Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Golden State Ballroom - Session CM-ThP
Advanced Characterization, Modelling and Data Science for Coatings and Thin Films Poster Session

CM-ThP-1 Artificial Intelligence for Predictive Design of Semiconducting Thin Films: Bandgap, Conductivity, and Activation Energy in Se–Sb–In Alloys, ***Maninder Kamboj [maninderk@gmail.com]***, *Farah Mohammadi,* Toronto Metropolitan University, Canada

Semiconducting chalcogenide thin films are central to next-generation optoelectronic and memory technologies, where precise control of bandgap and transport properties dictates device performance. Se–Sb–In alloys, in particular, offer rich compositional flexibility, yet experimental mapping of their structure–property space remains slow and resource-intensive. To address this challenge, we demonstrate an artificial intelligence (AI) framework for predictive design of Se–Sb–In thin films, focusing on three key parameters: optical bandgap (Eg), electrical conductivity (σ), and DC activation energy (Ea).

Physics-informed datasets were constructed from compositional variables and experimental trends, and gradient boosting regression models were trained with optimized hyperparameters and cross-validation. The models delivered high predictive accuracy (RMSE ≈ 0.05 eV for Eg, 0.11 log-units for σ, and 0.02 eV for Ea), while preserving interpretability. Crucially, AI predictions reproduced experimentally observed behaviors—bandgap narrowing with In incorporation and Ea reduction with Sb-induced defect states—while revealing nonlinear couplings between Se, Sb, and In that suggest unexplored pathways to enhanced performance.

Feature attribution analysis identified In content as the dominant driver of Eg, while Sb primarily shaped transport properties, consistent with defect-mediated conduction mechanisms. Beyond replication of prior results, the framework highlighted regions of compositional space where predictive uncertainty is highest, offering guidance for targeted experiments.

This study establishes AI as a powerful complement to semiconductor physics, enabling accelerated exploration of chalcogenide thin films. By integrating machine learning with physical insight, it opens a path toward data-driven discovery of optimized alloys for electronic, photonic, and memory applications.

CM-ThP-2 *Strata*PHI for Thin Film Surface & Interface Engineering: Depth-Resolved, Non-Destructive Analysis of Layered Materials, *Anthony Graziano,* ***Norbert Biderman [nbiderman@phi.com]***, Physical Electronics USA

Next-generation engineered materials increasingly demand new approaches as insights into ultra-thin films, surfaces, and interfaces are often obscured by the limitations of even traditional surface analysis techniques. As material systems become more complex, the need for precise, depth-resolved characterization of layered structures is critical for understanding performance, reliability, and process control. *Strata*PHI introduces a next-generation characterization platform designed for non-destructive analysis of multi-layer films composed of ultra-thin layers.

By leveraging X-ray photoelectron spectroscopy (XPS) and hard X-ray photoelectron spectroscopy (HAXPES), *Strata*PHI extracts key processing-dependent material parameters such as thickness and composition across stacks extending up to 30 nm beneath the surface. Fractional coverage analysis in *Strata*PHI also enables detection of partial film formation and interface quality such as incomplete Al_2O_3 growth, which is essential for optimizing atomic layer deposition (ALD) and other advanced coating processes.

The newest *Strata*PHI platform introduces an integrated analyzer acceptance angle mode that builds on the traditional model of a single photoelectron escape angle from the surface by including all escape angles as detected by the analyzer. This enables *Strata*PHI's application in engineered materials, delivering reliable thickness measurement of individual layers in a multi-layer thin film, equivalent to thicknesses traditionally obtained via angle-resolved XPS. The latest version of *Strata*PHI also enhances automated, real-time batch processing and full traceability of the relationship between material and processing parameters.

This presentation will demonstrate how *Strata*PHI enables researchers and engineers to model complex ultra-thin film stacks and extract insights into process-induced variations using its real-time batch processing capability, providing a comprehensive materials characterization suite for a deep understanding of ultra-thin films as well as their surfaces and interfaces.

CM-ThP-3 Active-Learning M3GNet-Accelerated Multiscale Pipeline for ALD/ALE Thin-Film Descriptors, ***Fedor Goumans [gouman@scm.com]***, *Nestor Aguirre, Nicolas Onofrio,* Software for Chemistry & Materials, Netherlands

We developed an automated multiscale pipeline that turns precursor/surface chemistry into device-relevant thin-film descriptors. Key components: (1) DFT reference calculations for representative surface terminations; (2) an active-learning M3GNet MLIP fine-tuned on DFT samples to accelerate PES exploration; (3) automated reaction-network extraction and selective DFT verification; (4) Bumblebee/Zacros 3D-kMC growth simulations that produce spatial maps of composition, nucleation density, defect/trap proxies and band-gap/dielectric indicators. The active-learning loop (ML uncertainty → targeted DFT → ML re-training) reduces the DFT budget by ~one order of magnitude in our tests while preserving energetics needed for kinetics. Results from the Ru–H ALE case study show: (a) ML-expanded PES discovery of alternative dissociative channels; (b) kMC–predicted trap-density maps that identify plasma flux / ion-energy windows minimizing interface damage; (c) sensitivity of band-gap and fixed-charge proxies to precursor chemistry and pulse timing. The poster presents the pipeline schematic, representative maps, and convergence plots showing ML error vs. cumulative DFT calls — demonstrating a practical route to speed up chemistry discovery for process engineers.

CM-ThP-4 Elastic Anisotropy and Stiffness Tensor Determination in TiN Thin Films, ***Rainer Hahn [rainer.hahn@tuwien.ac.at]***, CDL-SEC, TU Wien, Austria*; Rebecca Janknecht,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; Nikola Koutna,* TU Wien, Institute of Materials Science and Technology, Austria*; Anna Hirle,* CDL-SEC, TU Wien, Austria*; Anton Davydok,* Helmholtz-Zentrum Hereon, Germany*; Klaus Boebel,* Oerlikon Surface Solutions AG, Liechtenstein*; Szilard Kolozsvari, Peter Polcik,* Plansee Composite Materials GmbH, Germany*; Christina Krywka,* Helmholtz-Zentrum Hereon, Germany*; Paul H. Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria*; Helmut Riedl,* CDL-SEC, TU Wien, Austria

Direct experimental determination of elastic constants in thin films remains highly challenging due to small sample volumes, strong substrate constraints, and complex microstructures that differ fundamentally from bulk materials. While ab initio calculations provide valuable theoretical guidance, experimental validation has been limited by the lack of reliable, direction-dependent measurements on real thin film systems. This work advances the experimental methodology by combining in-situ micropillar compression with synchrotron X-ray microdiffraction to directly extract orientation-resolved elastic properties of polycrystalline TiN thin films. Building on earlier studies performed on Ti–B–N, this new approach benefits from a significantly expanded diffraction dataset, capturing multiple Debye–Scherrer rings that enable improved accuracy and statistical robustness. The simultaneous recording of mechanical and diffraction data during uniaxial compression allows tracking of elastic lattice strains as a function of applied stress, providing access to both macroscopic and crystallographic elastic responses. This comprehensive dataset forms the basis for reconstructing the stiffness tensor of TiN, thus linking macroscopic mechanical behavior to its crystallographic elasticity. The excellent correspondence between the experimentally derived constants and ab initio predictions underlines the reliability of this combined approach. The developed framework provides a robust method for determining the full elastic tensor of thin films, marking an important step toward quantitative micromechanical testing of complex coating materials.

CM-ThP-5 Hypulse XPSFemtoSecond Laser Ablation XPS Depth Profiling, ***James Lallo [james.lallo@thermofisher.com]***, Thermo Fisher Scientific, USA*; Tim Nunney, Robin Simposn,* Thermo Fisher Scientific, UK*; Mark Baker, Charlie Chandler,* University of Surrey, UK

The stability of novel perovskite photovoltaic devices is investigated via X-ray Photoelectron Spectroscopy. As XPS is a very surface sensitive technique, the experiment method involves depth profiling the material by interleaving analysis with removal steps, to characterize changes to the chemistry of these materials. XPS depth profiling is traditionally done usingmonatomic and gas cluster ion beam (GCIB) bombardment. However, ion beam methods induce changes in the material chemistry and morphology, affecting the validity of the results. By using Femtosecond laser ablation for XPS depth profiling it has been shown that analysis of thin film perovskite solar cell devices can be achieved without changing the chemistry.

Femtosecond laser Ablation XPS depth profiling has been performed here and compared with the traditional ion beam methods on different spin-coated formamidinium lead Iodide (CH5N2PbI3) based perovskite thin film solar cells, both pristine and following environmental testing. Fs-LA XPS depth profiles fully retained the true chemical composition of the 500 nm thick perovskite layer.

A femtosecond laser with a 1030 nm peak wavelength and a pulse duration of 160 fs was employed. The monatomic and cluster ion sputtering depth profiles exhibited chemical damage due to preferential sputtering of C, N and I.
Pb0 was also observed in the Pb 4f spectrum as a preferential sputtering artefact.

CM-ThP-6 Conditions for the Atom-by-Atom Growth of Maximum-Quality Thin Films, with a Focus on Ti-Al-N, ***Jiri Houska [jhouska@kfy.zcu.cz]***, *Hassan Ataalite,* University of West Bohemia, Czechia

The growth of metal, metal oxide and metal nitride thin films has been studied by molecular dynamics (MD) simulations. The overall aim is to reveal the relationships between the elemental composition, growth conditions, densification, stress, exact atomic structures (crucial for glasses) and conditions for the nucleation and uninterrupted growth of crystalline phases of interest (crucial for oxides and some of the nitrides). There are recent developments in this field, such as modelling the atom-by-atom growth of not only monocrystals but also nanocomposites or modelling based on machine learning interatomic potentials.

The first part of the contribution will summarize the methodology of growth simulations, materials' characteristics of interest and specifics of individual materials and individual mechanisms of interatomic bonding related to the modelling of the atom-by-atom growth. Because the success and reliability of classical MD in general and growth simulations in particular strongly depends on the interaction potential (force field), special attention will be paid to it.

The second part of the contribution will present very recent results of modelling the growth of technologically important Ti-Al-N. The process parameters include energy and momentum delivered into the growing films, energy distribution function of the film-forming flux, angle of the film-forming flux, temperature and crystal orientation. The specific results include particularly complex dependencies on the energy with multiple thresholds for individual atomic-scale processes, as well as dependencies of these threshold energies on the composition.

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