## Functional Thin Films and Surfaces
## Room Palm 5-6 - Session MB2-1-MoA

### Thin Films for Emerging Electronic and Quantum Photonic Devices I

**Moderators:** **Shirly Espinoza**, ELI Beamlines, ELI ERIC, Czechia, **Jaroslav Vlcek**, University of West Bohemia, Czechia

2:00pm **MB2-1-MoA-2 Optical and Electrical Properties of Nitrogen-doped p-type $Cu_2O$ Thin Films Prepared by Reactive HiPIMS**, ***Jan Koloros* [koloros@ntis.zcu]**, *Jiří Rezek, Pavel Baroch,* University of West Bohemia in Pilsen, Czechia

One of today's challenging scientific topics is finding a suitable p-type TCO that would at least approach the optoelectronic properties of the n-type counterpart [1]. Finding such p-type material is a necessary condition for further sustainable technological development of society. The realization of p-n junctions using transparent conductive materials will enable the development of a new generation of invisible electronics, contribute to reducing the energy requirements of various optoelectronic devices or lead to the production of more efficient solar cells. Transparent conductive materials based on $Cu_2O$ appear to be among the most promising. This is mainly due to the abundance of elements used, their non-toxicity and interesting optoelectronic properties. One of the limiting factors in $Cu_2O$ layers is the low mobility of holes. In our previous work [2], we demonstrated that post-deposition laser annealing can effectively enhance hole mobility.

In our work, we systematically investigated the role of nitrogen incorporated into $Cu_2O$ thin films, with a primary focus on their optical and electrical properties, including the optical band gap and electrical resistivity. The $Cu_2O$:N films were prepared by reactive HiPIMS of Cu circular target (100 mm in diameter) in Ar+$O_2$+$N_2$ atmosphere. The pulse-averaged target power density ($S_{da}$) was varied from ≈ 100-1300 $Wcm^{-2}$, and the fraction of $N_2$ in (Ar+$N_2$) mass flow was 0–90 %. A decreasing trend in resistivity has been observed with increasing nitrogen content. The prepared p-type $Cu_2O$:N films with the highest value of a nitrogen fraction of 90% exhibited a very low resistivity about $5x10^{-2}$ Ωcm exceeding the current state of the art [3].

[1] J. Singh, P. Bhardwaj, R. Kumar, V. Verma, Progress in Developing Highly Efficient p-type TCOs for Transparent Electronics: A Comprehensive Review, J Electron Mater (2024).

[2] J. Rezek, M. Kučera, T. Kozák, R. Čerstvý, A. Franc, P. Baroch, Enhancement of hole mobility in high-rate reactively sputtered $Cu_2O$ thin films induced by laser thermal annealing, Applied Surface Science, (2024).

[3] J. Rezek, J. Koloros, J. Houška, R. Čerstvý, S. Haviar, D. Kolenatý, J. Y. Damte, P. Baroch, Ultra-low-resistivity nitrogen-doped p-type $Cu_2O$ thin films fabricated by reactive HiPIMS, Applied Surface Science, (2025).

2:20pm **MB2-1-MoA-3 Fabrication and Manipulation of Weakly-Interacting Interfaces for Optoelectronic Applications**, ***Kostas Sarakinos* [kostas.sarakinos@helsinki.fi]**, University of Helsinki, Finland **INVITED**

A key challenge in the materials science community is to understand the correlation among nanoscale atomic arrangement, structure-forming mechanisms, and mesoscale morphology during material synthesis. Addressing this challenge will herald a new epoch in which tailor-made materials and devices with unprecedented macroscopic behavior will be created by controlling mesoscale structure via nanoscale manipulation. The present talk demonstrates the implementation of the above-outlined concept of multiscale materials design during the vapor-based synthesis of thin noble-metal films (and nanostructures) on weakly-interacting substrates, including oxides and van der Waals crystals. Such film/substrate systems exhibit a pronounced and uncontrolled three-dimensional (3D) morphology, which is a major obstacle toward fabricating high-quality multifunctional metal contacts in a wide array of devices. Using growth of sliver (Ag) on silicon dioxide (SiO2) as a model system—along with a combination of in situ film growth monitoring, ex situ microstructure and chemical characterization, and modelling—it is shown that the tendency for 3D growth morphology can be effectively reversed, without compromising key physical properties of the film and the substrate, when miniscule amounts of minority gaseous [1,2,3] and metal species [4,5] (surfactants) are deployed with high temporal precision at the film growth front, such that atomic-scale processes that govern key film-formation stages are selectively targeted and affected. The talk concludes with a discussion with regards to the implications and possibilities that this strategy opens for tuning macroscopic performance of devices in the areas of energy saving and generation.

[1] A. Jamnig *et al.*, "*3D-to-2D morphology manipulation of sputter-deposited nanoscale silver films on weakly-interacting substrates via selective nitrogen deployment for multifunctional metal contacts*", ACS Applied Nano Materials 3 (2020) 4728.

[2] N. Pliatsikas *et al.*, "*Manipulation of thin silver film growth on weakly-interacting silicon dioxide substrates using oxygen as a surfactant*", J. Vac. Sci. Technol. A 38 (2020) 043406.

[3] K. Sarakinos *et al.*, "*Unravelling the effect of nitrogen on the morphological evolution of thinsilver films on weakly-interacting substrates*", App. Surf. Sci. 649 (2021) 159209.

[4] A. Jamnig *et al.* "*On the effect of copper as wetting agent during growth of thin silver films on silicon dioxide substrates*", App. Surf. Sci. 538 (2021) 148056.

[5] A. Jamnig *et al.*, "*Manipulation of thin metal film morphology on weakly-interacting substrates via selective surfactant deployment*", J. Vac. Sci. Technol. A. 40 (2022) 033407.

3:00pm **MB2-1-MoA-5 Stability and Interlayer Formation at Epitaxial P-Type Oxides and $Ga_2O_3$ Interfaces**, ***Anna Sacchi* [anna.sacchi@nrel.gov]**, *Andriy Zakutayev, Brooks Tellekamp, Michelle Smeaton, Steven Spurgeon,* National Renewable Energy Laboratory, USA*; Shivashree Shivamade Gowda, Patrick Hopkins,* University of Virginia, USA

Research in power electronics is increasingly directed toward ultra-wide bandgap (UWBG) oxides such as $Ga_2O_3$, valued for its wide bandgap (≈ 4.5 eV), high breakdown field (≈ 8 MV/cm), as well as thermal and chemical stability. However, the impossibility to achieve p-type doping in $Ga_2O_3$ has motivated the exploration of heterojunctions based on different p-type oxides, among which NiO and $Cr_2O_3$ are considered the most promising.[1,2] To date, most studies on $Ga_2O_3$ based heterojunctions have focused primarily on device optimization rather than on the fundamental understanding of interface dynamics and long-term stability, except for a recent study[3] where the formation of a $NiGa_2O_4$ interlayer at the NiO/$Ga_2O_3$ interface after prolonged thermal cycling was found responsible for device performances degradation.

This work aims to provide a deeper understanding of NiO/$Ga_2O_3$ and $Cr_2O_3$/$Ga_2O_3$ interfaces. Pulsed laser deposition growth technique is exploited to run a detailed growth campaign for NiO and $Cr_2O_3$ on top of $Ga_2O_3$ substrates with various orientations, *i.e.*, (100), (001), and (−201). X-ray diffraction evaluated material quality and epitaxial relationships, revealing (-201) substrate orientation as common epitaxial match for both oxides. Transmission electron microscopy is used to examine interface stability and possible interlayer formation when thermal treatments are applied, simulating long-term high-temperature operations. Additionally, thermoreflectance measurements are performed to investigate heat dynamics at the interfaces, both with and without the interlayer presence.

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(1) Kokubun, Y.; Kubo, S.; Nakagomi, S. All-Oxide p–n Heterojunction Diodes Comprising p-Type NiO and n-Type β-Ga2O3. *Appl. Phys. Express* **2016**, *9* (9), 091101. https://doi.org/10.7567/APEX.9.091101.

(2) Callahan, W. A.; Egbo, K.; Lee, C.-W.; Ginley, D.; O'Hayre, R.; Zakutayev, A. Reliable Operation of Cr2O3:Mg/ β-Ga2O3 p–n Heterojunction Diodes at 600 °C. *Appl. Phys. Lett.* **2024**, *124* (15), 153504. https://doi.org/10.1063/5.0185566.

(3) Egbo, K.; Garrity, E. M.; Callahan, W. A.; Chae, C.; Lee, C.-W.; Tellekamp, B.; Hwang, J.; Stevanovic, V.; Zakutayev, A. NiGa2O4 Interfacial Layers in NiO/Ga2O3 Heterojunction Diodes at High Temperature. *Appl. Phys. Lett.* **2024**, *124* (17), 173512. https://doi.org/10.1063/5.0194540.

3:20pm **MB2-1-MoA-6 Investigation of High-temperature Morphology and Electrical Performance of YZr-alloyed Amorphous $Al_2O_3$ Thin Films**, 
***Norma Salvadores Farran [norma.salvadores@tuwien.ac.at]**, Florentine Scholz, Tomasz Wojcik,* TU Wien, Austria*; Astrid Gies, Jürgen Ramm, Klaus Böbel,* Oerlikon Balzers, Liechtenstein*; Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials, Austria*; Tobias Huber, Jürgen Fleig, Helmut Riedl,* TU Wien, Austria

Aluminium oxide ($Al_2O_3$) is a widely used insulating material, particularly in thin-film applications. In addition to its various polymorphs, $Al_2O_3$ can also exist in an amorphous phase, which is characterized by excellent oxidation resistance and high thermal conductivity. A key advantage of the amorphous form is its uniform structure, free from pinholes. Owing to these properties, amorphous $Al_2O_3$ being investigated as a dielectric material in electronic and semiconductor devices, as well as in energy storage technologies. Therefore, identifying cost-effective and sustainable deposition methods for the fabrication of high-quality $Al_2O_3$ insulating thin films is of great importance.

Amorphous $Al_2O_3$ films were synthesized using a reactive Modulated Pulse Power (MPP) sputtering process. All depositions were carried out in an in-house developed sputtering system equipped with a 3-inch aluminium target and operated in a mixed $Ar/O_2$ atmosphere. The primary aim of this study was to examine the influence of yttrium–zirconium (YZr) alloying on the thermal stability of the amorphous $Al_2O_3$ phase, with the goal of preventing phase transitions into crystalline states up to 1200 °C. To achieve this, varying amounts of YZr were incorporated into the aluminium targets. The effects of these YZr additions and their concentrations on process stability, as well as on the resulting film properties – including morphology, structure, and electrical resistivity – were analysed using advanced high-resolution characterization techniques.

Phase formation and evolution were investigated using X-ray diffraction (XRD) over a temperature range from room temperature up to 1200 °C. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were employed to assess the deposition rate and surface morphology of the coatings. The chemical composition of the films was analysed using X-ray photoelectron spectroscopy (XPS), which was also utilized to examine the bonding states of the constituent elements. Additionally, in-situ impedance spectroscopy was used to study variations in the electrical properties as a function of temperature. For electrical characterization, Ti/Pt electrode pads were fabricated via photolithography.

4:00pm **MB2-1-MoA-8 Ion-Beam Assisted Deposition of P-Type Oxide Semiconductor Thin Films in Room Temperature**, 
***Tsung-Yu Huang [huang.tsungyu@mail.mcut.edu.tw]**,* Ming Chi University of Technology, Taiwan **INVITED**

Transparent semiconductor oxides are an important class of materials in materials science, including $SnO_2$, $In_2O_3$, ZnO, and dozens of doped transparent semiconductor oxides. These materials have been widely used in various electronic and optoelectronic devices. Tin monoxide (SnO), due to the overlap between its 5s orbital and the oxygen 2p orbital, exhibits unique characteristics that enable hole transport. This makes it one of the most promising candidates for p-type oxide semiconductors. In this study, our p-type SnO thin film achieved a mobility of 4.52 $cm^2 V^{-1} s^{-1}$.

4:40pm **MB2-1-MoA-10 Influence of Bonding Temperature on Electromigration Suppression in Cu-Doped Ag Bumps**, 
***Chien-Cheng Chiang [johnson10678@gmail.com]**, Peng-Hsiang Hsu, Fan-Yi Ouyang,* National Tsing Hua University, Taiwan

The continuous advancement of technology has driven the demand for higher-performance electronic devices, leading to progressive miniaturization of device dimensions. However, further device scaling is fundamentally constrained by physical limits. To overcome these challenges, three-dimensional integrated circuits (3D ICs) have emerged as a promising alternative for enhancing device performance. Compared with conventional flip-chip solder joints, direct metal bonding (DMB) provides higher interconnect density, lower electrical resistance, and improved reliability, making it an attractive technique for advanced packaging. Nevertheless, as interconnect dimensions decrease, reliability issues become increasingly critical, with electromigration (EM) being one of the primary failure mechanisms.

In this study, Ag alloyed with 3.2 at.% Cu was employed as the interconnect material, and a nanotwinned structure was introduced to enhance EM resistance. Thermal compression bonding was performed at various temperatures to investigate the influence of bonding temperature on electromigration behavior and microstructural evolution.Compared with pure silver, Ag doped with 3.2 at.% Cu exhibits not only a better bonding interface at higher bonding temperatures but also retains a larger amount of twin structures, thereby achieving superior electromigration resistance. The results provide valuable insights into the relationship between bonding parameters and EM performance, offering practical strategies to improve the reliability of next-generation advanced packaging technologies.

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