{SH}$ ) is a representative odor gas molecule and a biomarker for diagnosing halitosis disease. However, its sensing detection properties have not yet reported. Here, we investigated  $\text{CH}_3\text{SH}$  sensing characteristics of the tellurene nanowire-based

sensor at room temperature. These gas responses increased from 52% (RH 0%) to 179% (RH 80%), with a faster response time of 24.5 s even under humid conditions. Furthermore, a superior limit of detection (LOD) of 18 ppb was achieved even at RH 80% for the first time. These noticeable detection performances are attributed to the synergistic interaction between water molecules and the surface of tellurene. We finally demonstrated a breath analysis module incorporating our Tellurene-based sensor to prove the feasibility for breath analysis application. This sensing platform represents a significant step toward practical gas sensors for oral health monitoring, combining high sensitivity, fast response, and humidity-enhanced performance to ensure reliable operation in real-time breath analysis.

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**MB-ThP-23 Enhanced Electrochemical Performance and Stability of Zinc-Ion Batteries Using Tellurium Nanowires, Hyun Tae Kim [qscft8536@gmail.com],** Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea; Gyeong Hee Ryu, Gyeongsang National University, Republic of Korea; Sang-Soo Chee, Korea Institute of Ceramic Engineering and Technology (KICET), Republic of Korea

Aqueous zinc-ion batteries (ZIBs) have attracted significant attention as a promising technology for next-generation energy storage systems due to their safety, environmental friendliness, and high cost-effectiveness. However, practical applications of ZIBs face critical issues including dendrite growth, corrosion, and dissolution of the metallic Zn anode. Additionally,  $\text{MnO}_2$ -based cathodes suffer from poor wettability and low electrical conductivity, leading to significant performance degradation.

1D tellurium (Te) nanowires exhibit a good electrical conductivity with a good chemical stability, enhancing ZIB performances. Furthermore, Te atoms can electrochemically interact with Zn ions, leading to improved energy storage performance.

Here, we introduce 1D Te nanowires as a conductive additive for  $\text{MnO}_2$  cathodes and as an anode protective coating layer, aiming to enhance the energy storage performance in ZIB.

First, Electrochemical analysis revealed that the integration of Te nanowires into the  $\text{MnO}_2$  cathode significantly reduced charge transfer resistance while simultaneously enhancing energy storage performance. This improvement originates from the intrinsic 1D structure of Te nanowires, which facilitates better electron pathways for faster charge transport.

Second, Te nanowire coating on anode surface effectively suppressed dendrite formation and promoted uniform nucleation, resulting in enhanced cycling stability. The modified Zn anode exhibited capacities ranging from 344 to 160 mAh/g at current densities ranging from 0.3 to 2.0 A/g, while maintaining excellent stability over 200 cycles.

This study demonstrates that Te nanowires in both the  $\text{MnO}_2$  cathode and Zn anode systems significantly enhance the electrochemical performance of ZIBs. This approach makes it a promising approach for next-generation aqueous ZIBs.

#### Acknowledgement

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**MB-ThP-24 Development of Functional Insulation and Wear Protection Layers for Coating Sensors, Martin Welters [welters@kcs-europe.com], Rainer Cremer,** KCS Europe GmbH, Germany

The mobility sector is one of the main emitters of greenhouse gases. Therefore, providers of mobility services and systems in particular are facing a profound transformation process towards climate neutrality. An important driver on the way to emission-free production is circular production. It enables a significantly lower primary resource requirement and thus reduced environmental impact. The overarching aim of the project is to improve the  $\text{CO}_2$  and environmental balance of structural and hybrid components by implementing a consistent increase in efficiency, the use of recyclates and a weight optimized component design.

One sub-project of the association is concerned with the development and design of sensory tool inserts for in-situ temperature measurement during the manufacture of automotive components from recycled materials. The sensory layer system consists of several individual layers (sensor layer,

electrical insulation layer and wear protection layer) which are applied on top of each other as a layer stack. KCS Europe is responsible for producing the insulation and wear protection layers. Vacuum coating processes such as physical vapor deposition or plasma-assisted chemical vapor deposition are used for this purpose. An essential requirement is usually that the coatings must meet the durability criteria required for the application in addition to the sensory requirements, especially for the use of polymer melts with recycled material components. In cooperation with the partners, new layer systems are being tested and systems are being provided for large-scale implementation.

**MB-ThP-25 Sub-10nm Superlattice HZO on CMP-Planarized Metal Surfaces Achieving High Remanent Polarization and Endurance**, *Zefu Zhao, Dun-Bao Ruan*, FZU-Jinjiang Joint Institute of Microelectronics, College of Physics and Information Engineering, School of Advanced Manufacturing, Fuzhou University, China; *Qian Cheng Yang [455783022@qq.com]*, FZU-Jinjiang Joint Institute of Microelectronics, College of Physics and Information Engineering, School of Advanced Manufacturing, Fuzhou University, Fuzhou University, China; *Kai-Jih Gan*, FZU-Jinjiang Joint Institute of Microelectronics, College of Physics and Information Engineering, School of Advanced Manufacturing, Fuzhou University, China; *Kuei-Shu Chang-Liao*, Department of Engineering and System Science, National Tsing Hua University, Taiwan

This work presents a novel approach to fabricating high-performance ferroelectric capacitors through atomic layer deposition (ALD) of sub-10nm  $\text{Hf}_{0.5}\text{Zr}_{0.5}\text{O}_2$  (HZO) superlattices on chemically-mechanically polished (CMP) metal electrodes. The ultra-flat electrode surface (RMS roughness = 0.3 nm) enables precise control of crystallographic orientation, as confirmed by electron diffraction patterns showing c-axis alignment of orthorhombic-phase HZO along the deposition direction.

The optimized flat electrode system demonstrates superior interface quality with HZO, achieving a high remanent polarization ( $2P_r = 63 \mu\text{C}/\text{cm}^2$ ) in the sub-10nm thickness regime.

The ALD-grown HZO superlattice architecture, combined with CMP planarization, enables uniform electric field distribution. This interfacial engineering strategy results in outstanding endurance characteristics, maintaining 90% of initial polarization ( $56 \mu\text{C}/\text{cm}^2$ ) through  $1 \times 10^{12}$  switching cycles.

**This study establishes a manufacturable pathway for implementing high-performance ferroelectric memories in advanced nodes, demonstrating the critical role of metal electrode engineering in achieving reliable ferroelectricity in ultrathin HZO films.**

**MB-ThP-26 The duality of Thermal and Magnetic Properties of Ni-Ta Thin Films: A New Generation of Sensing Devices**, *Armando Ferreira [armando.f@fisica.uminho.pt]*, *Filipe Vaz, Cláudia Lopes*, University of Minho, Portugal

Nickel-Tantalum (Ni-Ta) thin films have emerged as promising candidates for multi-sensing applications, combining electrical, magnetic, and thermoelectric functionalities. In this study, Ni-Ta nanostructures were synthesized via DC magnetron sputtering and integrated into a prototype to evaluate their dual capability: sensing temperature variations and generating an electrical potential under a constant magnetic field. By tuning the Ta content, three compositional groups were identified, significantly affecting their structural and functional properties. Ni-rich films exhibited the lowest sheet resistance ( $\sim 14 \Omega/\text{sq}$ ), while increasing Ta content induced higher magnetic disorder and enhanced the temperature coefficient of resistance (TCR), reaching  $5.43 \times 10^{-1} \text{ K}^{-1}$  for a Ta/Ni ratio of 0.48. These results highlight the potential of Ni-Ta thin films as functional surfaces for thermoelectric energy harvesting and multi-sensing applications, making them promising materials for next-generation sensor technologies.

**MB-ThP-27 Electrical and Physical Properties of Dual-Active Channel TFTs Composed of Controlled Hf Doped InGaSnO Layer and an InGaSnO-Only Layer**, *Seungjin Kim [epicus87@naver.com]*, *Byoungdeog Choi*, Sungkyunkwan University (SKKU), Republic of Korea

In this study, a dual-channel layer TFT was fabricated using  $\text{HfO}_2$  and IGTO co-sputtering, and its electrical and physical properties were analyzed. Enhancing the reliability of amorphous metal oxide (AOS) based TFTs by strengthening metal-oxygen bonds through doping to reduce oxygen vacancies has been extensively studied. However, some reliability improvements achieved through doping have also been observed to cause side effects, such as reduced mobility and decreased on-current. To address these issues, this study fabricated TFTs with a dual-layer structure consisting of a pure InGaSnO layer and a Hf-doped layer, and examined

their electrical and physical properties. Through the dual-layer channel structure, we were able to achieve both the high mobility characteristics of IGTO-only TFTs and the reliability improvement effects of the Hf-doped layer. The reliability changes were evaluated by measuring bias stress (PBS, NBS, PBIS, NBIS) according to the Hf doping concentration in the doped layer, and physical property changes were analyzed through optical transmittance, XPS, UV-vis, and AFM measurements. This study suggests an optimal device fabrication method that can improve the reliability issues caused by stress, a persistent problem in oxide semiconductors, without performance degradation.

**MB-ThP-28 3D Structured Local Thin Film Deposition by Direct Atomic Layer Deposition (DALP™)**, *Mira Baraket [mbar@atlant3d.co]*, ATLANT 3D Nanosystems, Denmark

Advancements in chemical and physical deposition techniques for thin films and coatings are paramount for academic research and industrial applications in many technologies such as electronics, energy, and MEMS. Recent trends point to deposition technologies that combine flexibility, scalability, and material versatility. While traditional methods like Chemical Vapor Deposition (CVD) and Atomic Layer Deposition (ALD) offer high-quality film deposition, they often face challenges in patterning, complex structure fabrication, and process adaptability. Overcoming these limitations typically requires additional pre- or post-processing steps (such as lithography), which increase both processing time and cost, limiting their efficiency for next-generation applications.

Here, we introduce Micro Direct Atomic Layer Processing ( $\mu\text{DALP}^{\text{TM}}$ ), a novel, atmospheric-pressure, direct-write deposition technology that expands ALD into localized, high-precision thin film printing (Figure 1). Unlike conventional ALD,  $\mu\text{DALP}^{\text{TM}}$  enables complex structured coatings and seamless material transitions. Moreover, it allows deposition in ambient pressure, eliminating vacuum-related throughput limitations, and eliminates the need for lithography for some applications, significantly enhancing scalability for industrial applications. In particular,  $\mu\text{DALP}^{\text{TM}}$  allows 3D designs with sub-nanometer control over the thickness profile of the film (Figure 2), making structures such as gradients, wells, and combs accessible easily.

$\mu\text{DALP}^{\text{TM}}$  adaptability and versatility open new possibilities for designing, developing, and producing next-generation thin film-based devices. By leveraging  $\mu\text{DALP}^{\text{TM}}$ 's capability for pre-programming the print shape and material transitions during deposition, we significantly accelerate device validation and optimization, dramatically reducing R&D costs.

In this talk, we will present the key advantages of  $\mu\text{DALP}^{\text{TM}}$  for disruptive devices, multi-material integration, rapid material discovery, and direct-write patterning of functional thin film

**MB-ThP-29 Effect of Amino Ligands of Aminosilane Precursors in Low-Temperature Silicon Nitride Plasma-Enhanced Atomic Layer Deposition (PEALD) for Moisture Barrier Films**, *Hyeonjin Choi [hyonjin0918@gmail.com]*, *Jinmyeong Kim, Youngju Ko, Heeyeop Chae*, Sungkyunkwan University (SKKU), Republic of Korea

In this work, the effect of amino ligands in aminosilane precursors on low-temperature plasma-enhanced atomic layer deposition (PEALD) of silicon nitride ( $\text{Si}_3\text{N}_4$ ) for moisture barrier films was investigated. Silicon precursors including (tert-butylamino)dimethylsilane (TBADMS), bis(tert-butyl)aminosilane (BTBAS), and tris(dimethylaminosilane) (TDMAS) were compared in the PEALD process. TBADMS contains one tert-butylamine ligand, BTBAS contains two, and TDMAS contains three dimethylamine ligands. Quadrupole mass spectrometry (QMS) was used to analyze reactive species during the precursor dosing step. For TBADMS and BTBAS, the detected species included H,  $\text{CH}_x$ ,  $\text{SiH}_x$ , tBu, and NHTBu, whereas for TDMAS, H,  $\text{CH}_x$ , and  $[(\text{CH}_3)_x\text{N}]_y\text{Si}$  were identified. The radicals CN, NH,  $\text{N}_2$ , and H were identified for all three precursors using optical emission spectroscopy (OES) during the  $\text{NH}_3$  plasma process. TBADMS has fewer amino ligands than BTBAS and TDMAS, enabling efficient silicon delivery through rapid dissociation. This feature minimizes precursor adsorption issues caused by the larger molecular sizes of BTBAS and TDMAS, resulting in differences in growth per cycle (GPC) [1,2]. TBADMS exhibits the highest GPC (0.7 Å/cycle), a high N/Si ratio (1.23), the lowest water vapor transmission rate (WVTR) of  $5.695 \times 10^{-3} \text{ g}/\text{m}^2\text{day}$ . These results indicate that a lower number of amino ligands reduces steric hindrance, enhances the N/Si ratio, and lowers WVTR in  $\text{Si}_3\text{N}_4$  films. This work supports the development of high-quality thin-film silicon nitride for moisture barrier applications in flexible OLED encapsulation.

**MB-ThP-30 Morphology Sustainable Synthesis of Calcium Phosphate 1D Nanostructures via Electrospinning for Advanced Functional Applications,** *Yao Mawuena Tsekpo, Weronika Smak*, Department of Engineering Materials and Biomaterials, Faculty of Mechanical Engineering, Silesian University of Technology, Poland; *Adrian Radoń, Łukasiewicz Research Network- Institute of Non-Ferrous Metals, Poland; Paweł Jarka, Tomasz Tanski [tomasz.tanski@polsl.pl]*, Department of Engineering Materials and Biomaterials, Faculty of Mechanical Engineering, Silesian University of Technology, Poland

Calcium phosphate compounds are a sustainable material with applications in biomedicine and environmental remediation. Among these compounds, calcium pyrophosphate can be prepared from biogenic materials; however, its fabrication into one-dimensional nanostructures via electrospinning remains understudied. This work presents a novel method for synthesizing calcium pyrophosphate nanowires using *Galatea paradoxa* clamshells as a calcium source. The process integrates electrospinning and sol-gel techniques to achieve 1D nano calcium pyrophosphate and aims to elucidate the influence of temperature on the process. Thermogravimetric analysis (TGA), Scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) were employed to characterize the nanostructures. Calcination at 600 °C reveals the formation of wire-like structures at the nanoscale with diameters ranging from 96 – 296 nm. XRD analysis confirmed the presence of  $\beta$ -calcium diphosphate [1001556], corroborating the presence of calcium pyrophosphate and aligning with the Fast Fourier Transform (FFT) diffraction patterns obtained in TEM. These findings indicate the successful formation of 1D nanostructures of calcium pyrophosphate. The observed structure and morphology of the prepared nanostructure exhibit properties suitable for application in bone regeneration and biomedicine, adsorption of harmful heavy metals, and as a host material for semiconductors in creating sustainable catalysts.

**MB-ThP-31 Investigation of Optical Constants in Nanostructured MoS<sub>2</sub>, ws<sub>2</sub>, and MoS<sub>2</sub>-WS<sub>2</sub> Thin Films by Spectroscopy Ellipsometry,** *Prachi Gurawal [prachi@ic.iitr.ac.in]*, Indian Institute of Technology Roorkee, India

The material structure-property relationships are crucial for the optimization and integration to enable the manipulation of material characteristics, such as electrical and optical properties. This work explored the synthesis and controlled growth of molybdenum disulfide (MoS<sub>2</sub>), tungsten disulfide (WS<sub>2</sub>), and the composite of both MoS<sub>2</sub>-WS<sub>2</sub> as a thin film in a single step using pulsed laser deposition (PLD). The morphology of the thin films was analyzed using scanning electron microscopy (SEM), revealing distinct surface features for each film. The topography with surface roughness and elemental composition has been investigated employing atomic force microscopy and X-ray photoelectron microscopy, respectively. Spectroscopic ellipsometry (SE) has been used to determine optical dispersion, such as extinction coefficient  $k$ , refractive index  $n$ , and optical bandgap under wavelength range 246-1688 nm. The experimentally determined SE data were fitted with the theoretical Drude-Lorentz and Bruggeman effective approximation model.

**MB-ThP-32 Optical and Protective Coatings Synthesized by Magnetron Sputtering,** *Eric Aubry, Pascal Briois [pascal.briois@utbm.fr]*, FEMTO-ST, France

The consortium of Opti-Reve project is composed by Surcotec and HE-Arc for the Swiss part and Gaggionne and UTBM for the French part. This project aims to develop a new technological solution (optical and protective coatings) in order to improve the quality of optical polymer components thanks to new functionalities brought to the surface by PVD technology, notably the corrosion resistance and the wear, as well as the brightness.

As part of this study, we first theoretically defined the material presenting the best reflection for the application and its thickness. The aluminium offers the best compromise between optical performance and cost production. With a thickness of about 50 nm, its reflection is only lowered by a few percent compared to that obtained with a silver mirror. In order to protect it from external environmental aggressions, a transparent layer such as aluminum oxide or nitride and also silicon oxide or nitride is implemented. Optical modeling reveals that the  $a^*$  and  $b^*$  components are lowest for thicknesses of about 125 nm and 350 nm. The importance of thickness will be studied in terms of its protective properties and corrosion resistance.

From the experimental point of view, the films were sputtered by magnetron sputtering from metallic targets in a neutral argon atmosphere for the reflective layer, then in a reactive atmosphere for the protective

layer. First, the stability of the Al-O, Al-N, Si-O and Si-N systems is studied for fixed conditions of plasma gas flow rate and current dissipated on the target. Once the reactive gas flow rates are determined for the synthesis of ceramics, the bilayer thin films is synthesized under specific substrate. The thin films are characterized by scanning electron microscopy, X-ray diffraction for the morphological and structural properties, by spectrophotometry for the optical properties, and with a nanohardness test for the mechanical properties.

Funding:

This project is carried out within the framework of the INTERREG VI France-Switzerland 2021-2027 European territorial cooperation program. The total cost of the project amounts to €571 663.57. It benefits from financial support from the EU through the European Regional Development Fund (ERDF) for €186 634.06, from the Swiss Federal INTERREG for €105 547.65 and from Swiss cantonal funds for an amount of €105 547.65 (Canton of Geneva = €40 322.58 and canton of Neuchâtel = €65 225.07)

**MB-ThP-33 Influence of Substrate Temperature on the Structural and Mechanical Properties of Ti-Zr Oxynitride Thin Films,** *Rogelio Ospina [rospinao@uis.edu.co], Sergio Andres Rincon, Jorge Hernan Quintero*, Universidad Industrial de Santander, Colombia

Titanium and zirconium oxynitrides have garnered significant attention due to their unique physicochemical properties. Titanium oxynitrides are extensively utilized in the medical and chemical industries owing to their exceptional combination of mechanical strength and chemical stability. Meanwhile, zirconium oxynitrides have attracted considerable interest in the electronics industry due to their promising electrical properties. These materials exhibit the advantageous characteristics of nitrides, such as high hardness and wear resistance, as well as those of metallic oxides, including tunable optical properties, chemical stability, and coloration effects. Given these attributes, the development of Ti-Zr oxynitride thin films is of particular scientific interest, especially in understanding how substrate temperature influences their structural and mechanical properties.

This study aims to investigate the effect of substrate temperature on the structural and mechanical characteristics of Ti-Zr-O-N thin films deposited via pulsed laser deposition (PLD). The deposition process was performed on commercial titanium substrates using an Nd:YAG excimer laser with a wavelength of 355 nm, a pulse duration of 8 ns, and a source energy of 150 mJ. The samples were subjected to controlled temperature variations in an oxidative atmosphere within a high-pressure chamber integrated with the X-ray Photoelectron Spectroscopy (XPS) system to assess surface chemical modifications. Furthermore, variations in the hardness of the substrate-coating system were evaluated using microindentation testing before and after oxidative treatment.

The microstructural evolution of the coatings was characterized using X-ray diffraction (XRD), while the surface morphology of the processed films was analyzed via Atomic Force Microscopy (AFM). The findings of this study provide valuable insights into the correlation between deposition parameters and the physicochemical properties of Ti-Zr oxynitride coatings, contributing to the optimization of their applications in advanced engineering fields.

**MB-ThP-34 Functionalization of SnO<sub>2</sub> Electron Transport Layer with Phosphonic Acid Derivative for Enhanced Perovskite Solar Cell Performance,** *Biplav Dahal [biplav.dahal@udc.edu], Akhil Prio Chakma, Hongmei Dang*, University of the District of Columbia, USA

Interfacial engineering is critical in optimizing charge transport, mitigating recombination losses, and improving the long-term stability of perovskite solar cells (PSCs). In this work, we explore the functionalization of the SnO<sub>2</sub> electron transport layer (ETL) with (2-chloro-2-phenyl-vinyl)-phosphonic acid (CPVPA), a phosphonic acid derivative, to enhance interfacial properties and device performance. CPVPA contains key functional groups that contribute to interface engineering: the  $-PO_3H_2$  group facilitates strong chemical bonding with SnO<sub>2</sub>, potentially passivating defect sites and tuning energy levels; the phenyl group may aid in charge transport and surface energy alignment; and the chlorine atom could introduce dipole effects or modulate the electronic environment, thereby improving band alignment with the perovskite absorber. Additionally, the structural stability provided by the phenyl group may further contribute to enhanced device stability. The impact of CPVPA modification was examined through structural and morphological characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM), and atomic force microscopy (AFM), which revealed improved perovskite crystallinity, enlarged grain sizes, and a more uniform film morphology with reduced surface roughness and pinholes. To further probe the chemical interactions and electronic structure changes at

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the SnO<sub>2</sub> interface, X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared spectroscopy (FTIR) are planned. Photovoltaic performance evaluations have demonstrated improved power conversion efficiency (PCE) for CPVPA-modified devices compared to unmodified controls. Additionally, preliminary stability studies suggest that CPVPA-modified perovskite film exhibits enhanced moisture resistance. This study highlights the potential of phosphonic acid-based interfacial engineering to improve efficiency and enhance the stability of PSCs. The findings contribute to ongoing efforts toward developing more reliable and scalable perovskite photovoltaics.

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