

Functional Thin Films and Surfaces

Room Golden State Ballroom - Session MB-ThP

Functional Thin Films and Surfaces (Symposium MB) Poster Session

MB-ThP-2 Porous Metal/Metal-Oxide Nanostructured Coatings Produced Using Gas Aggregation Sources of Nanoparticles as Recyclable SERS-Active Platforms, A. Hanková, D. Novák, N. Khomiakova, E. Kočíšová, M. Procházka, Ondřej Kylián (ondrej.kylian@matfyz.cuni.cz), Charles University, Prague, Czech Republic

Due to their low cost, chemical and thermal stability, and unique electronic, optical or bioresponsive properties, metal-oxides (MeO) have become almost irreplaceable materials in an impressive range of modern technologies, such as (photo)catalysis, sensing, detection, or energy harvesting. In many cases, the functional properties of MeO may be enhanced by their nanostructuring that increases the specific surface and facilitates physicochemical phenomena like adsorption and diffusion of chemical species. One possibility of producing these materials relies on the deposition of highly porous transition metal (e.g. Ti, V, Nb, W) nanoparticle films by magnetron-based gas aggregation sources followed by the subsequent annealing of such formed nanoparticle films that assures their controllable oxidation and crystallization. The aim of this study is to demonstrate that further improvement of the functional properties of MeO nanoparticle-based films may be achieved if they are decorated with sputter-deposited noble metal nanostructures. In this way, different functionalities intrinsic to metal-oxide and metal components may be successfully combined or enhanced. As shown in this study, such metal/MeO nanomaterials are highly interesting as novel platforms for surface-enhanced Raman spectroscopy (SERS), in which the noble metals act as highly SERS-active component, while the transition MeO due to its photocatalytic characteristics provides the possibility of highly effective recycling of the platforms after cleaning them with UV light irradiation.

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MB-ThP-4 A Carbon Nanotubes-Based Microwave Resonator for Ammonia Gas Sensing, Hsuan-Ling Kao (snoopy@mail.cgu.edu.tw), Y. Tsai, Chang Gung University, Taiwan

Carbon nanotubes (CNTs) have been used as gas-sensing material owing to their high specific surface areas and structural porosities that enable rapid responses and high sensitivity at room temperature. Fully inkjet printing technology promotes the green process using by digital controlled pattern in required location to offer fast, material saving, low cost, high substrate selectivity, and low annealing temperature. In this work, Inkjet-printed CNT films can be conferred with the appropriate resistance for embedding into transmission-type resonators for gas sensing by controlling droplet spacing (DS) and layer number. CNTs films as sensing layers and silver films as conductive layers to realize gas sensors using fully inkjet printing technology. Gas sensors, including resistive and microwave resonator sensors, were inkjet-printed on CLTE-MW to measure their response in the presence of ammonia. Gas responses of CNT films with regular electrode and interdigital electrode patterns were compared by resistive-type gas sensors. CNTs with the IDE pattern can provide large contact areas between the silver film and CNTs for the provision of more effective conductive paths, this resulting in stable sheet resistance and high response. The resistance of the sensing films embedded into the transmission-type microwave resonators should be as low as possible to avoid affecting loss. A microwave resonator consisting of two open-loop ring resonators coupled to each other by an interdigital structure was proposed as a microwave gas sensor. CNT films with the IDE pattern were embedded at the edge of the interdigital structure. The repeatability of the resonator under exposure to 700 ppm NH₃ for 20 cycles was examined. The exposure time to NH₃ gas at each step was 60 s and then, pure N₂ was injected into test chamber for 90 s at the recovery step. The average sensitivities of insertion loss and resonant frequency were 9.5 mdB and 353 kHz for 20 cycles, respectively. The results demonstrated that the CNT films with IDE pattern embedded in transmission-type microwave resonator provided two-dimensional response values in NH₃ sensing through electromagnetic transduction, thereby providing wireless sensor applications.

MB-ThP-5 Investigating 2D-Materials Using Correlative Spectroscopy & Microscopy, T. Nunney, Thermo Fisher Scientific, UK; James Lallo (james.lallo@thermofisher.com), Thermo Fisher Scientific, USA; P. Mack, R. Simpson, H. Tseng, Thermo Fisher Scientific, UK

Across a wide range of application areas, understanding the chemistry and structure of surfaces and interfaces is crucial. In the last fifty years, X-ray photoelectron spectroscopy (XPS) has become established as a one of the key techniques for measuring surface and interface chemistry, and advances in instrumentation have enabled it to keep pace with the requirements for both academia and industry. XPS can deliver quantified surface chemistry measurements, and by using depth profiling, an understanding of layer and interfacial chemistry, but the limit on spatial resolution for XPS can prevent it from determining how the surface structure is related to the measured chemical properties. For example, how the changing morphology of the surface during a depth profile could influence the measured composition would be challenging to determine using just XPS.

Other experimental techniques which are unable to match the surface selectivity of XPS are able to provide complementary information to extend the data from XPS. Electron microscopy can provide high resolution imaging, with elemental composition provided by energy dispersive X-ray microanalysis, but without the same surface selectivity seen with XPS or Auger electron spectroscopy (AES). This can be a perfect complement to XPS analysis, so long as the same points of interest can be identified. Molecular spectroscopy, such as FTIR or Raman, can also provide complementary information to XPS, albeit with different sampling depths, which can be extremely useful to validate measurements or confirm particular molecular structures using the wide range of spectral libraries available for those techniques.

In this poster, we will describe how a correlative approach using both surface analysis instrumentation and scanning electron microscopy can be used to characterize 2D nanomaterials. Samples of MoS₂ grown on Si substrates have been investigated using XPS, Raman and SEM to determine their composition and structure. To facilitate co-alignment of the analysis positions when moving between the instruments, special sample carriers and software alignment routines have been developed.

MB-ThP-6 CsPbI₃-Based Perovskite Thin Film Using All Vacuum Deposition Process, HYO SIK CHANG (hschang@cnu.ac.kr), M. Jeong, J. Park, Chungnam National University, Republic of Korea

We deposited CsPbI₃ films using a co-evaporation method, and optimized the film thickness and heat treatment. UV-vis and PL analysis confirmed the presence of a peak at 710nm wavelength, indicating the absorption and emission properties of the a-phase CsPbI₃ perovskite film. The use of vacuum co-deposition for CsPbI₃ deposition allows for excellent uniformity and thickness control, leading to optimized film thickness. To make inorganic CsPbI₃ perovskite solar cell, the phase change temperature must be lowered and a low phase change temperature of less than 200 °C is required. We have developed low phase change temperature CsPbI₃ with additive deposition. In this study, we manufactured a perovskite solar cell by combining the co-deposited CsPbI₃ perovskite with an inorganic charge transport layer using atomic layer deposition (ALD). ALD NiOx and SnO₂ films used as a hole transport layer and electron transport layer (ETL). Efforts are underway to apply vacuum co-deposition of FAPbI₃ and CsPbI₃ perovskite to tandem perovskite-Si solar cell applications.

MB-ThP-7 Synthesis and Characterization of AlCrTiZrSiW High Entropy Alloy Coating by High-Power Impulse Magnetron Sputtering, C. Chang, Ming Chi University of Technology, Taiwan; J. Tang, Lughwa University of Science and Technology, Taiwan; Bo-Ruei Lu (M11188027@mail2.mcut.edu.tw), J. Tsao, M. Lin, Ming Chi University of Technology, Taiwan; F. Yang, National Taiwan University of Science and Technology, Taiwan

High-entropy alloy coating feature high hardness, excellent thermal stability, and corrosion resistance. They have been considered as promising candidates for next-generation surface coating material because of their advantageous properties. In recent years, the popular high power impulse magnetron sputtering (HIPIMS) surface technology has attracted considerable attention due to the ability to produce coatings with excellent properties. It is preferable to replace high entropy alloy target with a co-sputtering method involving the use of more targets (single element metal target) simultaneously, which can greatly reduce the process cost.

In this study, AlCrTiZrSiW high-entropy alloy coating deposited on the various substrates (SKH-9 high-speed steel, SUS304 stainless steel, Si wafer)

by HIPIMS technology. To obtain the Non-equimolar high-entropy alloy coatings was adjusted by varying the output power of Al and CrSi target (Zr, TiSi, W target power was fixed). Detailed investigation was performed on the microstructure, mechanical properties and corrosion resistance of the resulting coatings. XRD and nanoindenter measurement results indicated that the coating exhibited an amorphous structure with a hardness value between 9.0 to 10.8 GPa. In addition, the coating with hydrophobic and corrosion resistance was verified via contact angle and electrochemical potentiostat test. The corrosion resistance of the AlCrTiZrSiW high-entropy alloy coating ($R_p=28.3 \Omega\text{cm}^2 \times 10^5$) is ~27 times that of the SUS304 stainless steel.

MB-ThP-9 Location-Dependent Super-amphiphobic Nano-Structured Films Deposited by Tubular Microwave Plasma, Ta-Chin Wei (tcwei@ccu.edu.tw), Y. Shen, Chung Yuan Christian University, Taiwan

Super-hydrophobic and oleophobic surfaces have attracted much interest for both fundamental research and practical applications. In this study, Teflon-like fluorocarbon films with different nano-structures were deposited on various substrates by microwave-generated C₂H₂F₄/CF₄ plasma. The reactor was a tubular quartz tube with diameter of 5 cm and length of 80 cm. The substrates were placed in 20 different locations along the gas flow direction in upstream region, discharge region, and afterglow region. It was found that the surface morphology of the deposited film was very location dependent. The fluorocarbon films deposited in upstream and afterglow region consisted of nano-particulate structure with F/C atomic ratio of about 2.0, namely the Teflon-like structure. However, the fluorocarbon film was rough and thick with a low F/C atomic ratio when substrate was located in the discharge region. Interestingly, Teflon-like fluorocarbon films with vertical nano-wall structure could be deposited only on substrates located in the end of upstream region and in the beginning of the afterglow region. It was also found that water contact angle on the Teflon-like nanowall or nano-particulated film was above 160° and the CH₂I₂ contact angle was above 140°. Moreover, by using the same operating parameters, we successfully deposited transparent super-amphiphobic fluorocarbon nanowall film onto various substrates such as glass, copper, polycarbonate, and etc. Moreover, we found that Teflon-like films with nano-wall structure could also be deposited onto various porous substrates. Finally, from the time evolution of the deposited film, the growth mechanism of nano-wall structure film was realized.

MB-ThP-10 Enhancing Oxygen Evolution Reaction Performance with Sputter-Deposited High Entropy Alloy Thin Film Electrocatalysts, Siang-Yun Li (m9810217@gmail.com), T. Nguyen, Y. Su, Y. Shen, C. Liu, J. Ruan, K. Chang, J. Ting, National Cheng Kung University, Taiwan

Thin film catalyst, giving a different morphology, provides a significant advantage over catalyst particles for gas evolution reaction. Taking the advantages of sputter deposition, we hereby report high entropy alloy (HEA) thin film electrocatalyst for oxygen evolution reaction (OER). We investigate the catalyst characteristics not only in its as-deposited state but also during and after the OER. For comparison, unary, binary, ternary, and quaternary thin film catalysts were prepared and characterized. The surface electronic structure modification due to the addition of a metal is studied experimentally and theoretically using density function theory calculation. We demonstrate that sputtered FeNiMoCrAl HEA thin film exhibits OER performance superior to all the reported HEA catalysts with robust electrocatalytic activity having a low overpotential of 220 mV at 10 mA cm⁻², and excellent electrochemical stability at different constant current densities of 10 and 100 mA cm⁻² for 50 h. Furthermore, we have investigated the microstructure transformation during the OER, which is important for the understanding of the OER mechanism provided by HEA electrocatalyst. Such finding would contribute to future catalyst design.

MB-ThP-11 Transition Metal Nitride Anti-Reflective Coatings, Barbara Schmid (barbara.schmid@tuwien.ac.at), B. Hajas, N. Koutná, TU Wien, Institute of Materials Science and Technology, Austria; J. Blaschke, TU Wien, Austria; P. Polcik, Plansee SE, Germany; P. Mayrhofer, TU Wien, Institute of Materials Science and Technology, Austria

Anti-reflective (AR) coatings are of high importance for our everyday lives in the field of optics, for example in visual aids and photography equipment. Lesser known, those coatings are also essential in the realm of photovoltaics like solar cells, because they are able to reduce the reflectivity of the material surface. There is a plethora of different design approaches to this topic. Within our work, we want to change the optical properties of hard TiC/TaC superlattice protective coatings without sacrificing superior mechanical properties. Using DC magnetron sputtering, we create nano-scale transition metal nitride-based (AlN and ZrN) thin films

exhibiting different material characteristics. We investigate the influence of deposition parameters and film thickness on the optical properties of our materials system. Apart from structural and morphological investigations and the determination and comparison of mechanical properties of our material systems, we conduct optical investigations using differential reflectance spectroscopy (DRS).

MB-ThP-12 Enabling Robust Chemical State Analysis of Sn-Based Perovskites via Auger Parameter Analysis in XPS, A. Wiczorek, Sebastian Siol (Sebastian.Siol@empa.ch), Empa – Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Sn-based perovskites exhibit compelling properties such as reduced toxicity and lowered band gaps over those purely based on Pb. As a result, they are of increasing interest for photovoltaic applications in single-junction and all-perovskite tandem applications.^[1]

For high performances, control of the oxidation state and interfacial chemistry is paramount, which can be determined using X-Ray photoelectron spectroscopy (XPS). However, the minor chemistry related shifts of the Sn core level emission complicate the analysis, especially for semiconducting materials. Here, surface band-bending as well as differences in the work function can be particularly pronounced.

In this presentation, we demonstrate that studies based on the modified Auger parameter α' provide a robust method to resolve different chemical states in Sn-based perovskites. Using a set of reference samples, we identified a high sensitivity to the halide, resulting in a shift of up to $\Delta\alpha' = 2$ eV between ASnI₃ and ASnBr₃-type polycrystalline perovskite thin-films.^[2] Observed dependencies of α' on the Sn oxidation state and local chemistry provide a framework that enables reliable tracking of degradation as well as X-site composition for Sn-based perovskites and related compounds. Recently, we successfully applied this framework on Sn-based perovskite nanocrystals to ensure the absence of Sn(IV) impurities upon optimized synthesis procedures.^[3]

The higher robustness and sensitivity of such studies not only enables more in-depth surface analysis of Sn-based perovskites than previously performed, but also increases reproducibility across laboratories. Due to the facile data analysis, this method is ideal for high-throughput studies that are increasingly being adopted in the development of new semiconducting materials.^[4]

References

- [1] H. Lai, J. Luo, Y. Zwirner, S. Olthof, A. Wiczorek, F. Ye, Q. Jeangros, X. Yin, F. Akhundova, T. Ma, R. He, R. K. Kothandaraman, X. Chin, E. Gilshtein, A. Müller, C. Wang, J. Thiesbrummel, S. Siol, J. M. Prieto, T. Unold, M. Stalterfoht, C. Chen, A. N. Tiwari, D. Zhao, F. Fu, *Adv. Energy Mater.* **2022**, *12*, 2202438.
- [2] A. Wiczorek, H. Lai, J. Pious, F. Fu, S. Siol, *Adv. Mater. Interfaces* **2023**, *10*, 2201828.
- [3] D. N. Dirin, A. Vivani, M. Zacharias, T. V. Sekh, I. Cherniukh, S. Yakunin, F. Bertolotti, M. Aebli, R. D. Schaller, A. Wiczorek, S. Siol, C. Cancellieri, L. P. H. Jurgens, N. Masciocchi, A. Guagliardi, L. Pedesseau, J. Even, M. V. Kovalenko, M. I. Bodnarchuk, *Nano Lett.* **2023**, *23*, 1914.
- [4] S. Zhuk, A. Wiczorek, A. Sharma, J. Patidar, K. Thorwarth, J. Michler, S. Siol, *Chem. Mater.* **2023**, *35*, 7069.

MB-ThP-13 Pvd Deposition of Tin Based Antimultipacting Thin Films for Applications in Particle Accelerators, Yanis Pisi (yanis.pisi@grenoble-inp.fr), CNRS, Université Paris-Sud, France

The multipactor phenomenon is a critical issue that can occur in particle accelerators. To improve the performance of components used in particle accelerators, we have chosen to develop a materials approach with innovative coatings.

The SEY is the ratio of the number of secondary electrons to the number of incident electrons (primary electrons). To avoid the multipactor effect, the ratio must be less than 1. Currently, most materials have an SEY greater than 1 [1]. The investigated coatings based on nitride or carbide titanium because the SEY ratio is intrinsically low [2,3]. My work consists to elaborate based TiN (TiO_xN_y, TiN, TiN_xC_y) thin films and study their properties. Another approach concerns the investigation of thin layers consisting of alternating layers of NbN and TiN. The preferred deposition method is PVD (Physical Vapor Deposition) by cathodic pulverisation. We will present the results obtained as a function of coating nature: (i) firstly, the physical properties (such as electrical properties by 4-point measurements) and chemical characterisations (such as the layer composition determined by XPS analysis); (ii) the values of secondary

electron emission yields at the fully conditioned state (see Table, the surface was conditioned by electron bombardment). In this work, we study the SEY without the effects of roughness, which is known to significantly influence the SEY.

Reference	Layer	Substrat	Roughness (nm)	SEY
This work	TiNC	Si	0,5	1,01
This work	Multilayer NbN/TiN	Si	1	0,99
[1]	TiNC	Si	High	0,97
[2]	TiZrVC	Si	High	0,93

Table: SEY values of different thin films obtained PVD

REFERENCES

- [1] N. Hilleret, SPS & LEP Performance Workshop, Chamonix, 2000.
 [2] P. C. Pinto et al., Particle Accelerator Conference, New York, 2011.
 [3] I. Montero, et al., Journal of Applied Physics, vol. 101, n° 11, p. 113306, juin 2007, doi: 10.1063/1.2736861 [https://doi.org/10.1063/1.2736861].

MB-ThP-14 Influence of Oxygen Partial Pressure and Temperature on the Optical and Electrical Properties of NiO_x Thin Films obtained by r.f. Sputtering, *E. Osorio-Urquiza, Francisco David Mateos-Anzaldo (dmateos@uabc.edu.mx), M. Curiel-Alvarez, R. Nedev, O. Pérez-Landeros, B. Valdez-Salas, N. Nedev*, Instituto de Ingeniería-Universidad Autónoma de Baja California, Mexico

Nickel oxide (NiO_x) thin films were deposited by r.f. magnetron sputtering on n-type silicon and corning glass substrates. The deposition conditions were 60 W of power during 6 minutes, a pressure of 5 mTorr and different substrate temperatures in the range of 25-200 °C. The partial pressure between O/Ar was varied between 0 and 4 %. Prior to deposition, the substrates were cleaned in an ultrasonic bath with acetone, isopropyl alcohol and deionized water for 5 min each and dried with high-purity nitrogen after each step. Besides, the target was pre-sputtered for 15 min. MOS capacitors were fabricated by deposition of gold and aluminum as top and back contacts using thermal evaporation. The thickness and optical constants of the films were obtained by spectroscopic ellipsometry. Measurements of current-voltage (I-V) and capacitance-voltage (C-V) dependences were carried out to study the effect of temperature and oxygen partial pressure on the electrical properties of the NiO_x thin films. The obtained results indicate that it is possible to obtain high quality films at low r.f. power that are viable for applications in electronic devices.

MB-ThP-17 Effect of the R.F. Power and Thermal Annealing on the Properties of NiO_x Thin Films, *Roumen Nedev (roumen.nedev@uabc.edu.mx), F. Mateos-Anzaldo, M. Curiel-Alvarez, O. Pérez-Landeros, E. Osorio-Urquiza, B. Valdez-Salas, N. Nedev*, Instituto de Ingeniería-Universidad Autónoma de Baja California, Mexico

NiO_x thin films were deposited by RF sputtering in Ar atmosphere on n-Si and glass substrates. During the deposition the RF power was varied between 5 W and 60 W, while the deposition time was fixed at 9 min. Three deposition temperatures of 25 °C, 50 °C and 100 °C were used. The samples deposited on Si were separated in three groups. The first group was furnace annealed at 450 °C in N₂ atmosphere for 1 h. The second one was treated by Rapid Thermal Annealing (6 min, 550 °C), while the third group was kept as control. Metal/NiO_x/n-Si heterostructures were prepared by deposition of Au electrodes through a mask.

The thicknesses and optical constants of the layers were determined by spectroscopic ellipsometry. XRD measurements were used to determine the effect of deposition temperature and thermal annealing on the crystallinity of the films. The Au/NiO_x/c-Si structures were electrically characterized by current-voltage (I-V) and capacitance-voltage (C-V) measurements. The I-V dependences showed formation of p-n heterojunction diodes with properties, which depend on the r.f. power, deposition temperature and annealing.

MB-ThP-20 Nano Indentation Pop-in Response on Basal Plane of 4H Hexagonal SiC Surface, *Jacob C. Huang (jacobc@faculty.nsysu.edu.tw)*, National Sun Yat-sen University, Taiwan

The nano-scaled mechanics for the hexagonal 4H SiC single-crystal surface (with a bandgap of 3.26 eV) is examined by using nanoindentation testing on the {0001} basal plane. The 4H SiC material was prepared by Prof. M. C. Chou's lab via the Czochralski process. The as-grown crystal surface has been examined carefully by X-Ray diffraction (XRD) to confirm the 4H hexagonal structure, with the basal plane lying on the horizon plane and the c-axis parallel to the growth direction. The (0004) peak at 2 θ =35.5° is the only peak appeared, ensuring the well-grown surface orientation with minimum defects. The lattice parameters, a and c, are determined to be

0.3073 and 0.1006 nm, respectively. Through the analysis of XRD rocking curves, it is confirmed that there should be minimum defects inside the as-grown SiC surface.

Nanoindentation tests were performed using the continuous stiffness method (CSM), up to a maximum depth of ~950 nm on the (0001) basal plane surface. The average elastic modulus and hardness calculated from depth ranging from 300~800 nm over nine indents were ~500 GPa and ~42.5 GPa, respectively. In addition, the first few pop-in loads and displacements are captured from the deviations from a perfect Hertzian contact curve fitted to the load-displacement curve. By using rough estimation for the yield stress from hardness by a factor about 2.5 (Tabor's assumption), we estimate the yield stress to be about 42.5/2.5 ~ 17.0 GPa. The first pop-in loads, pop-in hardness, and pop-in stresses can all be measured. The first pop-in stress is usually termed as the incipient stress, associated with the first initiation of the activation of dislocations (nucleation or gliding of dislocations). The average incipient stress for the first dislocation activity is about 16.1 GPa, slightly below the overall yield stress. From the first pop-in displacement, about 10 nm, it is likely to be a result of the micropipe threading screw dislocations (with a Burger's vector of c-axis, namely, ~1 nm). This suggests that the first pop-in could be caused by these screw dislocations gliding for 10 Burger's vectors. The understanding of dislocation incipient pop-in as a function of applied load would give the insight for subsequent influence for various functional properties of 4H SiC.

MB-ThP-21 2D Chemical Mapping of Nanoscale Functional Material using Soft X-ray STXM, *Namdong Kim (east@postech.ac.kr)*, Pohang Accelerator Laboratory, Republic of Korea

Soft x-ray nanoscopy employing the scanning transmission x-ray microscope (STXM), which can provide chemical structural information of materials at tens of nanometer scale, has become a powerful study in analytical microscopic research. The nanoscopy beamline in the Pohang Light Source is operating currently at the optimum condition in its focused beam size ~30 nm and photon energy resolution < 0.1 eV in the soft x-ray energy range (200-1650 eV).

Basically, based on different x-ray absorption contrast depending on chemical states, we have studied structural and electronic properties of nanoscale defects or domains formed on various two-dimensional (2D) materials including graphene, hBN, MoS₂, WSe₂, and topological insulators such as Bi₂Se₃ thin film as well as energy materials. We will here introduce briefly the 2D nanoscale chemical mapping of such functional materials.

Moreover, as for Li-ion batteries, we investigated in-situ annealing effect on Ni-rich NCM cathode materials from RT to high temperature by measuring Ni, Co, Mn L₃, and O K-edge absorption spectra. In-situ thermal degradation is induced by annealing. And oxygen reduction is preferentially observed on the edges of smaller particles at 400 °C.

KEYWORDS: 2D chemical mapping, soft x-ray nanoscopy, STXM, 2D materials, energy materials

MB-ThP-23 Exploring HiPIMS-Deposited TixN and TixAl_yN Films for Oxygen Evolution Reaction (OER) Catalysis, *Wan-Yu Wu (wywu@nuu.edu.tw)*, National United University, Taiwan; *J. Ting*, National Cheng Kung University (NCKU), Taiwan; *Y. Tsai*, National United University, Taiwan; *S. Li*, National Cheng Kung University (NCKU), Taiwan; *Y. Lin*, National Chung Hsing University, Taiwan

Sustainable energy technologies are fundamentally linked to electrochemical reactions, notably the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), which are critical in electrolysis cells. OER, characterized by its sluggish kinetics, is a bottleneck in the efficiency of molecular oxygen generation, highlighting the necessity for advanced catalyst development. While precious metals like Ir, Ru, and their oxides (IrO₂, RuO₂) are prevalent in current research, their scarcity, cost, and low durability limit practical applications, urging the discovery of viable alternatives. This study explores metal nitrides, specifically TixN and TixAl_yN films deposited on nickel foam using High Power Impulse Magnetron Sputtering (HiPIMS), as potential OER catalysts. Despite traditionally higher OER overpotentials, these heterostructured metal nitrides demonstrate promising activity and remarkable long-term stability, even in strong alkaline electrolytes. The capability of producing these films with precise crystalline structure and stoichiometry via scalable magnetron sputtering positions them as compelling substitutes to conventional precious metal catalysts, showing lower overpotentials compared to commercial RuO₂ and paving the way for their application in large-scale clean energy solutions.

MB-THP-24 Characterization of Protective AlCrON Thin Films for Application on Sensor Thin Films in Fused Layer Modeling Processes, *W. Tillmann, Julia Urbanczyk (julia.urbanczyk@tu-dortmund.de), M. Mainz, P. Bengfort, N. Lopes Dias, TU Dortmund University, Germany*

In plastic processing, the use of sensor thin films is gaining interest for inline measurement to ensure stable process control. However, due to the corrosive and abrasive characteristics of molten plastics, the application of an appropriate protective coating becomes imperative to ensure the functionality of the sensor films. AlCrON thin films demonstrate favorable protective attributes for this purpose. The tribo-mechanical and electrical properties are inherently influenced by the oxygen content. Therefore, a systematic variation of O₂ gas flow rates (10 to 30 sccm in steps of five) during the mid-frequency magnetron sputtering process was employed resulting in the O contents rise from 12.2 at.-% for 10 mln O₂ to 57.6 at.-% for 30 mln O₂. Simultaneously, a change of a polycrystalline structure containing CrN, Cr₂N, and hexagonal AlN to an amorphous structure with increasing O content for AlCrON is observed. This affects the tribo-mechanical properties. The highest polycrystallinity was reached at 25.2 at.-% O resulting in a H/E maximum, with a maximum in hardness of (37.6 ± 2.8) GPa and an elastic modulus of (361.2 ± 20.7) GPa. Here, also the lowest coefficient of friction (CoF) at elevated temperatures was reached with 0.43 against polypropylene (PP) and 0.23 against polyamide (PA). The low CoF correlates with a lower wetting ability of the AlCrON thin film. Regarding the electrical properties AlCrON thin films show insulating characteristics dependent on the O content. The electrical resistance increases with higher O content while the dielectric strength tends to increase with higher crystallinity.

A first attempt to apply a functional copper layer within an Al₂O₃ and AlCrON system was successful, showing promise for enhanced functionality. However, further investigation is needed to fully understand its potential and optimize its performance.

The results show that AlCrON thin films offer promising protective qualities for sensor applications in plastic processing. By adjusting the oxygen content, their tribo-mechanical properties can be optimized for reduced friction and enhanced durability, while their insulating properties are promising for maintaining the functionality of the sensors.

MB-THP-25 Synthesis of Highly-Textured Wurtzite AlN Thin Films on Nitrogen-Terminated Metal Surfaces, *Oleksandr Pshyk (oleksandr.pshyk@empa.ch), J. Patidar, S. Zhuk, S. Siol, EMPA (Swiss Federal Laboratories for Materials Science and Technology), Switzerland*

AlN thin films in wurtzite structure are used in a broad range of piezoelectric applications such as microelectromechanical systems (MEMS) due to their high acoustic velocity, chemical resistance, thermal stability and linear piezoelectric response. Especially, for piezoelectric applications AlN thin films have to demonstrate a high crystalline quality and exhibit a pronounced out-of-plane c-axis orientation.

Typically, this necessitates the growth at elevated temperatures. It has been demonstrated that deposition on certain metallic substrates can improve the crystallinity and texture of sputter-deposited AlN [1]. However, despite the widespread application of metallic templates for the deposition of AlN, only few systematic studies of the stabilization mechanisms are reported.

In this work, we present a systematic study of AlN thin film growth on chemically and structurally different metallic seed layers. The deposition sequence used in these experiments is pre-sputter metal targets in Ar (1)/ RF magnetron sputter deposition of a metal layer (2)/ pre-sputter Al-target in Ar (3)/ pre-sputter Al target in Ar+N₂ (4)/ AlN deposition by reactive DCMS (5). All steps are performed at room temperature to eliminate the effects of temperature while (4) ensures metal layer exposure to N₂ for 1 min.

We demonstrate that AlN films grown on different low-work function metals show markedly improved texture and crystallinity compared to films grown on glass. To differentiate between either a chemical or a structural templating effect we vary the metal-layer thickness from 115 nm down to less than 1 nm and to tune their crystallinity and their substrate coverage. The AlN grain size strongly correlates with the glass substrate coverage by the metal layers. However, it appears much less important if the metal templates are crystalline or amorphous. It is therefore likely that the stabilization mechanism is chemical in nature.

UHV-transfer XPS studies on freshly sputtered metal layers demonstrate the formation of a thin layer of metal nitride on the surface of W and Al thin

films upon short-term exposure to the N₂-containing process gas, even at room temperature. The conditions were chosen equivalent to the environment in the sputter chamber leading up to the AlN deposition. We therefore assign the promotion of AlN nucleation and growth on low-work function metal substrates to the chemical effect set by a complete N₂ substrate surface termination and the associated preferential c-axis polarization. The revealed mechanism extends the fundamental understanding of the AlN growth process on different metallic substrates beyond strain-driven mechanism or AlN/metal interface symmetry considerations.

MB-THP-26 Synthesis of Epitaxial α -Ga₂O₃ Thin Films on Sapphires by Pulsed Laser Deposition, *Heungsoo Kim (heungsoo.kim.civ@us.navy.mil), M. Mastro, A. Piqué, Naval Research Laboratory, USA*

Gallium oxide (Ga₂O₃) is an emerging ultrawide-bandgap semiconductor for high power electronics and ultraviolet photonics. Among various Ga₂O₃ crystal structures, a α -Ga₂O₃ has gained a great interest because its bandgap (>5.3 eV) is far wider than that of common β -Ga₂O₃ (4.5 – 5.3eV). Thermodynamically stable β -Ga₂O₃ thin films have been successfully synthesized by various deposition techniques. However, the growth of metastable α -Ga₂O₃ thin films is more challenging process because the formation of α -Ga₂O₃ is only stable for the first few monolayers and easily converted from α -Ga₂O₃ to β -Ga₂O₃ during high temperature post growth treatment. In this work, we have explored an effective route for growing relatively thick epitaxial α -Ga₂O₃ films on *m*-plane and *a*-plane sapphire substrates by pulsed laser deposition (PLD). First, we have grown Ga₂O₃ films at various substrate temperatures (560 – 720 °C) while the background pressure was kept at 3 mTorr of oxygen. Second, the effect of oxygen background pressure was investigated in an oxygen pressure range between 1 and 50 mTorr while the substrate temperature was fixed at 720 °C. The crystal structure and film quality of all Ga₂O₃ thin films were then investigated by high-resolution X-ray diffraction (XRD). For films grown on *a*-plane sapphires, pure α -Ga₂O₃ films can be obtained at only high growth temperatures (> 720°C) while the β -Ga₂O₃ peaks are appeared as the growth temperature is lowered below 720 °C. For films grown on *m*-plane sapphires, pure α -Ga₂O₃ film can be obtained at all temperature ranges (560 – 720 °C) while the film crystallinity improved as the growth temperature increases. We will present details of optimization processes to grow pure α -Ga₂O₃ films along with structural and optical properties of Ga₂O₃ films.

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MB-THP-27 High Responsivity GaS Nanobelt Metal-Semiconductor-Metal Photodetector with Ni Contact, *Chun-Yi Lin (gary12305112@gmail.com), C. Wang, National Taiwan University of Science and Technology, Taiwan*

Two-dimensional GaS is an important member of group III_A-VI_A semiconductors possessing exceptional optoelectronic properties. In this work, 2D GaS nanobelts (NBs) were successfully synthesized via the vapor-liquid-solid (VLS) method and the structure, morphology, and chemical composition of the as-prepared nanobelts are extensively investigated. Furthermore, GaS nanobelts are fabricated into photodetector with Ni contacts through electron beam lithography (EBL), electron beam evaporation and lift-off processes. The photodetector determines the photodetectors exhibited a dark current smaller than 500 fA while demonstrating remarkably high responsivity, external quantum efficiency (EQE) and detectivity is tens mA W⁻¹, ~10⁴ % and ~10¹³ Jones, respectively. Moreover, they displayed repeatable ON-OFF switching behavior, which with a fast response time is ~60 ms under the 405 nm excitation. Given the very low dark current, the GaS nanobelts were characterized as p-type semiconductors via MOSFET measurements under 405 nm excitation, with a measured mobility of ~10⁻³ cm² V⁻¹ s⁻¹.

To further enhance the performance of the devices, GaS/Ni heterostructure devices were formed through rapid thermal annealing (RTA). Post-annealing, the devices exhibited metallic behavior with a conductivity of ~10³ Ω⁻¹cm⁻¹ with high annealing temperature. On the other hand, low-temperature annealing resulted in the formation of Ni_xGaS/GaS heterostructures. These findings present a novel approach to enhancing the responsivity of GaS photodetectors with Ni contacts, offering promise for future high-performance optoelectronic systems.

MB-ThP-29 The Effect of the Precursors and Chemical Vapor Deposition Process on the Synthesis of Two-Dimensional Molybdenum Nitride Nanomaterials, C. Peng, B. Lin, H. Chen, L. Chen, *Sheng-Kuei Chiu (skuechiu@o365.fcu.edu.tw)*, Feng Chia University, Taiwan

Transition metal nitrides (TMNs) are crucial in influencing a wide range of physical and chemical characteristics due to their layered structure. They find applications in energy storage, sensors, electronics, spintronics, and catalysis. TMNs have a 2D structure that contains several active sites on the surface or edge, which contribute to their exceptional catalytic activity. Ongoing research is increasingly focused on developing methods to synthesize 2D TMNs. There are several defects in the structure of 2D TMN created using solution-based chemical synthesis, such as the hydrothermal technique. When fluorine, hydroxyl, or other oxygen-containing groups are on the surface of 2D TMNs, they become less reactive than they were before. Obtaining the desired effect from the use of TMNs synthesized by the hydrothermal process is challenging. The chemical vapor deposition (CVD) method has recently been approved as a way to make high-quality 2D transition metal nitrides (TMNs) that do not have any functional groups on the surface. We present a novel technique for producing an extremely thin, two-dimensional molybdenum nitride nanomaterial via chemical vapor deposition. Molybdenum nitride can be synthesized on a SiO₂/Si wafer by the CVD process. It undergoes an ammoniation reaction with the transition metal disulfide (MoS₂) and substitutes it with the transition metal nitride (MoN). By using a range of material testing devices, the precise composition and structure of the material are verified. This verification process aims to synthesize exceptionally reactive TMNs by carefully manipulating experimental conditions. The ultimate goal is to further the use of 2D TMNs in nanoelectronic components in the future.

MB-ThP-30 Optical Properties of Nanoscale Multi-Layered Ti/tac Thin Films, K. Oh, *JiWon Park (pjw000605@naver.com)*, Korea Aerospace University, Republic of Korea; J. Kim, KIMS, Republic of Korea; Y. Kim, Yonsei University, Republic of Korea; S. Lee, Korea Aerospace University, Republic of Korea

For the decade, it has been shown that diamond-like carbon (DLC) coatings are very promising anti-reflection (AR) and protective coatings for solar cell. However, tetrahedral amorphous carbon (ta-C) coatings with extremely high hardness, smooth surface, excellent wear resistance, and better thermal stability than DLC have been paid much attention to an alternative protective coating materials. Additionally, optical properties of the taC coating could be improved by various metals doping. In this study, various contents of Si were doped in the taC coating to improve the mechanical and optical properties of taC coatings. A filtered cathodic vacuum arc (FCVA) and magnetron sputter hybrid system was used to synthesize the metal doped taC coating. As the Ti concentration increased, the mechanical properties of the coatings decreased. The hardness and elastic modulus of the taC coating (50 and 435 GPa) decrease down to 14 and ~223 GPa. X-ray photoelectron spectroscopy (XPS) C 1 s spectra showed that both the Ti atomic percent and TiC bond percent increased with sputtering power. In addition, Ti-doped taC coatings showed an improved transmittance in all wavelength ranges when the sputtering powers were relatively low, comparing with undoped taC coating. Tribological behaviors of the Ti-doped taC coatings were investigated and the results showed that with increasing sliding distance, the CoF and the wear rate increased regardless of the Ti and Ti-C content in the Ti-doped taC coatings. Experimental details and further results will be presented.

MB-ThP-31 Vernier Ellipsometry Sensing with Ultralow Limit-of-Detection and Large Dynamic Range by Tuning of Zero-Reflection Points, Y. Zhang, M. Thawda Phoo, F. Yishu, X. Li, Y. Lam, *Juan Antonio Zapien (apjazz@cityu.edu.hk)*, City University of Hong Kong

Optical sensors using zero-reflection points (ZRP) enable excellent sensitivity due to accompanying phase singularities and the steepest slope of the reflectivity curve. Reflection zeros have been demonstrated at different spectral regions under very specific conditions in the angle of incidence (AoI) and polarization state. However, manipulation of the darkness points for multiple spectral positions and polarizations has not been achieved yet. Here, we report the collaborative and synergic operation of three ZRPs in a simple platform formed by a lithography-free, three-layer, metal-dielectric-metal structure where careful design and efficient manipulation of these ZRPs results in an optical sensor with unsurpassed, experimentally demonstrated, limit of detection $\sim 2 \times 10^{-8}$ RIU. The synergic operation of the proposed sensor relies on: i) strong coupling between *p*-pol surface plasmon polariton and *p*-pol photonic waveguide modes with experimentally demonstrated reflection suppression, Rabi

splitting and phase singularities; ii) simultaneous implementation of two orthogonally polarized ZRPs and wavelength-interrogation mode of operation leads to spectral overlap of *s*-pol photonic modes with the coupled, *p*-pol resonances; and iii) ellipsometry-based sensing where the relatively insensitive *s*-pol ZRPs provide internal references to boost the sensor performance in terms of the amplitude ratio (ψ) and phase difference (Δ) of the *s*- and *p*-polarized reflectance thereby naturally forming a refinement measuring scale akin to a Vernier scale. Remarkably, the precise manipulation of the double dark points via the AoI control enables a second metric that yields ultrahigh sensitivity and can be reset to the original spot over a large dynamic range, thereby avoiding the trade-off between sensitivity and dynamic range. This occurs because the AoI acts an additional degree of freedom to tune and reset the sensor to its original ZRPs while keeping track of the total accumulated change. The strength of these capabilities has been demonstrated for a biosensor of SARS-CoV-2 spike (S2) protein that can track the full functionalization process of the chip surface and then reset to its best sensing conditions to perform real-time dose-dependent detection of the S2 spike protein. Our work provides a new and powerful strategy for the development of optical sensors, perfect light absorbers, pyroelectric detectors, and phase modulators.

This work was supported by the Research Grants Council of Hong Kong, SAR, Project number CityU 11219919.

MB-ThP-32 Optical and Protective Coatings Synthesized by Magnetron Sputtering, E. Aubry, FEMTO-ST (UMR CNRS6174)/UTBM, France; *Pascal Briois (pascal.briois@utbm.fr)*, FEMTO-ST (UMR CNRS 6174)/UTBM, 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 but also its thickness. Based on the theoretical results, an adequate protective coating is determined. 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. The thin films were characterized by SEM, XRD for the morphological and structural parameters, the optical properties were determined by spectrophotometry. The first results obtained will be presented as well as future work.

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