Functional Thin Films and Surfaces
Room Palm 1-2 - Session MB1-WeA

Optical Materials and Thin Films

Moderators: Jiri Houska, University of West Bohemia, Czechia, **Juan Antonio Zapien**, City University of Hong Kong

2:00pm **MB1-WeA-1 Ultrafast Phenomena in Optical Materials with fs–ns Time-Resolved Spectroscopic Ellipsometry***, **Shirly Espinoza [shirly.espinoza@eli-beams.eu]***, ELI Beamlines. ELI ERIC, Czechia **INVITED**

Static, imaging, and time-resolved ellipsometry link microstructure and optical function in thin films. Using time-resolved spectroscopic ellipsometry (TRSE), we access amplitude and phase simultaneously (angles Ψ and Δ) to recover the complex dielectric function (ε) with femtosecond resolution, a capability that conventional transient probes do not provide directly and that is key to disentangling overlapping ultrafast processes. As complementary techniques, time-resolved X-ray diffraction (TR-XRD) correlates lattice strain and structural pathways with the optical response, while imaging ellipsometry maps, with spatial resolution, thickness and optical constants (n, k), assessing uniformity and device-level variability.

In ZnO thin films, TRSE separates bleaching by Pauli blocking, band-gap renormalization, and intra-valence-band absorption, together with the evolution of excitonic features under strong photoexcitation; this yields the full-time evolution (real and imaginary parts) of ε(ω,t) and clarifies electron–electron and electron–phonon coupling on sub-ps time scales.

In $LaCoO_3$ thin films, TRSE reveals a photoinduced insulator-to-metal transition with spectral-weight transfer to low energies, followed by an ultrafast relaxation and, between 1–30 ps, a second maximum whose kinetics and thickness dependence evidence coherent acoustic phonons that transiently modulate the optical constants.

Complementarily, imaging ellipsometry applied to spin-coated oxides demonstrates its utility for metrology and function: thickness/optical-constant mapping and fabrication of Co_3O_4/CeO_2 diodes with reproducible rectification, all within a low-cost deposition platform.

Finally, for layered chalcogenides, recent results obtained outside our TRSE setup show that GaS acts as a reconfigurable optical material: laser-induced structural modification persistently tunes the band structure and refractive index with low loss, enabling sub-wavelength patterning and programmable optical elements.

Taken together, TRSE, TR-XRD, and imaging ellipsometry form a quantitative toolbox to read and design ultrafast optical functionalities in oxides and chalcogenides, from fundamental dynamics to scalable device integration.

2:40pm **MB1-WeA-3 The Role of Contaminants in the Microstructural Evolution of Defects in Low-Emissivity Glazing at High Temperatures***, **Phillip Rumsby [phillip.rumsby@etud.polymtl.ca]**, Bill Baloukas, Oleg Zabeida, Ludvik Martinu,* Polytechnique Montréal, Canada

Silver-based coatings present exceptional optical and electrical properties, garnering them significant interest in applications requiring multifunctional optical filters. Amongst these are low-emissivity (low-E) windows. These dramatically reduce radiative heat transfer, improving the energy efficiency of window units while simultaneously providing highly transparent and aesthetically pleasing glass facades. However, Ag films present specific challenges in terms of their chemical and high-temperature stability, which must be managed with an appropriate combination of protective layers (hard coatings, diffusion barriers, metallic interface layers).

In this work, we investigate the processes by which minor mechanical defects in said protective layers evolve during glass tempering. This process, in which coated glass is heated at temperatures in excess of 650 °C, can cause small, practically invisible scratches, formed during glass cutting and handling, to develop into highly visible features. This can lead to entire panes of glass being rejected late in the fabrication process.

First, the multiple mechanisms participating in coating degradation are isolated and their interplay is analyzed: indeed, in addition to purely microstructural changes, disruption of the protective films allows diffusion of both atmospheric and substrate contaminants to the Ag layer, such as O_2, H_2O, and Na. The effect of different combinations of contaminants is thus evaluated by annealing partial stacks with various barrier layer configurations in controlled environments and on substrates of different composition, allowing one to control contaminant availability. Subsequent optical, electrical and microstructural analyses reveal key differences in the Ag dewetting behavior induced by O_2 and Na exposure.

Defects with repeatable morphological features are then generated using a microscratch tester with a diamond tip indenter. The effect of defect types and tempering conditions on scratch visibility is then compared quantitatively by image analysis of dark-field photographs. This reveals that atmospheric contaminants play a dominant role in scratch intensification. Investigation of the coating microstructural features leading to this increase in visibility is performed by both scanning and transmission electron microscopies; this indicates that large Ag particles (≈ 1 µm) formed at the scratched surfaces are not the main contributor. Rather, particles formed inside the coating, with restricted sizes (≈ 100 nm) contribute to scattering much more strongly, as evidenced by Mie scattering calculations.

3:00pm **MB1-WeA-4 Thermochromic VO_2-Based Coating for Energy-Saving Smart Windows: Design and Scalable Synthesis***, **Jaroslav Vlcek [vlcek@kfy.zcu.cz]***, University of West Bohemia, Czechia **INVITED**

Vanadium dioxide (VO_2) exhibits a reversible phase transition from a low-temperature monoclinic VO_2(M1) semiconducting phase to a high-temperature tetragonal VO_2(R) metallic phase at a transition temperature of approximately 68 °C for the bulk material. The automatic response to temperature and the abrupt decrease of infrared transmittance with almost the same luminous transmittance at the transition into the metallic state make VO_2-based coatings a promising candidate for thermochromic smart windows reducing the energy consumption of buildings.

We report two different types of high-performance thermochromic coatings synthesized on standard soda-lime glass at a low substrate temperature of 320-350 °C: three-layer $YSZ/V_{0.855}W_{0.018}Sr_{0.127}O_2/SiO_2$ coatings, where YSZ is yttria-stabilized zirconia, prepared using a scalable (proved by a successful transfer to a large-scale roll-to-roll deposition device with ultrathin flexible glass substrate) sputter deposition technique, and even higher-performing coatings with four layers of subwavelength W-doped VO_2 nanoparticles dispersed in SiO_2 matrix prepared using a two-step process, combining magnetron sputter deposition and postannealing in oxygen. The coatings exhibit a transition temperature of 22-33 °C with an integral luminous transmittance $T_{lum} > 60\%$ and a modulation of the solar energy transmittance $\Delta T_{sol} > 10\%$. Such a combination of properties, together with the low substrate temperature in both cases, fulfill the requirements for large-scale implementation on building glass (glass panes, or flexible glass and polymer foils laminated to glass panes) and have not yet been reported in the literature.

We present and explain the fundamental principles of both developed low-temperature (usually used temperatures are higher than 450 °C) preparation techniques and the design of these thermochromic coatings. Moreover, we explain the effect of Sr in the W and Sr co-doped VO_2 on the electronic structure and the enhanced thermochromic properties of the three-layer $YSZ/V_{0.855}W_{0.018}Sr_{0.127}O_2/SiO_2$ coatings, and the effect of the discontinuous W-doped VO_2 microstructure on the very promising thermochromic properties ($\Delta T_{sol} > 15\%$) of the coatings with four layers of W-doped VO_2 nanoparticles dispersed in SiO_2 matrix.

3:40pm **MB1-WeA-6 Designing Light-Active Thin Film Heterojunctions: Band Alignment and Layer Engineering for Efficient Photocatalysis***, **Monserrat Bizarro [monserrat@materiales.unam.mx]***, UNAM, Mexico **INVITED**

The design of functional thin films capable of harvesting visible light for photocatalytic processes relies critically on controlling charge transport and interfacial phenomena. While the formation of semiconductor heterojunctions in nanoparticles or powdered materials has proven to be a powerful approach to improve carrier separation and extend light absorption, the actual mechanisms that govern the performance of *thin-film* heterostructures—where photocatalysis is inherently surface-dominated—remain poorly understood.

In this work, we explore how stacking order and interfacial electric fields define the photocatalytic response in two representative systems: ZnO/Bi_2O_3 and BiOBr/BiOI thin-film heterojunctions prepared by spray pyrolysis. Each semiconductor was first deposited as an individual layer to establish its structural, optical, and electronic properties, and then combined in two configurations (A/B and B/A) to evaluate the influence of layer sequence. Detailed microstructural analyses confirmed the formation of well-defined physical junctions and excluded the presence of new ternary phases. Band positions, carrier concentrations, mobilities, and Fermi levels were determined to construct energy band diagrams that explain the observed photocatalytic trends.

Under blue or simulated sunlight irradiation, the heterostructures exhibited a pronounced dependence of activity on stacking order. Configurations in which the semiconductor with the wider band gap and less negative conduction band (ZnO or BiOBr) occupied the surface achieved superior photocatalytic efficiency toward dye degradation, attributed to favorable band alignment, internal electric fields that drive charge migration, and reduced recombination at the interface. Conversely, reversing the stacking sequence quenched the photocatalytic response, highlighting the delicate interplay between layer order, thickness, and interfacial charge transfer.

These findings demonstrate that thin-film heterojunctions can be rationally designed to enhance surface photocatalytic activity through precise control of band alignment and interface fields. Beyond their relevance for environmental photodegradation, such insights are broadly applicable to solar energy conversion, photoelectrochemical devices, and other light-assisted surface reactions, positioning thin-film heterostructures as a versatile platform for functional materials engineering.

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