Functional Thin Films and Surfaces
Room Pacific C - Session C1-WeM
Optical Materials and Thin Films
Moderator: Nikolas Podraza, University of Toledo, USA

8:00am **C1-WeM-1 Engineering Ultra-thin Films for Extreme Optics and Photonics**, ***Jeremy Munday (jnmunday@ucdavis.edu)***, University of California at Davis, USA **INVITED**

Ultra-thin optical coatings have a variety of applications from antireflection coatings to optical sensors. The simplicity of using a single optical film makes it an excellent candidate for large scale applications; however, this simplicity also results in design space constraints and limitations. In this talk, I will discuss how we are able to circumvent a number of these issues using specially designed ultra-thin films in unique ways. I will discuss how ultra-thin metal films can convert a visible silicon detector into a near-infrared detector, how hydrogen can be optically detected in ultra-thin metal films, how materials with epsilon-near-zero (ENZ) optical properties can enhance these effects, and how high-melting-point materials can be used to create custom thermal emitters and their application to thermophotovoltaics. I will conclude with an outlook on these technologies and future applications.

8:40am **C1-WeM-3 Study of $Cs_x(CH_3NH_3)_{1-x}PbBr_3$ Perovskite with XPS Imaging and Small Area Spectra**, ***Tatyana Bendikov (tatyana.bendikov@weizmann.ac.il)***, Weizmann Institute of Science, Israel; *Y. Rakita,* Columbia University, USA; *H. Kaslasi, G. Hodes, D. Cahen,* Weizmann Institute of Science, Israel

Interest in halide perovskite (HaPs) is motivated by the combination of superior optoelectronic properties and ease in synthesizing these materials with a surprisingly low density of electrically active defects. HaPs possess high chemical sensitivity, especially those having an organic cation at their *A* position (AMX_3). Although a direct role of the *A* cation in this sensitivity is unclear, and the structural and optoelectronic backbone lie within the *M-X* bond, the type of the *A* cation was shown to impact the chemical stability and, usually indirectly, affect optoelectronic properties of HaPs.

X-ray Photoelectron Spectroscopy (XPS), is a surface sensitive technique with a sensitivity that goes down to a single atomic layer, and can provide unique information that relates the elemental composition with the chemical and electronic states of the different elements in the material. Our study focuses on the XPS imaging in combination with selected small area XPS spectra and uses solution-grown, single crystals of mixed *A*-cation $Cs_xMA_{1-x}PbBr_3$(MA = $CH_3NH_3^+$) HaPs as a candidate for investigating heterogeneity within the crystals. With XPS we followed the variations in chemical composition of these crystals. By observing the surface, we found significant changes in the N/Cs ratio, which increases towards the interior of the crystal. Similar variations in N/Cs, but also in Pb/(N+Cs) ratios were found when we studied cross-sections of cleaved crystals. This compositional heterogeneity within the HaPs crystal was not previously reported and was discovered and monitored due to exclusive capabilities of the XPS technique.

9:00am **C1-WeM-4 Tuning the Optical Properties of PVD Deposited SiC Coatings by a Design of Experiments Approach**, ***Vincent Tabouret (vincent.tabouret@grenoble-inp.Fr)***, *A. Crisci, M. Morais, G. Berthomé, E. Garel, G. Renou, D. CHaussende,* CNRS, France

Silicon carbide (SiC) is a wide bandgap semiconductor that is currently driving a profound evolution in power electronics, thanks to a unique combination of outstanding physical properties. In addition, SiC also exhibits very promising optical properties, making it very suited for applications in photonics, such as waveguides and frequency combs. For this purpose, amorphous SiC (a-SiC) thin films are deposited at very low temperature with the main challenges being the control of bulk properties and the formation of perfects interfaces. Today, the relationships between the deposition conditions and the optical properties of the films is still not clear. This paper aims to provide a comprehensive picture of these relationships and finally to give some hints for further optimization.

Coatings of a-SiC were deposited by Physical Vapor Deposition (PVD) on different types of substrates, such as sapphire and silica on silicon wafers, and using a polycrystalline SiC target as source material.A design of experiments (DOE) methodology was implemented to identify and weight the main deposition parameters with respect to the optimization of the refractive index and attenuation coefficient of the films, measured by spectroscopic ellipsometry. In parallel, a systematic investigation of the chemical and structural properties of the films was carried out, using a combination of XRD, FTIR, XPS and TEM.

9:20am **C1-WeM-5 Submicron Structures Obtained by Laser Dewetting of Metallic Thin Film Stacks**, ***Bruno Felipe Leitao Almeida (bruno.almeida2@saint-gobain.com)***, *L. Gallais,* Institut Fresnel, France; *J. Fonné, D. Guimard,* Saint-Gobain Research Paris, France

Patterned thin films can have interesting applications in functional glazing provided by their optical and electrical properties. Some examples are: Plasmonic effects of the dewetted structures, anisotropic electrical properties (polarizers) and high resistivity and good transparency, that could be used as transparent electrodes. In this context, dewetting is an interesting way of patterning thin films, including metallic ones.

Although most of the literature work on the laser induced dewetting is on uncapped metallic films (substrate / metallic film) using pulsed laser, the laser induced dewetting can also take place in metallic thin films encapsulated by dielectrics using a continuous wave laser. An example is the stack of Glass / Si_3N_4 / Ag / Si_3N_4 deposited on soda-lime glass by magnetron sputtering, depicting morphologies of lines and islands after laser annealing. According to the temperatures achieved during laser treatment, different mechanisms can take place in continuous wave laser dewetting (solid-state or liquid-state dewetting).

In this stack configuration, our work was interested in studying the different structures that could be obtained. The structuration substantially changed the optical properties of the films. A set of *ex-situ* characterizations has been done on the stack before and after structuration. The techniques used were: ellipsometry, spectrophotometry, Fourier-transform infrared spectroscopy, SEM, AFM and XRD.

In order to obtain more information on the mechanisms responsible for these structures in our systems, a set of *in-situ* techniques (fast microscopy and thermal measurements) has been developed and used to obtain the thermal and temporal dependency of the phenomena. *In-situ* thermal measurements were afterwards confronted to results obtained through numerical simulation. These results showed good accordance for temperatures below the structuration threshold regarding the temporal evolution and the spatial distribution of temperature. For temperatures above the structuration threshold, this is no longer the case. From this point on, the film presented changes in the morphology that affects the optical properties (emissivity and absorption).

We shall present in more details these unique structures and their characterizations, the strategies used to take these changes in account to obtain a better correlation measurement/simulation in elevated temperatures and our interpretation of the mechanisms responsible for its structuration.

11:00am **C1-WeM-10 Design of High-Performance VO_2-Based Thermochromic Coatings, and Pathway for Their Industry-Friendly Preparation**, ***Jiri Houska (jhouska@kfy.zcu.cz)***, *D. Kolenaty, T. Barta, J. Rezek, J. Vlcek,* University of West Bohemia, Czechia **INVITED**

The contribution reports our latest results [1-5] concerning energy-saving thermochromic multilayered VO_2-based coatings for smart window applications prepared by reactive magnetron sputtering. First, we show that and how reactive high-power impulse magnetron sputtering with a pulsed O_2 flow control allows reproducible preparation of crystalline VO_2 of the correct stoichiometry under exceptionally industry-friendly deposition conditions: on soda-lime glass substrates without any substrate bias or post-deposition annealing at a low temperature of around 300 °C. Second, doping of VO_2 by W is employed in order to shift the thermochromic transition temperature (68 °C for bulk, 57 °C for our thin film VO_2) toward the room temperature (40 °C for $V_{0.988}W_{0.012}O_2$, 20 °C for $V_{0.982}W_{0.018}O_2$), without concessions in terms of transmittance and its modulation. Third, we employ ZrO_2 antireflection layers both below and above the thermochromic $V_{1-x}W_xO_2$ layer, and explain an optimum design of the resulting $ZrO_2/V_{1-x}W_xO_2/ZrO_2$ coatings. While utilizing a first-order interference on ZrO_2 leads to a tradeoff between the luminous transmittance (T_{lum}) and the modulation of the solar energy transmittance (ΔT_{sol}), utilizing a second-order interference allows one to optimize both T_{lum} and ΔT_{sol} in parallel. Fourth, we discuss multilayered designs leading, without any further doping, to thermochromic coatings of optimized color (chromaticity as close to white as possible). The state-of-the-art T_{lum} and ΔT_{sol} values achieved under the aforementioned industry-friendly deposition conditions and at lowered transition temperature are in agreement with those predicted during the coating design.

[1] J. Vlcek et al., J. Phys. D Appl. Phys. 50, 38LT01 (2017), 10.1088/1361-6463/aa8356

[2] J. Houska et al., Sol. Energy Mater. Sol. Cells 191, 365 (2019), 10.1016/j.solmat.2018.12.004

[3] D. Kolenaty et al., Sci. Rep. 10, 11107 (2020), doi.org/s41598 020 68002-5

[4] J. Houska, Sol. Energy Mater. Sol. Cells 230, 111210 (2021). 10.1016/j.solmat.2021.111210

[5] J. Houska et al., Design and reactive magnetron sputtering of thermochromic coatings (invited perspective paper), J. Appl. Phys., submitted (2022)

Author Index

Bold page numbers indicate presenter