Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country A - 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-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.

CM-ThP-7 AI-Optimized Afterglow Functional Coatings for Enhanced Plant-Based Carbon Capture*, Yu-An Chen, Amit Kumar Sharma,* National Cheng Kung University, Taiwan*; Fei Pan,* ETH Zürich, Switzerland*; **Yen-Hsun Su [yhsu@mail.ncku.edu.tw]**,* National Cheng Kung University, Taiwan

Functional coatings offer a powerful yet underutilized platform for integrating advanced materials with biological carbon capture systems. In this study, we present an AI-optimized afterglow-enabled coating strategy designed to enhance photosynthetic carbon sequestration in indoor plants, positioning thin-film engineering as an active component in next-generation carbon capture solutions.A red-emitting afterglow phosphor system based on strontium sulfide (SrS) co-doped with europium (Eu) and praseodymium (Pr) was engineered to serve as a photonic energy storage layer. To ensure environmental stability and biocompatibility, the phosphor particles were encapsulated with a silica (SiO_2) shell and subsequently embedded into a transparent polymeric coating. This functional thin film was applied directly to the leaf surface of Monstera deliciosa, forming a conformal light-management layer that acts as a “light battery,” continuously supplying photosynthetically active radiation during low-light and dark periods.

To maximize luminescence performance and carbon fixation efficiency, an artificial intelligence–driven optimization framework was developed. A Genetic Algorithm–Neural Network (GA–NN) model was constructed to predict photoluminescence intensity as a function of Eu and Pr co-doping concentrations. The training dataset consisted of experimentally synthesized samples across multiple doping ratios and batch processes. A two-hidden-layer neural network architecture was selected to balance nonlinear representational capability with overfitting avoidance. The genetic algorithm employed a crossover rate of 0.7 and a mutation rate of 0.007, enabling rapid convergence while preserving population diversity. Model convergence was achieved within 30,000 generations and 300 evaluation cycles. The optimized dopant composition was further refined using a generative reinforcement learning strategy to jointly maximize afterglow intensity and photosynthetic response. As a result, the afterglow-functionalized coating increased net photosynthetic assimilation to 2.352 $\mu mol\cdot m^{-2}\cdot s^{-1}$ and enhanced sustained carbon capture efficiency by 20.55% compared to untreated controls. Beyond measurable performance gains, the coating provides aesthetic and functional value for indoor environments. This work demonstrates a novel paradigm in which AI-guided thin-film engineering directly augments biological carbon capture. By coupling functional coatings with machine-learning-driven materials optimization, the proposed approach offers a scalable and integrative pathway toward high-efficiency biosequestration in built environments.

CM-ThP-8 Development of an Electrical Waste Plastic Sorting System Using Laser-Induced Breakdown Spectroscopy and Convolutional Neural Networks*, **Guan Wen Chen [m13188009@o365.mcut.edu.tw]**, Tsung-Yu Huang,* Department of Materials Engineering, Ming Chi University of Technology, Taiwan

With the rapid growth in global consumption of electronic products, the management of waste electrical and electronic equipment (WEEE) plastics has become a critical environmental challenge. According to reports by the United Nations, a record 62 million tons of electronic waste were generated worldwide in 2022, while the global recycling rate remained as low as 22%. Current recycling systems largely rely on manual sorting, which faces significant limitations in efficiency and accuracy when dealing with discarded electronic plastics of complex compositions that often contain hazardous additives. These challenges severely hinder the realization of closed-loop resource recycling.

The objective of this study is to develop an automated intelligent sorting system by integrating laser-induced breakdown spectroscopy (LIBS) with a convolutional neural network (CNN). A total of 256 WEEE plastic samples were collected and classified into six material categories based on their polymer properties including acrylonitrile butadiene styrene (ABS), acrylonitrile butadiene styrene/polycarbonate blend (ABS/PC), polypropylene (PP), polystyrene (PS), poly(methyl methacrylate) (PMMA), and polystyrene/poly(methyl methacrylate) blend (PS/PMMA).

As for the model development of CNN, this study systematically investigated the key parameters of CNN, including input data representation, spectral matrix construction, the number of convolutional layers, the number of convolutional kernels, and kernel size. The experimental results indicate that when the LIBS spectra were reshaped into two-dimensional matrices with a size of 79 × 144, and the CNN architecture consisted of three convolutional layers, each with 64 kernels and a kernel size of 3 × 3, the proposed model achieved a classification accuracy of approximately 98% on the test dataset, demonstrating excellent classification performance and robustness.

This study confirms the feasibility of integrating spectroscopic techniques with multidimensional deep learning models for rapid, non-contact sorting of WEEE plastics, and highlights its strong potential as a technological solution for achieving industrial-scale automated recycling.

CM-ThP-9 Corrosion Resistance of Titanium Boride (TiB_X) Layers Formed on the Biomedical Ti6Al4V Alloy in Simulated Body Fluid*, **Tania Cabrera-Yacuta [tcabreray1800@alumno.ipn.mx]**,* Instituto Politécnico Nacional, Mexico*; J. Pérez-Alvárez, C. D. Rivera-Tello,* Universidad de Guadalajara, Mexico*; G. A. Rodríguez-Castro,* Instituto Politécnico Nacional, Mexico*; J.G. Quiñones-Galván,* Universidad de Guadalajara, Mexico*; A. Meneses-Amador, H. Martínez-Gutiérrez,* Instituto Politécnico Nacional, Mexico

The Ti6Al4V alloy is a benchmark material in biomedical applications due to its biocompatibility; however, its performance can be optimized through surface modifications to enhance durability in physiological environments. This study evaluates the corrosion resistance of Ti6Al4V modified by powder-pack boriding at 900, 1000, and 1100 °C for 20 h in simulated body fluid (SBF) at 37 °C. X-ray diffraction (XRD) confirmed the presence of TiB and TiB_2 phases. Furthermore, the results showed a progressive increase in the cumulative layer thickness (TiB_2 + TiB) with increasing temperature, reaching approximately 25 µm. Nanoindentation measurements evidenced a significant increase in surface hardness around 40 GPa, compared ~4 GPa for the base alloy. Electrochemical evaluations conducted via electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization confirmed that the borides layers act as effective passive barriers against ion transfer. The 900 °C treatment exhibited the best performance, recording the highest impedance modulus ($\sim 1.8 \times 10^5\ \Omega\cdot cm^2$) and a phase angle of 75°, indicating superior polarization resistance and slower charge transfer kinetics. In contrast, the 1100 °C condition showed lower impedance values ($\sim 4–5 \times 10^4\ \Omega\cdot cm^2$) and a reduced pseudo-capacitive response, which are associated with faster electrochemical processes and diminished protective capacity. Polarization tests corroborated this trend: the 900 °C condition achieved the lowest corrosion rate ($0.21\ \mu m\cdot y^{-1}$), representing a 50% improvement compared to the 1100 °C sample. These results suggest that corrosion protection is governed by the structural integrity and homogeneity of the borided layer rather than thickness alone

CM-ThP-10 Rapid Thickness Quantification of Coating Layers Using PLSR and Parallel Rietveld Analysis of XRD Data*, **Thomas Degen [thomas.degen@malvernpanalytical.com]**, Mustapha Sadki, Nicholas Norberg,* Malvern Panalytical, Netherlands*; Namsoo Shin,* Deep Solution Inc.,, Korea (Democratic People's Republic of)

Accurate monitoring of coating thickness in continuous galvanizing lines requires methods that are both rapid and statistically representative. In contrast to SEM, which probes only a limited number of local cross–sectional spots, **X-ray diffraction (XRD) and X-ray fluorescence (XRF) analyse a significantly larger illuminated surface area**, providing **more robust and representative layer–thickness values**. This makes XRF–derived layer thickness an ideal basis for calibrating both model–based and data–driven XRD approaches.

Building on our earlier work using a full-pattern Rietveld refinement approach to model layer thickness from XRD absorption effects, we now demonstrate that **Partial Least Squares Regression (PLSR)** applied to XRD patterns offers a **fast, calibration-driven route to direct thickness prediction**. PLSR captures subtle diffraction–pattern variations linked to changes in layer absorption, density, and microstructure without requiring explicit structural modelling. When trained using reference values obtained from **XRF and, where needed, SEM**, the PLSR model provides accurate and stable thickness predictions suitable for real–time process control.

We further show that both methods—**XRD–PLSR and XRD–Rietveld**—can be executed in parallel within the HighScore Plus [2] environment. This dual workflow delivers fast PLSR–based results for on-line feedback, while the Rietveld refinement provides full structural insight, including unit-cell parameters, crystallite size/strain, and texture. Importantly, **both XRD–derived thicknesses show excellent agreement with reference values from XRF and SEM**, confirming the robustness of the combined methodology.

This integrated approach enables **reliable, representative, and high-speed layer-thickness quantification** suitable for industrial environments.

References

[1] H.M. Rietveld, J. Appl. Cryst. (1969) 2, 65–71.
[2] T. Degen et al., Powder Diffr., 29 (2014), 13–18.

CM-ThP-11 Investigation of Epitaxial Silicon Growth Mechanisms from Chlorosilane–H2 Systems on Si(100) Substrates

*, **Seokmin Oh [min12002@yonsei.ac.kr]**, Dongmin Yoon, Seonwoong Jung, Hyerin Shin, Jungwoo Kim, Dae-Hong Ko,* Yonsei University, Republic of Korea

Silicon film growth using chlorosilane-based precursors is commonly employed in semiconductor manufacturing, including complementary metal–oxide–semiconductor devices and silicon solar cells. Despite their widespread use in high-temperature hydrogen environments, the elementary reaction steps involved in silicon epitaxial growth from chlorosilane–H_2 systems are not yet fully clarified. In this study, we examine the reaction pathways associated with chlorosilane-assisted silicon epitaxy by considering both gas-phase decomposition and surface reactions. Gas-phase reaction networks were analyzed using detailed chemical kinetics modeling, while surface reaction energetics were evaluated through first-principles calculations. Density functional theory calculations were performed using slab models of reconstructed Si(100) surfaces to describe adsorption, surface transformation, and desorption processes relevant to epitaxial growth. Transition states were explored using nudged elastic band–based methods to identify feasible reaction pathways. By combining gas-phase kinetics with surface-level reaction analysis, this work aims to improve the mechanistic understanding of silicon growth in chlorosilane–H_2 environments. The insights from this approach are expected to support the interpretation of precursor reactivity and surface chemistry in chlorosilane-based silicon epitaxy.

Acknowledgment

This work was supported by the Technology Innovation Programs (RS-2023-00235609 & RS-2025-02306457) and the K-CHIPS program (25065-15FC) funded by the Ministry of Trade, Industry & Energy (MOTIE, Korea).

CM-ThP-12 Machine-Learning Based Prediction of Carbon Quantum Dot Fluorescent Properties Using Molecular Representations

*, **Yehyeon Shin [yehyeon23@yonsei.ac.kr]**, Jong-souk Yeo, Chae-won Lee, Jong-Seok Lee,* Yonsei University, Korea

Carbon quantum dots are promising fluorescent nanomaterials which potentially offer reasonable synthetic routes with low cytotoxicity. They have been widely studied in various fields, including bioimaging, biosensing, drug delivery, and light-emitting devices. However, their broad methods of synthesis and many precursors make it difficult to predict the fluorescent properties of carbon quantum dots. Their fluorescent properties are influenced by many different factors, such as the dopant concentration within the core structure, particle size, synthesis conditions, and surface functional groups. These factors are regulated by complicated interactions of molecular structures, precursor interactions, and reaction conditions.

In this work, we adopt machine-learning based approaches to the prediction of synthesizing carbon quantum dots. These approaches are generally more suitable for modeling complex and non-linear relationships than other simulation methods. Applying these approaches would require input parameters of both reaction conditions and molecules. But there are difficulties in numerical encoding of molecular information, because molecules involve complex three-dimensional structures. Thus, we utilize molecule representations like graphs, 2D matrices, and SMILES (Simplified Molecular Input Line Entry System), which have commonly used in computational methods for predicting chemical formulas. Since molecule representations in these approaches focus on atoms and their bonds rather than the molecular information itself, our models allow extensive precursor inputs, unlike previous studies that restrict prediction to predefined and limited precursors.

In fact, our study shows a minimum mean average error (MAE) of 42.4 nm between predicted emission wavelengths and experimentally measured values, when precursors are introduced into the 2D matrix model. Although the current results indicate room for further refinement, this value is comparable to previous studies that predicted emission based on predefined precursors. Our approach is not restricted to specific molecular libraries, enabling scalable molecular design exploration and providing insight into the atomic and bonding features that contribute to emission properties of carbon quantum dots. Therefore, we systematically compare models based on different molecular representations and identify highly performing and broadly suitable models.

CM-ThP-13 Structural and Morphological Assessment of a Si/SiO_2/Cr/Au Thin-Film Electrode Stack via Correlative AFM with SEM & EDX

*, **Satyam Ladva [Satyam@qdusa.com]**,* Quantum Design, USA

Si/SiO_2/Cr/Au thin-film stacks are widely used as planar electrode platforms in electrochemical sensors, microelectrode arrays, MEMS, and FET-based devices due to their mechanical stability, chemical inertness, and electrical performance. Device reliability depends strongly on the integrity of each layer: a thermally stable Si substrate (~525 µm), an insulating SiO_2 layer (~90 nm), a Cr adhesion layer (30–50 nm), and a functional Au electrode layer (30–50 nm). Defects such as SiO_2 pinholes, poor Cr adhesion, or non-uniform Au growth can result in leakage currents, delamination, elevated contact resistance, and unstable electrochemical response.

We performed correlative scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and atomic force microscopy (AFM) using Quantum Design's FusionScope system on samples prepared by Moorfield's NanoPVD system, to assess morphology, roughness, and elemental distribution across representative regions of interest. This was performed under one environment, utilizing a single workflow, without needing to move the sample in and out of separate systems, reducing traditional workflow times by over 50%, whilst improving positional accuracy of the AFM.

Whilst the individual techniques utilized acquired traditionally common data e.g. SEM acquired surface morphology of the films, AFM acquired uniformity, roughness and mechanical properties of the film whilst EDS acquired elemental information – all implying a pure, uniform sample of roughness 1 – 5nm – the uniqueness resulted from the correlation of this data in real time allowing direct comparative analysis to be acquired in-situ rather than having to do much post-acquisition analysis on a separate platform.

This correlative technique can also be implemented on a range of other thin films, coatings, membranes etc... to provide precise and controllable AFM positioning and elemental information in an environment that is, traditionally, elementally blind.

Author Index

Bold page numbers indicate presenter