New Horizons in Coatings and Thin Films
Room Pacific Salon 6-7 - Session F4-1-WeM

Functional Oxide and Oxynitride Coatings I

Moderators: Anders Eriksson, Oerlikon Balzers, Oerlikon Surface Solutions AG, **Marcus Hans**, RWTH Aachen University, **Jörg Patscheider**, Evatec AG

8:00am **F4-1-WeM-1 Microstructure and Piezoelectric Properties of Hexagonal $Mg_xZn_{1-x}O$ and $Mg_xZn_{1-x}O/ZnO$ Films at Lower Mg Compositions***, **Hsin Hung Chen**, C Liu, J Huang,* National Cheng Kung University, Taiwan

We investigate the piezoelectric coefficient(d33) of MgxZn1-xO and MgxZn1-xO/ZnO with various Mg content. The films were grown on Si (111) substrate using MgO and ZnO targets by radio frequency magnetron sputtering. Thickness of all films are fixed at around 600nm for MgxZn1-xO and 300/300nm for MgxZn1-xO/ZnO. There shows high crystallinity with preferred orientation along c-axis in XRD pattern, and columnar structures are clearly observed in SEM images, indicating that the films still remain wurtzite structures. Besides, XRD pattern, PL and XPS spectra proved that substitution of smaller magnesium ions at zinc sites causes lattice distortion and therefore enhance the d33 at maximum 48.7pm/V of MgxZn1-xO and 39.1pm/V of MgxZn1-xO/ZnO (x=0.17 for both) by PFM measurement. These values are nearly four and three times larger than pure ZnO films. We consider these films as a promising candidate for nanogenerators(NGs) and ultraviolet photodetectors(UV-PDs).

8:20am **F4-1-WeM-2 Structure Optimization of Ta-O-N Films Prepared by Reactive HiPIMS for More Effective Water Splitting***, **Šárka Batková**,* Department of Physics and NTIS - European Centre of Excellence, University of West Bohemia, Czech Republic*; J Čapek, S Haviar, J Houška, R Čerstvý,* University of West Bohemia, Czech Republic*; M Krbal,* University of Pardubice, Czech Republic*; T Duchoň,* Charles University, Czech Republic

The TaON material is a promising candidate for application as a visible-light-driven photocatalyst splitting water into H_2 and O_2 and thus converting solar energy into chemical energy. The photo-generated electron-hole pairs act here as the active water splitting species. In order to work as a water splitting photocatalyst, the material must satisfy certain conditions: (i) band gap of proper width (preferably corresponding to visible light absorption) and (ii) suitable alignment of the band gap with respect to the water splitting redox potentials. The subsequent transport of the charge carriers through the material (particularly across the films thickness) plays an important role in the effectivity of the process.

In this work we first demonstrate that using reactive high-power impulse magnetron sputtering (HiPIMS) as the deposition technique followed by post-annealing of the amorphous as-deposited film at 900°C in a vacuum furnace allows us to prepare a polycrystalline film exhibiting a pure TaON phase. Such film satisfies the above mentioned conditions for a water splitting photocatalyst (band gap of ~2.6 eV). However, as it is desirable to prepare the TaON phase in situ, we investigate the possibilities of substrate heating and biasing during deposition while focusing on fine-tuning of the elemental composition. Additionally, as the monoclinic TaON phase exhibits anisotropic charge carrier conductivity, tailoring of the texture of the film can further improve the charge carrier transport in a desired direction. In this work, we therefore also investigate the possibilities of deposition at high power densities in a pulse (up to 4 kW/cm^2) and/or deposition onto suitable substrates providing proper seeding layers (e.g., Pt, ZrO_2) to prepare textured TaON film allowing enhanced charge carrier mobility across the film thickness.

8:40am **F4-1-WeM-3 A Sustainable and Viable Alternative to Low Cost Electronics based on Metal Oxides***, **Elvira Fortunato**, R Martins,* New University of Lisbon, Portugal **INVITED**

In the last 50 years we observed a drastic change in our daily life since society was never before so efficient and interconnected. This provides a collaborative environment that is essential for economic growth and progress like: Silicon Valley for microelectronic technology and Boston for biotechnology. This breakneck development has been in part dictated by an empirical technologically and economically driven rule know as "Moore's law". Indeed today a microprocessor has more than 7 billion integrated transistors in an area of 350 mm2. This unbelievable integration capability with higher processing speeds, memory capacity and functionality gives rise to what we call today: ubiquitous electronics. Despite the importance of silicon technology there are applications where it is impossible, either technically or economically use it. Displays are the most notorious example, more if we want them to be flexible and conformable. On the other hand, 10 years ago it was pure science fiction the notion of fully transparent, flexible and conformable displays, like those used by T. Cruise in the Minority Report movie fully based on materials away from silicon! Thanks to the Hollywood vision and the hard work of scientists this is now a reality. After the huge success and revolution of transparent electronics where we must highlight the low process temperatures that turn possible the use of low cost eco-friendly materials and substrates such biopolymer or paper, where CENIMAT is pioneer and with the worldwide interest in displays/smart interfaces where metal oxide thin films have proved to be truly semiconductors, display backplanes have already gone commercial due to the huge investment of several high profile companies such: SAMSUNG, SHARP, LG, BOE, in a very short period of time. Recently IDTechEx estimated that 8 km sqr of metal oxide-based backplanes will be used in the OLED and LCD industry by 2024, enabling a 16 billion USD market at the display module level alone. We can anticipate that the metal oxide based industry will be in the near future a so-called multi billion euro market similar to what is observed with the pharmaceutical industry, due to the number of different applications that can serve, ranging from information technology, biotechnology/life sciences and energy to food/consumer products. In this talk we will present results on recent new technologies developed at CENIMAT|i3N where it is possible to have the use of sustainable materials used in disruptive applications.

9:20am **F4-1-WeM-5 Photocatalytic Study for Indium Tantalum Oxide Thin Film in Visible Light***, **Chuan Li**,* National Yang Ming University, Taiwan*; J Hsieh,* Ming Chi University of Technology, Taiwan*; P Hsueh,* National Central University, Taiwan

Indium tantalum oxide thin film was deposited by sputtering using three different designs: 5-7 and 10-14 nm alternative layers of Ta_2O_5 and In_2O_3, and co-sputtering of In_2O_3 and Ta_2O_5. Then as-deposited films were rapid annealed at different temperatures to assess the thermal effects on microstructures and photocatalytic functions. Results from XRD and EDS indicates that crystalline $InTaO_4$ emerges in 5-7 and 10-14 nm stacks of films but absent in the co-sputtered films. Since crystalline $InTaO_4$ is capable of photocatalysis under both ultraviolet and visible light, we particularly tested the annealed films in water to degrade methylene blue under visible light. The photo-induced degradation on methylene blue by 5-7 and 10-14 nm stacks can reach 45% after 6-hour continuous exposure. Using UV-Visible-NIR spectroscopy, we can estimate the optical band gaps in these annealed films and from these estimations, a mechanism for the photocatalysis is discussed following. This mechanism is similar to other electron-hole separation and transfer across the heterogeneous junctions in semiconductors.

9:40am **F4-1-WeM-6 Tailoring the Microstructure of ZnO Thin Films for Antimicrobial Applications***, P Pereira-Silva, J Borges, A Costa-Barbosa, D Costa, M Rodrigues, **Filipe Vaz**, P Sampaio,* University of Minho, Portugal

Nosocomial infections are microbial infectious diseases that are acquired in healthcare settings, and are a worldwide health problem. The surfaces are involved in the spread of these infections, thus there is an urgent need to eliminate this route of transmission. Nanotechnology allows the production of materials with improved properties and effective action against pathogens. Zinc oxide (ZnO) is frequently used due to its excellent antimicrobial properties.

This work focused on the evaluation of the antimicrobial activity of ZnO thin films. All the samples were produced by reactive DC magnetron sputtering and tested against the fungus *Candida albicans*. A first set of thin films were produced with different O_2 flows, which affected the thin films' chemical composition and morphology. Additionally, some of the thin films were subjected to an annealing treatment, which promoted the crystallization of the ZnO matrix. A second set of thin films was produced modifying the deposition angle, using the Glancing Angle Deposition technique, GLAD, with a fixed O_2 flow. These changes were performed to increase the porosity and roughness of the thin films, which may allow the tailoring of the film's biological response. To evaluate the ZnO thin films surface antimicrobial properties, a direct contact assay was performed, and the results revealed no significant cell growth after five hours of incubation. Analysing possible molecular mechanisms responsible for the antimicrobial activity, it was observed that the loss of membrane integrity and the increase of Reactive Oxygen Species (ROS) within *C.albicans* cells was correlated with the incapacity of the cells to grow.

As a general conclusion, one may claim that all the thin films showed a significant antifungal activity, and the observed differences among them can be correlated with the evolution of the (micro)structural features.

11:00am **F4-1-WeM-10 Exploring Thin Film Zn-Sn-O (ZTO) Composition Spreads Using Combinatorial Sputtering***, **Siang-Yun Li**, Y Shen, K Chang, J Ting,* National Cheng Kung University, Taiwan

Transparent conducting oxide (TCO) films are extensively applied as electrodes in the fields of solar cells and displays, due to their high transparency and excellent electrical conductivity. Multicomponent oxides such as Zn-Sn-O (ZTO) have attracted much attention due to the low cost elements of indium (In). In addition, thermal stability and mechanical strength of ZTO can be tailored by varying its stoichiometry. However, making compounds having different ratios of Zn/Sn systematically is not trivial.

Combinatorial methodology has been proven its validity in such an application. This approach allows the Zn/Sn ratio continuously to change across a single sample area and a feasible intimate mix of Zn and Sn. Therefore, a single ZTO composition spread sample essentially includes a full spectrum of properties to be investigated. A Zn-Sn-O (ZTO) composition spread, consisting of thickness wedges of SnO and ZnO, was prepared using a state-of-the-art combinatorial sputtering system, equipped with a moving shutter and two RF guns for the targets of Zn and Sn, respectively. The thickness gradient was determined using SEM, α-step and SIMS. It was found a smooth thickness variation across the sample area for both ZnO and SnO with the coefficient of determination (R2) $\cong$ 0.99, indicating a good control of the ZTO composition spread. Structure evolution was characterized using XRD. We found in-situ 500 ºC annealing resulted in crystallization of the samples, where ZnO, Zn_2SnO_4, $ZnSnO_3$, and SnO_2 phases were observed, depending upon the ZnO/SnO ratios on the ZTO composition spread. The resistivity was characterized using a four-point probe on different substrates, which revealed lower resistivity near ZnO-rich. Morphology and optical characteristics were studied as well using AFM, SEM and UV-Vis spectrometry. A clear variation trend of both properties was observed. A systematic study of physical properties of ZTO has been successfully demonstrated.

11:20am **F4-1-WeM-11 Can Thin-Film Technology Help to Realize The Einstein Gravity Quantum Computer?***, **Norbert Schwarzer**,* SIO, Germany

After it became clear that quantum computers are more powerful than originally thought [1], we were asked by the industry to find the most fundamental form of a Turing machine based on Quantum Theory. Do this job in a very comprehensive manner, we found that the deepest layer for the Quantum Computer was not to be found inside the theoretical apparatus of Quantum Theory. Surprising as this may be, it is the General Theory of Relativity which “contained it all”. We found that an extremely simple solution of the Einstein-Field-Equations, using pairwise dimensional entanglement, sports the principle structural elements of computers [2]. We will derive these structural elements and show that the classical computer technology of today and even the quantum computers are just degenerated derivatives of this general solution. In the talk we will discuss thin-film technology- and smart material-options potentially helping us to one day realize the general computer concept.

[1] J. Aron, “Quantum computers are weirder and more powerful than we thought”, www.newscientist.com/article/2170746

[2] N. Schwarzer, “Einstein had it, but he did not see it – Part XXXIX: EQ or The Einstein Quantum Computer”, www.amzon.com, ASIN: B07D9MBRS3

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