Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country D - Session CM3-1-MoA

Data-Driven Thin Film Design: High-Throughput Experimentation, Simulation, and Machine Learning I

Moderators: Kevin Kaufmann, Oerlikon, USA, **Po-Liang Liu**, National Chung Hsing University, Taiwan , **Sebastian Siol**, Empa, Switzerland

1:40pm **CM3-1-MoA-1 Predicting Outcomes of Thin-Film Synthesis from First Principles**, ***Vladan Stevanovic [vstevano@mines.edu]***, Colorado School of Mines, USA **INVITED**

The laws of thermodynamics are often used to predict outcomes of materials synthesis. However, thermodynamics alone cannot explain why some materials are easier and some much harder to grow, or why some systems exhibit strong tendencies toward forming stable amorphous phases and others do not. The situation is much more complicated for non-equilibrium synthesis methods (e.g. vacuum deposition), which often produce states that are not the thermodynamic ground states. In this talk I will describe the computational, first-principles technique we have developed to predict the likelihood for experimental realization of different states. We have found that many of the observed synthesis outcomes across material systems and growth methods can be explained using probabilistic arguments. The critical quantities are the sizes ("widths") of various local minima on the potential energy surface representing the states available to the system. By measuring the "widths" of local minima using the first-principles random structure sampling we have found that wider the local minimum (more probable in the random sampling) higher are its chances for experimental realization.[1] [#_edn1] This hypothesis has been validated against experiments and used to predict and explain synthesis outcomes more broadly. Examples include our recent work explaining why many layered ternary nitrides preferentially adopt a disordered rocksalt structure in as-grown thin-films despite the existence of ordered ground states much lower in energy.[2] [#_edn2] Or why Y_2WN_4 exhibits a strong tendency toward forming amorphous films, which are shown experimentally to be particularly resistant to crystallization.[3] [#_edn3] I will also discuss our approach to modeling kinetics of structural transformations and its utility in predicting the results of post-growth annealing.

[1] [#_ednref1] V. Stevanovic, Phys. Rev. Lett. 116, 075503 (2016)

[2] [#_ednref2] A. Zakutayev, M. Jankousky, L. Wolf, Y. Feng, C. L. Rom, S. R. Bauers, O. Borkiewicz, D. A. LaVan, R. W. Smaha, and V. Stevanovic, Nat. Synth. 3, 1471 (2024)

[3] [#_ednref3] O. V. Pshyk, S. Zhuk, J. Patidar, A. Wieczorek, A. Sharma, J. Michler, C. Cancellieri, V. Stevanovic, S. Siol, Adv. Mater. 2501074 (2025)

2:20pm **CM3-1-MoA-3 A Refined Toolbox for Predicting Phase Formation in PVD Thin Films**, ***Christian Gutschka [christian.gutschka@tuwien.ac.at]***, TU Wien, Austria; *David Holec,* Montanuniversität Leoben, Austria; *Jochen Schneider,* RWTH Aachen University, Germany; *Helmut Riedl-Tragenreif,* TU Wien, Austria

In recent decades, there has been a growing trend in the use of experimental and simulation-based screening methods across various fields of Materials Science. The main goal of these methods is to reduce the time and costs associated with laboratory experimentation. In the area of thin film technologies, especially regarding Physical Vapor Deposition (PVD) methods, combinatorial sputter deposition has emerged as a well-established experimental technique. However, ab initio methods, such as Density Functional Theory (DFT), often face limitations in accurately predicting essential properties like mechanical properties and the solubility of alloy components. The latter is of particular importance when novel thin film materials, such as carbides, nitrides, or borides, are engineered, as the extreme cooling rates during PVD promote the formation of metastable, often uncharted, solid solutions. Here trustful predictions in unexplored phase spaces, would be very helpful to optimize experimental work. However, one reasons why ab initio techniques frequently fail to yield satisfactory results for PVD thin films is that the resulting phase diagrams are markedly different compared to their equilibrium states – typically obtained from CALPHAD.

Nevertheless, over a decade ago, a model was proposed that connected combinatorial sputter deposition experiments with data obtained from DFT and CALPHAD. This model was capable of incorporating the effects of substrate temperature, target power and residual stress in the films. According to literature, the model has proven to be of adequate predictive accuracy, in the case of the metallic $W_{1-x}Cu_x$ and $V_{1-x}Cu_x$ [1] and the ceramic $Ti_{1-x}Al_xN$ and $V_{1-x}Al_xN$ [2,3] systems.

The present study aims to extend the methodology by virtue of two principal factors. Firstly, it negates the necessity for existing CALPHAD databases. Secondly, it incorporates the effects of interfacial energies stemming from microstructural causes, such as preferred crystal orientation and grain geometry. The present study focuses on ceramic thin films, and the initial stage involves a concise analysis of model dependencies regarding data from experiment and DFT. Subsequently, a reproduction and extension for the $Ti_{1-x}Al_xN$ and $V_{1-x}Al_xN$ systems is presented, with an outlook and presentation of ongoing work to test the method for established carbide and boride systems.

[1] Chang K., et al. Sci. Technol. Adv. Mater. 2016;17:210.

[2] Liu S., et al. Acta Mater. 2019;165:615.

[3] Liu S., et al. Acta Mater. 2020;196:313.

2:40pm **CM3-1-MoA-4 Pathways for the Preparation of Functional Coatings by Multiscale Modelling**, ***Jiri Houska [jhouska@kfy.zcu.cz]***[1], University of West Bohemia, Czechia **INVITED**

The lecture will cover different ways how to support the experimental research in the field of functional coatings by computer simulations. Various levels of theory (ranging from solid-state physics through atomic-scale ab-initio simulations to atomic-scale simulations based on empirical interaction potentials) and various simulation algorithms (ranging from static calculations of properties through searching for a local energy minimum to reproducing the time evolution of growing films) will be considered. Special attention will be paid to recent developments of the methodology. In all cases, the results will be compared to the experiment.

The first part will deal with a design of multilayered VO_2-based thermochromic coatings for smart energy-saving windows. Integral luminous transmittance and modulation of integral solar energy transmittance will be optimized in parallel, instead of a tradeoff between them. Prediction of coating color will be mentioned as well.

The second part will deal with an identification of maximum N content in amorphous Si–B–C–N networks of various compositions, assuming that it is limited by the formation, presence and loss of N_2 molecules. For example, the difficulties with the preparation of C_3N_4 will be explained by a maximum achievable stable N content in CN_x of 42%.

The third part will deal with reproducing the atom-by-atom growth of functional coatings in a wide range of conditions, using examples such as ZrO_2, Cu-Zr or Ti-Al-N. Effects of energy distribution function (not only average energy delivered into the films), mass of arriving particles (momentum delivered into the films) and growth temperature will be explained.

3:20pm **CM3-1-MoA-6 HADB Database: From Data Generation to AI-Supported Predictions of Properties of Hard-Coating Alloys**, ***Igor Abrikosov [igor.abrikosov@liu.se]***, *Sheuly Ghosh, Lalith Kumar Gurram, Jonatan Wästlund, Davide Sangiovanni, Ferenc Tasnádi,* Linköping University, IFM, Sweden **INVITED**

We introduce the HADB, a Hard-coating Alloys DataBase, available at https://hadb.funmat-ii.se/. HADB addresses a critical gap in existing materials databases by focusing on random alloys, important for industrial hard coatings applications such as metal cutting tools, with key data on thermodynamic, elastic, and mechanical properties. Focusing on ternary nitride alloys in two prototype crystal structures, rocksalt and zincblende, we present a reproducible workflow for high-throughput data generation in the framework of the Density Functional Theory (DFT). The framework integrates structure preprocessing, strategic composition selection to maximize successful data generation while minimizing usage of computational resources, automated DFT job submission, robust error handling, and post-processing analysis into a scalable pipeline. Further, data generated in DFT calculations at zero temperature is complemented by data at finite temperatures generated through ab initio Molecular Dynamics simulations. We discuss the technical implementations of the database infrastructure including support for browse, query, retrieval, and API access through the OPTIMADE API to make this data findable, accessible, interoperable, and reusable (FAIR). Finally, we demonstrate the potential of HADB to facilitate efficient alloy design in combination with a machine-learning (ML) Predictor. Our ML Predictor utilizes Crystal Graph Convolutional Neural Network (CGCNN) that has been trained on elastic properties for around 8000 compounds from Materials Project database as

[1] **Bill Sproul Awardee Honorary ICMCTF Lecture**

well as data for about 100 nitride alloys containing elements Ti, Hf, Zr, Al from HADB. Given an alloy composition beyond the data generated with DFT and its crystal structure, the model predicts with high accuracy single crystal elastic constants, bulk modulus, shear modulus, Young's modulus and Poisson ratios for the alloys.

4:00pm **CM3-1-MoA-8 The Intersection of Energy, Entropy, and Exploration: Data-Driven Discovery of High-Entropy Materials**, ***Corey Oses [corey@jhu.edu]***, Johns Hopkins University, USA **INVITED**

High-entropy materials, including oxides, metal alloys, and halides, are opening transformative possibilities for hydrogen generation, fuel cells, catalysis, energy storage, waste-heat recovery, radioactive waste immobilization, and radiation tolerance. However, the immense combinatorial complexity of these systems presents significant challenges for discovery and optimization. We employ data-driven approaches rooted in thermodynamics and chemistry to accelerate materials exploration, integrating high-throughput simulation, machine learning, and experimental feedback in a closed-loop workflow. This strategy efficiently guides exploration toward stable, high-performance compositions. Case studies demonstrate robust agreement with experimental results in mapping phase stability and uncovering functional materials. By advancing closed-loop discovery, we highlight scalable pathways to next-generation materials for critical energy applications.

4:40pm **CM3-1-MoA-10 Optimal Catalysts for Methane Pyrolysis by Atomistic Modelling of Molecule-Surface Interactions**, ***David Holec [david.holec@unileoben.ac.at]***, *Martin Matas,* Montanuniversität Leoben, Austria **INVITED**

Methane pyrolysis, heat decomposition into solid C and gas H_2, offers a promising technology for converting natural gas into hydrogen without causing CO_2 emissions. However, the necessary operating temperatures are too high for large-scale hydrogen production by catalyst-free methane pyrolysis. Therefore, catalytic methane pyrolysis, using liquid-metal bubble column reactors, has gained widespread interest. In this context, finding suitable catalysts that lower the operating temperatures and thus make methane pyrolysis economically viable and environmentally bearable has become an important scientific goal.We approach this topic by modelling interactions between CH_n (n=4, 3, ..., 1) molecules with different metallic surfaces using first-principles simulations. In the first part, we will present the results of the Sabatier analysis employing 0K adsorption energies on elemental metal surfaces. The results yield so-called volcano plots, which can be used for guiding the selection of the most efficient catalyst for selected conditions, i.e., temperature and methane partial pressure. In the second part of the talk, we will employ ab initio molecular dynamics to study the decomposition process directly at finite temperatures. We will also discuss the impact of the actual metal alloy composition and show that the catalytic efficiency is not a linear function between the two end members of the binary alloy. We will discuss quantities suitable for automatic statistical evaluation of the AIMD trajectories (such as bond-length and bond-length oscillations, or molecule-surface distance).These case studies will present state-of-the-art in gas–surface interaction modelling at the atomistic level: on the one hand, reliable qualitative predictions of trends guiding the experiments, and, on the other hand, the limitations for quantitatively capturing the complex experimental scenarios.

5:20pm **CM3-1-MoA-12 Multiscale Simulations from Precursors and Surface Chemistry to Thin Film Properties**, ***Fedor Goumans [goumans@scm.com]***, *Nestor Aguirrre, Nicolas Onofrio,* Software for Chemistry & Materials, Netherlands

Advanced device integration requires process-aware material descriptors that capture how precursor chemistry, plasma species and growth kinetics determine thin-film properties. We present a multiscale pipeline that couples DFT energetics, an active-learning M3GNet interatomic potential, automated PES exploration, and 3D kinetic Monte-Carlo growth simulations to produce spatially resolved property descriptors (growth rate, composition maps, defect/trap proxies, band-gap and dielectric indicators).

Starting from a foundation M3GNet universal machine learning interatomic potential (MLIP) and a small DFT seed set, we fine-tune and use uncertainty-guided sampling to automatically find intermediates and transition states; high-uncertainty configurations are re-computed with DFT and fed back to the MLIP, accelerating accurate exploration of the Potential Energy Surface (PES) at a little over MLIP cost with near-DFT accuracy. The verified reaction network parameterizes kMC to predict thin flim formation and etching, as functions of precursor, pulse timing, temperature and flux. We demonstrate the workflow on a Ru–H ALE case study: ML-accelerated PES exploration uncovered dissociative channels that shift band-gap and fixed-charge proxies; kMC maps reveal process windows minimizing interface trap formation while preserving selectivity. The approach provides compact, validated descriptors for process tuning and device correlation, shortening R&D cycles and guiding targeted experiments.

Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Palm 1-2 - Session CM1-1-TuM

Spatially-resolved and in situ Characterization of Thin Films, Coating and Engineered Surfaces I

Moderators: Damien Faurie, Université Sorbonne Paris Nord, France, **Naureen Ghafoor**, Linköping University, Sweden, **Aparna Saksena**, Max Planck Institute for Sustainable Materials, Germany

8:00am **CM1-1-TuM-1** ***Accelerated Atomic-Scale Exploration of Phase Evolution in Compositionally Complex Solid Solution Using Combinatorial Processing Platforms (CPP), Yujiao Li [yujiao.li@rub.de],*** Ruhr University Bochum, Germany **INVITED**

Combining microtip arrays with combinatorial thin film deposition and processing, along with direct atomic-scale characterization, we recently developed a new approach-combinatorial processing platform (CPP), which enables accelerated exploration of temperature- and environment-dependent phase evolution by (1) simultaneous synthesis of 36 identical volumes of nanocrystalline thin films on commercially-available Si tips; (2) rapid phase evolution upon successive thermal treatments; (3) direct near-atomic-scale analysis by atom probe tomography (APT), complemented by transmission electron microscopy (TEM).

Traditional methods of studying phase stability, evolving time-consuming material production process, long-term annealing for phase evolution, and sample preparation for microscopy, often take months or even years [1]. In contrast, our accelerated CPP approach dramatically reduces investigation time from months or years to several days.

In this talk, I will present the application of the CPP approach to study the phase stability of compositionally complex solid solution (CCSS) with a focus on the Cantor alloy (CrMnFeCoNi) [2] and CrCoNi alloy [3]. While these alloys are known for their unusual mechanical properties, they are susceptible to phase decomposition under elevated temperatures or reactive conditions. This can alter their superior properties and lead to potential failure. Therefore, understanding and controlling phase stability is crucial to optimizing their performance in real applications. We also extend this approach to investigate the oxidation [4] and electrochemical reactions [5] of CCSS. The results of these studies will also be presented.

[1] F. Otto, A. Dlouhý, K. G. Pradeep, M. Kubenova, D. Raabe, G. Eggeler and E. P. George, Acta Mater., 2016, 112, 40–52.

[2] Y. J. Li, A. Savan, A. Kostka, H. S. Stein and A. Ludwig, Accelerated atomic-scale exploration of phase evolution in compositionally complex materials, Mater. Horiz., 2018, 5,86–92.

[3] Y. J. Li, A. Kostka, A. Savan and A. Ludwig, Phase decomposition in a nanocrystalline CrCoNi alloy, Scr. Mater., 2018, 766, 1080–1085.

[4] Y. J. Li, A. Kostka, A. Savan and A. Ludwig, Atomic-scale investigation of fast oxidation kinetics of nanocrystalline CrMnFeCoNi thin films, J. Alloys Compd., 2018, 766, 1080–1085.

[5] V. Strotkötter, Y. Li, A. Kostka, F. Lourens, T. Löffler, W. Schuhmann and A. Ludwig, Self-formation of compositionally complexsurface oxides on high entropy alloys observed by accelerated atom probe tomography: a route to sustainable catalysts, Mater. Horiz., 2024, 11, 4932-4941 [tel:4932-4941] .

8:40am **CM1-1-TuM-3 Advanced Thin Film Characterization Through the Combination of New GD-OES System and Raman Analysis*, Kayvon Savadkouei [Kayvon.savadkouei@horiba.com],*** Horiba, USA*; Suyeon Lee, Patrick Chapon, Lionel Garrido,* Horiba Europe Research Center, France

Surface and interface studies require the use of complementary analytical techniques, as each instrumentation provides only partial information based on the interaction between the probing medium and the investigated material [1]. Here, we introduce a novel coupling of **Glow Discharge Optical Emission Spectroscopy (GD-OES)** with **Raman spectroscopy** for element-specific thin film characterization.

By combining GD-OES depth profiling with Raman spectroscopy, both elemental and molecular information of multilayers at different depths can be obtained [2]. This integrated approach provides a unique correlation between compositional and structural changes, enabling in-depth investigations of multi-layer thin films, conversion coatings, and organic coating systems. Representative results from multi-layered paint coatings for automobile applications demonstrate how the coupling of these two techniques enhances the understanding of complementary information from each layer.

Recent developments in GD-OES instrumentation, particularly the introduction of a new *Echelle* spectrometer and complementary metal-oxide-semiconductor (CMOS) camera detection system, have significantly expanded analytical possibilities. The *Echelle* system enables ultra-fast, simultaneous and automatic detection of all elements from hydrogen (and deuterium) to uranium at high acquisition rates, which is crucial for capturing transient phenomena and resolving nanometric interfacial layers. These improvements allow for more precise, comprehensive, and time-efficient investigations when GD-OES is coupled with Raman spectroscopy, ultimately enhancing the overall analytical performance of this hybrid approach.

These **hybrid analytical strategies**, coupling GD-OES with Raman spectroscopy, enable **quantitative, depth-, and time-resolved** characterization of complex materials.

[1] Compendium of Surface & Interface Analysis, Springer Raman and glow discharge optical emission spectroscopy studies on structure and anion incorporation properties of a hydrated alumina film on aluminum. Applied Surface Science 592 (2022) 153321.

[2] Advances in RF Glow Discharge Optical Emission Spectrometry Characterization of Intrinsic and Boron-Doped Diamond Coatings. *ACS Appl. Mater. Interfaces* 14, 5 (2022) 7405–7416.

9:00am **CM1-1-TuM-4** ***In Situ*** **Micromechanical Characterization of Nanocrystalline Materials Coupled with X-Ray Nanodiffraction*, Michael Meindlhumer [michael.meindlhumer@unileoben.ac.at],*** *Juraj Todt,* Technical University of Leoben, Austria*; Manfred Burghammer, Martin Rosenthal, Asma A. Medjahed,* ESRF, Grenoble, France*; Noel Sheshi,* University of Udine, Italy*; Michal Zitek, Anton Hohenwarter,* Technical University of Leoben, Austria*; Enrico Salvati,* University of Udine, Italy*; Doris Steinmüller-Nethl,* CarbonCompetence GmbH, Austria*; Daniel Kiener, Jozef Keckes, Markus Alfreider,* Technical University of Leoben, Austria **INVITED**

In order to improve our understanding of the mechanical behavior of nanocrystalline materials, it is essential to elucidate the multiaxial stress and strain fields throughout their irreversible deformation, especially in the regime where simplified homogeneous linear elastic assumptions are not valid anymore. Here, *in situ* micromechanical testing coupled with cross-sectional X-ray nanodiffraction (CSnanoXRD) with a spatial resolution down to 80 nm was used to resolve the individual multi-axial stress and strain fields throughout deformation history in two unique model experiments.

First, the capabilities of *in situ* CSnanoXRD will be showcased for monolithic ZrN and multi-layered ZrN-CuZr indented by a diamond wedge indenter tip coated with nanocrystalline (nc) diamond. Therefore, a diamond wedge indenter tip was coated with a nc diamond thin film, which was subsequently removed at the edges of the wedge using focused ion beam milling to ensure uniform signal during the CSnanoXRD experiment. Additionally, wedge samples for indentation were prepared from monolithic ZrN and a CuZr-ZrN multilayer thin films. This new kind of indentation experiment allows for tor the first time to directly assess the multi-axial stress distributions across the contact area for both the indenter tip and tested volume, thus, extending the classical single degree-of-freedom and single contact load-displacement response into a locally resolved a three-dimensional high-resolution probe.

In the second part of the contribution, we extend the CSnanoXRD capabilities further by nanoscale strain-mapping surrounding a growing crack tip in fracture specimens fabricated from a nc FeCrMnNiCo HEA. Thereby, one of two identical cantilevers was deformed *in situ* in a scanning electron microscope using the sequential loading-unloading approach to evaluate the incremental *J*-integral. Additionally, a point pattern was added on the surface of this cantilever allowing for the detailed analysis of the complete 2D surface strain components. CSnanoXRD was used to uncover the multi-axial stress fields associated with crack growth in the second HEA cantilever. This correlative approach for obtaining stress and strain data could be used for the first time to evaluate the *J*-integral around the crack tip in its original analytical form.

Altogheter, the quantitative experimental multi-axial strain and stress results give unprecedented insight into nanoscale deformation under severe loading conditions, which has significant implications in the development and assessment of modern damage-tolerant (thin film) materials and microstructures.

10:20am **CM1-1-TuM-8 Advanced Nanoscale 3D Tomography (APT) for Corrosion Barrier Healing in Steels*, Robert Ulfig [robert.ulfig@ametek.com],*** CAMECA Instruments Inc., USA **INVITED**

Stainless steels exposed to high temperatures undergo sensitization, a process that significantly reduces corrosion resistance due to chromium

carbide precipitation along grain boundaries [1]. This precipitation depletes chromium in the surrounding matrix below the threshold required for passivity, creating galvanically active regions prone to intergranular corrosion [2].

This study demonstrates the use of Ultrasonic Nanocrystalline Surface Modification (UNSM)—a high strain-rate surface peening technique—to rapidly desensitize sensitized AISI 304H austenitic stainless steel. High-resolution transmission electron microscopy and selected area electron diffraction confirmed that UNSM-induced localized strain and strain rate promote nanoscale deformation twinning in the austenite matrix.

Atom probe tomography (APT) revealed that deformation twinning facilitates nanoscale chromium homogenization near sensitization-induced grain boundary carbides. The minimum chromium content in the matrix increased from 7 at.% in the sensitized condition to ~12 at.% after UNSM treatment, surpassing the 11–12 at.% threshold for passivation. Crystallographic analysis of chromium distribution and carbide morphology suggests atomic transport during twin thickening as the underlying mechanism. These findings were enabled by recent advances in APT such as improved signal-to-noise ratio and a wide field-of-view. These capabilities will be discussed in relation to their impact on corrosion barrier characterization [4].

References:

1. ASM Handbook, Vol. 13B: Corrosion: Materials. ASM International, 2005.

2. E.L. Hall and C.L. Briant, Metall. Trans. A, 1984, vol. 15, pp. 793–811.

3. Ulfig, R. et al. LEAP 6000XR, New Applications, New Performance. Microscopy and Microanalysis 2022 vol. 28, pp. 3190–3191.

4. Sasidhar, K. N. et al. Understanding the protective ability of the native oxide on an Fe-13 at% Cr alloy at the atomic scale: A combined atom probe and electron microscopy study. Corrosion Science 2023 Vol. 211, pp. 110848.

Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Palm 1-2 - Session CM1-2-TuA

Spatially-resolved and in situ Characterization of Thin Films, Coating and Engineered Surfaces I

Moderators: Damien Faurie, Université Sorbonne Paris Nord, France, **Naureen Ghafoor**, Linköping University, Sweden, **Aparna Saksena**, Max Planck Institute for Sustainable Materials, Germany

2:00pm **CM1-2-TuA-2 Advancements in XPS Depth Profiling using Femtosecond Laser Ablation (fs-LA) for Thin Film and Metal Oxide Surfaces**, ***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

XPS depth profiling is a widely employed analytical technique to determine the chemical composition of thin films, coatings and multi-layered structures, due to its ease of quantification, good sensitivity and chemical state information. Since the introduction of XPS as a surface analytical technique more than 50 years ago, depth profiles have been performed using ion beam sputtering. However, many organic and inorganic materials suffer from ion beam damage, resulting in incorrect chemical compositions to be recorded during the depth profile. This problem has been resolved for most polymers by using argon gas cluster ion beams (GCIBs), but the use of GCIBs does not solve the issue for inorganics. We have introduced a novel XPS system, Hypulse, that employs a femtosecond laser rather than an ion beam for XPS depth profiling purposes. This novel technique has shown the capability of eradicating chemical damage during XPS depth profiling for all initial inorganic, compound semiconductor and organic materials examined. The technique is also capable of profiling to much greater depths (several 10s microns) and is much faster than traditional ion beam sputter depth profiling. fs-LA XPS depth profile results will be shown for selected thin films, coatings, multilayers and oxidized surfaces and the outlook for this new technique discussed.

2:20pm **CM1-2-TuA-3 Sample Charging During X-Ray Photoelectron Spectroscopy Analyses of Thin Film Insulators: From Understanding to Solution**, ***Grzegorz (Greg) Greczynski [grzegorz.greczynski@liu.se]***, Linkoping University, Sweden **INVITED**

Sample charging during X-ray photoelectron spectroscopy (XPS) analyses of electrically insulating samples is a widely recognized challenge of this essential technique. If the electron loss caused by the photoelectric effect is not compensated due to specimens' poor electrical conductivity, the positive charge building up in the surface region results in an uncontrolled shift of detected core level peaks to higher binding energy (BE). This seriously complicates chemical bonding assignment, which is based on measured peak positions, and accounts for a large spread in reported core level BE values. In this talk a new method for charging elimination is presented. The solution is based on the *ex-situ* capping of insulating samples with a few nm thick metallic layers that have low affinity to oxygen. The application examples include several industry-relevant oxides. The versatility of the charging elimination is demonstrated for different oxides/cap combinations and air exposure times. Results of the follow-up study aiming at a better understanding of physics behind charging and its elimination are also discussed. Although these studies are based on thin films, the conclusions give insights into critical factors that govern charging phenomena in any other type of insulating samples.

4:00pm **CM1-2-TuA-8 Is Platinum a Proton-Blocking Catalyst?**, ***Aparna Saksena [a.saksena@mpi-susmat.de]***, *Bingxin Li, Yujun Zhao, Manoj Prabhakar, Jörg Neugebauer, Mira Todorova, Dierk Raabe, Baptiste Gault, Yug Joshi,* Max-Planck-Institut for Sustainable Materials, Germany

Platinum, to date, is the most widely applied electrocatalyst for hydrogen evolution reaction (HER) in acidic media. It is assumed to be a proton-blocking catalyst with only surface-limited adsorption of the reaction intermediates. Here, we critically evaluate the bulk interaction of Pt with hydrogen (H), and its heavier isotope deuterium (D), by monitoring *operando* mass change of the Pt thin film electrode during galvanostatic heavy/water splitting by employing an electrochemical quartz crystal microbalance. Unexpectedly, we observe an irreversible temporal mass gain and a change in the reaction's overpotential, arising from diffusion of H/D into Pt, confirmed by atom probe tomography and thermal desorption spectroscopy. Sub-surface concentration of at least ca. 15 at. % of D in Pt was observed, diffusing down to a depth of more than 10 nm. Analytical description quantified the diffusion coefficient of D in Pt to be $(3.2\pm0.05)\times10^{-18}$ $cm^2 \cdot s^{-1}$. Density functional theory calculations supported the insertion of interstitial hydrogen as solid solution in Pt with a surface concentration of ca. 32 at.%. These findings challenge the existing credence of Pt-proton interaction being limited to the surface, prompting the expansion of the catalyst design strategies to account for property-modifying bulk diffusion of H/D in the Pt matrix.

4:20pm **CM1-2-TuA-9 Correlating Spectroscopic Ellipsometry Measurements in Imaging and Diffractive Modes**, *Md Rashedul Huqe, Yishu Foo, Kawshik Shikder, Yee Man Kwong, Zhang Yun, May Thawda Phoo,* ***Juan Antonio Zapien [apjazs@cityu.edu.hk]***, City University of Hong Kong

Non-imaging spectroscopic ellipsometry (SE) measurements provide extreme sensitivity on the fine details of subwavelength periodic samples and continue to be of importance because they are fast, contactless, and non-destructive. Such measurements, and corresponding modelling using Rigorous Coupled-Wave Analysis (RCWA), the Finite-Difference Time-Domain (FDTD) model, or the Finite Element Model (FEM), are done under the critical assumptions that i) the detected light includes only the zero-order specular reflection and ii) that the illumination area is sufficiently large to reasonably satisfy the ideal assumption of an infinite lattice. However, the increasing demand on photonic and plasmonic metamaterial applications provides fresh challenges for the SE strategies leading to renewed interest in imaging ellipsometry (IE). To date however, the use of IE for quantitative characterization of complex samples face significant challenges from experimental and modelling limitations when the aforementioned assumptions are not met. We recently proposed and build a dual-mode, imaging- and diffractive- spectroscopic ellipsometer to provide correlative and quantitative characterization of multiscale samples. We will discuss our current insights into the opportunities and challenges of this approach, including on-going efforts for the modelling and quantitative characterization of samples with complex structures.

We gratefully acknowledge the financial support from RGC (Projects CityU - 11215121 and 11310122) and ITC (Project ITS/461/18) of HKSAR, China.

4:40pm **CM1-2-TuA-10 Machine Learning Assisted Structure-Property Relationships by Nanoindentation**, ***Ude Dirk Hangen [ude.hangen@bruker.com]***, Bruker Nano GmbH, Germany; *Eric Hintsala, Bernhard Becker, Benjamin Stadnick, Kevin Schmalbach, Douglas Stauffer,* Bruker, Inc., USA

Nanoindentation can give a highly localized fingerprint of the materials elastic and plastic properties via the measured reduced modulus and hardness, respectively. Many thousands of indents can be done in a reasonable amount of time with modern instrumentation which can cover the sub-micron to mm-scale, allowing for structure-property relationships to be determined in complex heterogeneous materials. Machine learning can assist in this process in numerous ways, which will be discussed here. First, automatically identifying phases as regions of similar properties through clustering will be presented alongside a method to evaluate the uncertainty and bias of this approach.

Secondly, Bayesian optimization will also be employed to improve instrument efficiency in terms of placing indents in the most needed areas. Lastly, workflow improvements for the correlation of the indentation properties to co-located structural data will also be detailed.

Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM3-2-WeM

Data-Driven Thin Film Design: High-Throughput Experimentation, Simulation, and Machine Learning II

Moderators: Andrea Giunto, LBL, USA, **David Holec**, Montanuniversität Leoben, Austria

8:40am **CM3-2-WeM-3 Investigating growth twinning in NiCr and NiFe alloys by employing a combinatorial high throughput approach**, ***Ashley Maldonado Otero [ajmaldon@usc.edu]***, *Anthony Botros,* University of Southern California, USA*; Yi Liu,* University of California Irvine, USA*; Mohammad Hadi Yazdani, Aoyan Liang,* University of Southern California, USA*; Irene Beyerlein,* University of California Santa Barbara, USA*; Diana Farkas,* Virginia Tech, USA*; Paulo Branicio,* University of Southern California, USA*; Timothy Rupert,* Johns Hopkins University, USA*; Andrea Hodge,* University of Southern California, USA

Growth nanotwins (NT) are a special type of grain boundary associated with enhanced strength and thermal stability compared to nanocrystalline and ultra fine-grained materials. To date, research on nanotwinned materials has been limited to single and binary systems due to the lack of stacking fault energy (SFE) values and the high research time costs of exploring broader compositional ranges. By implementing combinatorial high throughput (CHT) techniques, it is possible to efficiently investigate NT formation and microstructural evolution over large compositional spaces. In particular, magnetron sputtering (MS) stands out as a versatile synthesis method because it offers the capability of depositing nearly any metallic alloy while providing a wide range of deposition parameters that can be modified to tune the resulting microstructure and morphology. In this study, a CHT methodology is employed to investigate growth nanotwinning in co-sputtered NiCr and NiFe alloys, which serve as precursors for Inconel 725. Regions across the compositional space where NT formation is either promoted or inhibited were identified, with Cr additions promoting a more densely and finely spaced NT microstructure than Fe. Attributed to the dependence of stacking fault energy—which is intrinsically linked to NT formation—on composition, this study demonstrates that CHT methodologies can be leveraged to understand growth twinning domains.

9:00am **CM3-2-WeM-4 High-Throughput Combinatorial Studies of Nanocrystalline Ni-Pt Thin Films**, ***Kyle Dorman [krdorma@sandia.gov]***, *Finley Haines, Heekwon Lee, Manish Jain, Tomas Babuska, Sadhvikas Addamane, Christian Harris, Luis Jauregui, Ping Lu, Brad Boyce, John Curry, David Adams,* Sandia National Lab, USA

Nanocrystalline thin films are a topic of interest in applications such as sliding metal contacts for their potential to enhance mechanical performance beyond that of their bulk polycrystalline counterparts. A wide-ranging combinatorial Ni-Pt survey was performed, seeking hard, electrically conductive coatings that might demonstrate enhanced wear resistance due to the catalytic potential of the material system encouraging lubricious tribofilm formation. The nanocrystalline thin film library was created by simultaneous confocal sputter deposition, with pulsed DC magnetron methods directing single element sources deliberately misaligned from ideal confocal geometry. The result, with the substrate fixed rather than rotated and the employment of photolithography, was a varied atomic composition across 112 samples on a single 150 mm diameter wafer. A series of such depositions, varying the gun angle and power at each cathode, allowed swift examination of nearly the full range of alloy compositions. Wavelength Dispersive Spectroscopy, X-ray Diffraction, X-ray Reflectivity, sheet resistance and nanoindentation were employed for high-throughput and fast-paced analysis. The binary collision Monte Carlo program SiMTra assisted with the deposition design and analysis. Promising tribological performance, high hardness, and low resistivity were observed.

9:20am **CM3-2-WeM-5 Experiment and Computation Meet in Mixed-Anion Thin Films**, ***Andrea Crovetto [ancro@dtu.dk]***, Technical University of Denmark **INVITED**

I will present initial results from a recently installed suite of vacuum deposition tools for combinatorial growth of “difficult” inorganic thin films, such as metal phosphochalcogenides and chalconitrides [1]. Thin-film synthesis of any material from these exotic mixed-anion chemistries is essentially unheard of. Such a lack of experimental studies is unfortunate because these material families have a remarkable degree of chemical diversity that could enable exciting applications in many fields.

We have been studying phosphosulfide compounds with an integrated experimental/computational work strategy inspired by the FAIR data principles. Density functional theory calculations indicate that many more of these compounds may be synthesizable than previously thought, including materials with previously unreported compositions and structures.

Backed by these computational results, we have so far explored five ternary phosphosulfide phase diagrams and one sulfonitride system by high-throughput experiments, targeting potential new semiconductors for photovoltaics. In this process, we have found promising materials for photoelectrochemistry, non-linear optics, and ultra-high refractive index applications.

[1] Mittmann, Crovetto, *J. Phys. Mater.* **2024**, *7*, 021002.

[2] Mittmann et al. *Chem. Sci.* **2025**, in press. https://doi.org/10.1039/D5SC05882A.

11:00am **CM3-2-WeM-10 Ion-Surface Interaction Models – Unraveling Microstructure Evolution in Oxides and Nitrides**, ***Denis Music [denis.music@mau.se]***, Malmö University, Sweden **INVITED**

Ion-surface interactions play a crucial role in microstructure evolution of thin films grown by magnetron sputtering and other plasma-based techniques. These processes affect adatom mobility, composition, nucleation kinetics, and stress. However, comprehensive models capable of describing the wide range of underlying mechanisms remain limited. Here, we introduce two models using accelerated density functional theory (DFT): one based on machine learning and the other referred to as the DFT thermal spike model. Oxides and nitrides were selected as benchmark systems. Sn-O thin films exhibit an unusual dendritic microstructure. To explain such behavior, a model was developed by integrating DFT with machine learning. The model identifies the average bond length and the number of nearest neighbors as key physical parameters governing surface adsorption, thereby enabling accelerated DFT simulations to uncover the fundamental growth mechanisms. Kinetic roughening is proposed as the initial stage of dendritic microstructure formation. Furthermore, the DFT thermal spike model was derived using TiN-based systems. Since conventional DFT is constrained by periodic boundary conditions and thus cannot accommodate high-energy ion impacts, the Kinchin-Pease equation was employed to parameterize thermally excited configurations that mimic such energetic events. This approach captures defect formation processes, such as Frenkel pair generation, which contribute to intrinsic stress. As the model operates at the electronic-structure level, it allows for the derivation of physical properties and provides insight into experimental observations. For example, applying this framework to oxynitrides such as TiAlON explains its exceptional thermal stability, exceeding that of TiAlN by approximately 300 °C. Overall, our approach enhances modeling of thin film behavior through atomistic insights and data-driven methods.

11:40am **CM3-2-WeM-12 Ai-Driven Prediction of Work Function Variations in $ZnGa_2O_4$(111) Under Multi-Gas Adsorption**, *Chao-Chang Shen,* National Chung Hsing University, Taiwan*; Sheng-Fang Huang,* China University of Science and Technology, Taiwan*;* ***Po-Liang Liu [pliu@dragon.nchu.edu.tw]***, National Chung Hsing University, Taiwan

Machine learning (ML), combined with first-principles density functional theory (DFT) calculations, establishes a data-driven workflow to predict the work function of the $ZnGa_2O_4$(111) surface under single-and dual-gas adsorption of NO, NO_2, CO, CO_2, H_2S, and O_3. We employ a set of regression models, including neural networks (NN), gradient boosting regressors (GBR), support vector regression (SVR), random forest regression (RFR), decision trees (DT), and linear regression (LR). Their predictive accuracy was evaluated using mean absolute error (MAE), mean absolute percentage error (MAPE), and the coefficient of determination (R^2). Results from fivefold cross-validation show that the NN achieves the lowest MAE and MAPE of 0.23 eV and 5.8%, respectively, with R^2 reaching 0.85, demonstrating robust discrimination among gas identities, adsorption sites, and surface conditions. Feature-importance analysis indicates that gas identity is the primary influencing factor, followed by the oxygen passivation state and adsorption site, suggesting that gas identity and the surface chemical environment play key roles in determining the work function. To improve usability, we developed an interactive web interface that allows users to upload crystal structure files. The system automatically performs structural analysis and feature extraction, returning real-time work-function predictions and structural visualizations to support interactive evaluation and iterative design of individual structures.

12:00pm **CM3-2-WeM-13 Artificial Intelligence Framework for Understanding Defect-Mediated Transport in Se–Te–Pb Thin Films**, ***Maninder Kamboj [maninderk@gmail.com]***, *Farah Mohammadi,* Toronto Metropolitan University, Canada

This work investigates the dark and photoconductive behavior of amorphous Se–Te–Pb thin films using an Artificial Intelligence (AI)–based framework that fuses experimental data with predictive modeling. Thin films of Se–Te–Pb with Pb concentrations ranging from 0 to 6 at.% were fabricated by thermal evaporation, and current–voltage characteristics were recorded under both dark and illuminated conditions. The resulting conductivity and activation-energy data were used to train and validate machine-learning models, including polynomial regression, multilayer perceptron (MLP), and adaptive boosting (AdaBoost).

Among these algorithms, the MLP model achieved the highest predictive accuracy, yielding an average R^2 = 0.982 for dark conductivity and R^2 = 0.975 for photoconductivity datasets. For the Pb = 0 sample, AI-predicted dark conductivity ($1.6 \times 10^{-8}\ \Omega^{-1}\ cm^{-1}$) closely matched the experimental value ($1.55 \times 10^{-8}\ \Omega^{-1}\ cm^{-1}$). Under illumination, the predicted conductivity increase by 3.1× corresponded well to the experimental enhancement of 3.3×. At higher Pb contents (4 % and 6 %), the AI model captured the observed reduction in activation energy from 0.48 eV to 0.32 eV with an overall deviation below 4 %.

The comparison between AI-predicted and experimental curves demonstrates strong agreement across all compositions, accurately reproducing both sublinear and saturation regimes of photoconductivity. Feature-importance analysis confirmed that Pb concentration was the dominant factor controlling dark resistivity, while illumination intensity most strongly influenced photoconductive gain.

By integrating AI-driven analytics with experimental validation, this framework provides a rapid, scalable route to decode the complex, defect-mediated transport mechanisms in amorphous chalcogenide thin films. The close AI–experimental correlation (R^2 > 0.97) highlights the potential of data-centric modeling to accelerate the predictive design of next-generation photoconductive and optoelectronic materials.

Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM2-1-ThM

Advanced Mechanical-Physical Testing of Surfaces, Thin Films, Coatings and Small Volumes I

Moderators: Hanna Bishara, Tel Aviv University, Israel, **Matteo Ghidelli**, Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France

8:40am **CM2-1-ThM-3 Ultra–High Vacuum Tribology: Industrial Relevance, Mechanisms, and Research Gaps**, ***Esteban Broitman [ebroitm@hotmail.com]***, *Sven Kelling, Rickmer Kose,* Sentys Inc., USA

Tribological behavior—friction, wear, and adhesion—depends critically on the local environment at contacting surfaces. In ambient air, adsorbed water, oxygen, and organic contaminants form boundary films that dominate contact mechanics and chemistry; as pressure is reduced these physisorbed layers thin and desorb, shifting surface interactions toward intrinsic solid–solid processes. Ultra–high vacuum (UHV), commonly defined as pressures below 10^{-9} mbar, represents an extreme limit in which physisorbed monolayers are effectively absent on laboratory timescales and surface chemistry is governed by atomic–scale adsorption and chemisorption. UHV conditions therefore provide a unique window onto fundamental friction and wear mechanisms that are masked at higher pressures.

For industrial applications, UHV tribology is directly relevant to sectors where components operate in extreme vacuum or require contamination–free contacts: satellite mechanisms and deployable structures, scientific instruments and space optics, semiconductor and thin–film processing tools, electron– and ion–beam systems, particle accelerators, and vacuum–operated MEMS/NEMS. Despite this industrial relevance, UHV tribology remains comparatively rare: most experimental work is performed in atmosphere or in high vacuum (HV, 10^{-3}–10^{-7} mbar), where residual gases and humidity continue to influence outcomes. The scarcity of UHV studies reflects practical barriers—specialized chambers, rigorous sample preparation and bakeout, vacuum–compatible instrumentation, and long pumpdown cycles—as well as a perception that UHV results have limited applicability to real–world service. Commercial UHV tribometry options are extremely limited; **PREVAC** currently offers a commercial UHV tribometer capable of reaching pressures on the order of 10^{-9} mbar, representing one of the few turnkey solutions for routine industrial UHV tribological testing.

This presentation evaluates UHV tribology through an industrial lens, bridging the gap between fundamental research and practical application. By comparing friction and wear data across UHV, high vacuum, and atmospheric conditions for common materials and coatings, we identify critical performance shifts. We conclude with actionable design recommendations aimed at accelerating the integration of UHV tribology into industrial hardware for product design and development.

9:00am **CM2-1-ThM-4 Atomic-Scale Revealing the Mechanical Response of Defect-Mediated Nitride Ceramics**, ***Zhang Zaoli [zaoli.zhang@oeaw.ac.at]***, Erich Schmid Institute, Austria*; Chen Zhuo, Yong Huang,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Nitride ceramic coating materials exhibit several advantages over metals, including superior hardness, wear resistance, thermal stability, and oxidation resistance [1-3]. With the growing need for industrial applications and environmental considerations, developing new composite nitride coatings that are both economically and environmentally friendly has become a challenging task. Using the architectural structure design of the interface and planar defects could be one approach. Along this line, we made some progress.

The extensive high-resolution transmission electron microscopy (HRTEM) observations of the TaN/TiN multilayer reveal that dissociation of full dislocations results in a network of stacking faults (SFs) and the formation of Lomer-Cottrell lock arrays within the TaN layer. Consequently, the high density of stacking faults dramatically strengthens the TaN/TiN multilayer [1]. Using valence electrons and inner shell electron spectroscopy, a combined experimental analysis of a multilayered structure of CrN/AlN allowed for the mapping of the multilayer's mechanical properties (bulk modulus) at the nanometer scale [2].

We observed atomic-scale intermixing in the nanoscale TiN/AlN multilayer by combining cross-sectional FIB cutting with atomic-resolution electron microscopy. A new solid-solution phase formed, as evidenced by mapping electronic structure differences. Using atomic EDS, we further corroborated that a homogeneous solid-solution zone formed upon loading [3].

From atomic-resolution observations, we first revealed that deformation in vacancy–engineered WNx/TiN multilayers can also be achieved through unit-unit disturbance. Instead of dislocation motion, multiple local unit-cell-scale disturbances can dissipate local strains, thereby releasing stress concentrations and enabling large-scale deformation. This mechanism leads to a significant enhancement of mechanical properties [4]. Moreover, one remarkable advancement is the discovery of an approach that successfully introduces a large density of nanotwins into nitride ceramics [5]. The synergy between the strength and toughness of nitride ceramics is enhanced. [5]

[1] Yong Huang et al., *Acta Materialia* 255 (2023) 119027

[2] Zaoli Zhang et al., *Acta Materialia*, 194(2020) 343

[3] Zhuo Chen et al., *Acta Materialia*, 214(2021)117004.

[4] Zhuo Chen et al., *Nature Communications*, (2023)14:8387

[5] Yong Huang, et al., Acta Materialia 299 (2025) 121475

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9:20am **CM2-1-ThM-5 Probing nanoscale deformation mechanisms in metastable metallic thin films using 4D-STEM**, ***Lukas Schretter [lukas.schretter@oeaw.ac.at]***, *Jürgen Eckert, Christoph Gammer,* Austrian Academy of Sciences, Austria **INVITED**

Understanding the deformation behavior of metallic thin films at small scales is essential for advancing nanoscale devices and coating performance. Mechanical properties are strongly governed by microstructural features such as grain size, defects, and interfaces, leading to pronounced spatial variations in elastic and plastic response and thus controlling failure. Conventional macroscopic testing is unable to resolve these local effects. In this talk, we present the recent progress in probing the nanoscale deformation mechanisms of metallic thin films at the nanoscale using four-dimensional scanning transmission electron microscopy (4D-STEM). This technique enables in-situ strain and crystal orientation mapping with nanometer spatial resolution during simultaneous mechanical loading inside the transmission electron microscope. Utilizing this advanced characterization technique, we aim to provide quantitative insight into the local strain evolution, stress redistribution, and defect activity that lead to material failure. The results demonstrate how 4D-STEM serves as a powerful tool for linking microstructure and mechanical performance. These insights provide a foundation for designing new material systems with tailored mechanical performance and improved reliability through nanoscale structural design.

10:20am **CM2-1-ThM-8 High-Speed Nanoindentation Mapping and Machine Learning as Enabling Technologies for Combinatorial Thin-Film Libraries**, ***Edoardo Bemporad [edoardo.bemporad@uniroma3.it]***, Roma tre university, Italy*; Rostislav Daniel,* Montanuniversität Leoben, Leoben, Austria*; Edoardo Rossi,* Roma Tre University, Italy*; Michal Zitek,* Montanuniversität Leoben, Leoben, Austria*; Marco Sebastiani,* Roma Tre University, Italy **INVITED**

Combinatorial thin-film libraries are rapidly transforming the exploration of complex metallic alloys, yet the ability to interpret their mechanical behavior across broad compositional gradients remains a significant challenge. High-speed nanoindentation mapping, combined with advanced data analytics, now provides the statistical depth and spatial resolution required to transform such coatings into quantitative mechanical datasets.

In this study, a compositionally graded Cr–Cu–Ti–W system was synthesized as a model platform to investigate how partial miscibility and non-equilibrium co-sputtering produce diverse architectures: from nanocrystalline solid solutions to amorphous metallic composites. More than 3,000 indents were acquired across 29 regions of interest, establishing position-resolved maps of hardness, modulus, and derived figures of merit (H/E, H^3/E^2). When correlated with local EDX composition and confirmed by STEM-EDS, the results reveal distinct mechanical regimes: Ti- and Cr-rich domains combine strength and compliance, whereas W-enriched regions exhibit high stiffness but limited deformability.

In this framework, unsupervised learning algorithms are applied to analyze the high-speed indentation dataset, identifying clusters of mechanical behavior. These mechanically defined clusters guide targeted investigations into microstructural and micromechanical properties. The analysis utilizes

micropillar compression data from over 200 pillars across different regions of interest to directly assess yield strength and strain-hardening behavior.

Unsupervised learning and dimensionality-reduction algorithms classify the pillars based on their deformation responses and connect these classifications to local indentation signatures and transmission electron microscopy (TEM) resolved microstructures. This approach allows for the identification of recurring deformation patterns, such as shear localization, homogeneous flow, or cracking, that are associated with specific compositional and microstructural configurations.

This combined experimental–computational framework provides a pathway for the rational design of multicomponent coatings, in which mechanical functionality emerges from quantitative correlations across scales.

11:00am **CM2-1-ThM-10 Deformation Twins, Kink Bands and Stacking Faults: Highlighting the Diversity and Complementarity of Deformation Mechanisms in the MAX Phase Cr_2AlC Through Micromechanical Testing**, ***Christophe TROMAS [christophe.tromas@univ-poitiers.fr]***, *Mohamed AKOU,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France*; Salomé PARENT,* institut pprime - CNRS - ENSMA - Université de Poitiers, France*; Anne JOULAIN,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France **INVITED**

In the process of determining the elementary mechanisms of plastic deformation, micromechanical testing has opened up a new avenue. Nanoindentation testing induces plasticity into a micrometer size volume, providing a localized plastic deformation structure that is easy to observe and identify. A spherical tip, instead of a classical pyramidal tip, avoid stress concentrations and produces a long-range stress gradient, with regions in tension and others in compression or shear, providing a broad sample of the possible mechanism in a given area. Complementarily, compression tests performed using a nanoindenter, equipped with a flat punch, on micrometer-sized pillars prepared by focused ion beam (FIB), generate a uniaxial and uniform compressive stress, easier to analyze. Furthermore, thanks to in situ experiments, observation of the free surfaces of the pillars under compression provides dynamic information on the deformation process.

In this study, the plastic deformation mechanisms of the MAX phase Cr_2AlC (a nanolamellar material with a hexagonal crystallographic structure) is investigated using micropillars compressions experiments and spherical nanoindentation. In both cases, the deformation microstructure is analyzed by Transmission Electron Microscopy (TEM) on lamella extracted along different orientations, in combination with surface observation by Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM), and with local crystallographic misorientation maps (ACOM ASTAR). This approach allows us to study the role played by deformation twinning, kink bands and stacking faults in the plastic deformation processes in this material.

11:40am **CM2-1-ThM-12 Analysis of the Mechanical Properties of APS Coatings Deposited on Agricultural Plough Components**, *Boris Nazar,* Technical University of Moldova*; Fabian Cezar Lupu, Corneliu Munteanu, Viorel Goanta,* ***Bogdan Istrate [bogdan.istrate@academic.tuiasi.ro]***, "Gheorghe Asachi" Technical University of Iasi, Romania*; Grigore Marian,* Technical University of Moldova*; Marcelin Benchea,* "Gheorghe Asachi" Technical University of Iasi, Romania

The present paper presents research conducted in the field of thermal spray coatings aimed at improving the properties of agricultural components. The studies focus on thermal plasma jet deposits using the APS (Atmospheric Plasma Spray) technique applied to agricultural plough components designed for soil processing. These components are subjected to extreme operating conditions during use, and their main required properties are wear and impact resistance - key performance factors that determine the plough's service life.

In the research, thermal coatings were produced using WC–12%Co–based metallic powders (commercial name WOKA 3101). On laboratory samples, mechanical properties were evaluated through tensile tests, micro-scratch testing, and determination of the coefficient of friction under both rotational and translational motion. Since these components experience significant operational stress, thermal spraying represents an effective method not only for improving the mechanical properties of newly manufactured parts but also for refurbishing worn elements to restore them to proper working condition.

Acknowledgment: This work was supported by a grant from the Ministry of Education and Research, CCCDI–UEFISCDI, project number PN-IV-PCB-RO-MD-2024-0336, within PNCDI IV

12:00pm **CM2-1-ThM-13 Thin Film Characterization by Ultrasonically Induced Nanofatigue During Nanoindentation**, ***Antanas Daugela [info@nanometronix.com]***, Nanometronix LLC, USA

In the era of fast product development thin film researchers are looking for fast and efficient methods of characterization.This is especially true in a semi-conductor industry where advanced multilayered chip/MEMS development process needs advanced characterization techniques. Nanoindentation based multi-cycle loading is offering insides into the real-time contact fracture dynamics [1]. A nanofatigue phenomenon can be observed on thin sub-micrometer films by monitoring the resulting multi-cycle nanoindentation loading-unloading curves where post-test imaging helps in identifying materials' behavior [2, 3].In addition, classical Mason-Coffin and ratcheting fatigue models derived for the nanoscale contact can be utilized in the predictions and correlate reasonably well with nanofatigue cycles obtained experimentally.

A newly developed ultrasonic nanoindentation tip operates at hundreds of kHz, therefore, inducing millions of load cycles within seconds.The resulting nanofatigue induces different thin film fracture modes such as radial, sink-in and produce unique acoustic signatures.The ultrasonic nanoindentation tip monitors associated waveforms, which can provide additional insides into nanofatigue process dynamics via advanced acoustic waveform analysis.Following our previous study [4], acoustic waveforms were processed using a combination of harmonics and Gauss noise base functions for signal decomposition. The proposed Deep Learning technique yields in reliable classification of acoustic signatures obtained during fracturing ofsub-micrometer thick coatings.Multiple SiC and GaAr semi-conductor thin films were tested.

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Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM3-3-ThA

Data-Driven Thin Film Design: High-Throughput Experimentation, Simulation, and Machine Learning III

Moderators: Kevin Kaufmann, Oerlikon, USA, **Sebastian Siol**, Empa, Switzerland

1:20pm **CM3-3-ThA-1 Transforming Thin-Film Research Through Autonomous Experimentation: From Synthesis to Long-Term Device Performance**, ***Davi Febba [davimarcelo.febba@nrel.gov]***, *Brooks Tellekamp, William Callahan, Andriy Zakutayev,* National Renewable Energy Laboratory, USA **INVITED**

The synthesis and characterization of thin-film materials traditionally require lengthy experimental campaigns, where processing conditions are iteratively adjusted to achieve desired compositions and properties. This challenge intensifies when studying complete devices, as interfacial phenomena play a decisive role in performance.

Autonomous experimentation is transforming this paradigm. By automating repetitive tasks and deploying AI-driven experiment planners, researchers can dramatically accelerate the materials discovery and optimization pipeline while reducing manual intervention.

In this presentation, I will summarize recent advances at NREL in (i) autonomous sputtering and molecular beam epitaxy (MBE) growth of thin films[1,2], and (ii) autonomous, long-term degradation studies of electronic devices under extreme environmental conditions[3]. These platforms integrate genetic algorithms, computer-vision feedback, and multidimensional Bayesian optimization to identify the most informative experiments in real time—maximizing information gain per unit time. I will also discuss the design and deployment of AI agents for direct instrument control, demonstrating how they enhance safety, reliability, and throughput.

Finally, I will highlight the practical aspects of retrofitting existing laboratories for autonomy, including instrument-level automation, workflow orchestration, data-management infrastructure, and networking strategies that link remote servers with local command-and-control systems. Together, these elements enable seamless, closed-loop operation across diverse scientific instruments, advancing the vision of fully autonomous research laboratories at NREL.

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2:00pm **CM3-3-ThA-3 HiPIMS Process-Optimization in an Autonomous Sputter Chamber via Active Learning**, *Alexander Wieczorek, Nathan Rodkey,* ***Sebastian Siol [sebastian.siol@empa.ch]***, Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

The growing demand for data-driven discovery in materials science has spurred rapid advances in autonomous experimentation. However, these developments have so far rarely extended to physical vapor deposition (PVD) methods, largely due to the technical challenges of automating such complex systems. Yet, the PVD community faces an urgent need for systematic data acquisition, as its processes continue to gain complexity. For instance, high-power impulse magnetron sputtering (HiPIMS) has become increasingly prevalent but introduces several additional process dimensions compared to conventional DC sputtering, such as frequency, pulse width, and peak current density. This expanding parameter space complicates experimental optimization and impedes a deeper understanding of the physical mechanisms governing HiPIMS.

To address this challenge, we developed an autonomous sputter deposition platform interfaced with LabView and controlled via a Python-based code utilizing Bayesian optimization. The system efficiently explores a defined parameter space through iterative, data-informed sampling. Large datasets of HiPIMS process parameters are collected autonomously and subsequently analyzed using Shapley Additive Explanations (SHAP), a machine learning approach capable of disentangling complex, high-dimensional relationships. This combination of automation, Bayesian statistics, and interpretive modeling enables data-driven insights into the underlying physics of advanced PVD processes. In this presentation we will show the experimental setup and workflow as well as first studies of HiPIMS parameter optimisation using in-situ plasma diagnostics.

2:20pm **CM3-3-ThA-4 Accelerating Experiments with AI and Automation: Powder Materials and their Compositional Characterization**, ***Andrea Giunto [agiunto@lbl.gov]***, *Yuxing Fei, Bernardus Rendy,* Lawrence Berkeley Lab, University of California, Berkeley, USA*; Pragnay Nevatia,* University of California at Berkeley, USA*; Nathan Szymanski, Gerbrand Ceder,* Lawrence Berkeley Lab, University of California, Berkeley, USA **INVITED**

Computational materials science, accelerated by AI, has enabled the prediction of thousands of new inorganic compounds. However, their experimental realization remains a key bottleneck. To close this gap, automated and AI-driven laboratories are emerging. In our group, we have developed the **A-lab**, a platform for automated solid-state synthesis and characterization of powder materials [1,2]. This talk will present the A-lab's capabilities, focusing on the challenges of reaction product characterization and our automated, AI-based solutions. We combine X-ray Diffraction (XRD) for structural analysis with automated compositional analysis by Energy-Dispersive X-Ray Spectroscopy (EDS) in a desktop SEM, using a framework developed in-house, and implemented in the Python package **AutoEMXSp** [3]. I will discuss strategies to obtain accurate compositional analysis of powders and how these methods can be extended to thin-film materials.

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3:00pm **CM3-3-ThA-6 Autonomous Experimentation with Quality Control and Cross-Facility Coordination**, ***Yongtao Liu [liuy3@ornl.gov]***, Oak Ridge National Laboratory, USA **INVITED**

Recent advancements in AI-driven autonomous experimentation (AE) are transforming the landscape of materials research These systems hold great promise for accelerating discovery, yet fully autonomous frameworks often struggle with the complexity, variability, and evolving nature of real-world experimental environments, sometimes misleading the AE process. In this talk, I will discuss our approach for overcoming these challenges by embedding quality control and expert guidance into active learning–based AE systems. Rather than relying solely on ML optimization, our framework allows experts to guide and refine the system's exploration in real time, leading to more meaningful experimentation. We have implemented this approach in autonomous thin-film synthesis and microscopy characterization, but its principles can be extended to many other AE platforms.In addition, as materials development increasingly relies on multimodal characterization to reveal the intricate chemical-structure-property relationships, most autonomous materials research platforms are limited to a narrow set of diagnostic tools due to constraints in lab space, available expertise, instrumentation capacity, etc. This hinders their ability to make informed decisions and generalize across diverse material systems. To address this gap, we further extend our approach to connect distributed AE platforms and supports hybrid integration of automated and manual tools, which broadens the diagnostic capabilities available to the autonomous research process. This framework enables real-time data exchange and coordinated decision-making across multiple systems, allowing independent platforms to collaborate seamlessly without requiring physical integration. This points toward an interconnect model of autonomous research by linking distributed facilities for more collaborative and adaptive autonomous materials discovery. Acknowledgments: This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory. This research and workflow development was sponsored by the INTERSECT Initiative as part of the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC for the US Department of Energy under contract DE-AC05-00OR22725.

4:00pm **CM3-3-ThA-9 Self-Navigating Thin Film Laboratory: Real-Time AI-Driven Optimization of Functional Thin Films**, ***Ichiro Takeuchi [takeuchi@umd.edu]***, University of Maryland, USA **INVITED**

Autonomous experimentation can be used to reduce the number of required experimental cycles for materials optimization by an order of magnitude or more by enlisting Bayesian optimization using Gaussian Processes. We have demonstrated autonomous control of unit cell-level growth of functional thin films implemented in pulsed laser deposition. Dynamic analysis of reflection high-energy electron diffraction images is used to autonomously navigate multi-dimensional deposition parameter space in order to rapidly identify the optimum set of growth parameters for fabricating the targeted materials phase. As an example, we have set up the autonomous system to synthesize the meta-stable hexagonal phase of $TbFeO_3$ and other rare-earth ferrites where substrate temperature, oxygen pressure, and the laser repetition rate are varied simultaneously. The self-navigating algorithm is able to consistently find the optimum conditions within 10-15 iterations resulting in thin films of the phase pure hexagonal phase. Our scheme can be applied to any type of thin film/semiconductor manufacturing setting where an effective in-situ characterization tool can be used to provide real-time autonomous feedback. This work is carried out in collaboration with Haotong Liang, Mikk Lippmaa, and A. Gilad Kusne, and is supported by the center for 3D Ferroelectric Microelectronics Manufacturing (3DFeM2), an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences under Award Number DE-SC0021118.

4:40pm **CM3-3-ThA-11 Advances in the Rapid Characterization of Sputter-Deposited, Binary Metal Thin Films Made by Combinatorial Techniques**, ***David Adams [dpadams@sandia.gov]***, *Finley Haines, Sadhvikas Addamane, Kyle Dorman, Remi Dingreville, Saaketh Desai, Brad Boyce, Mark Rodriguez,* Sandia National Laboratories, USA

Combinatorial sputter deposition techniques provide access to a rich variety of thin films that can be exploited for rapid design optimization and process refinement. Indeed, several combinatorial, magnetron sputtering approaches have been reported over the past decade demonstrating an ability to produce 10s or 100s of unique films in a single deposition experiment. In order to capitalize on the increased throughput provided by combinatorial methods, we seek to develop complementary, high-throughput film characterization techniques that accurately determine important film properties.

With this presentation, we describe two, new techniques that have accelerated the development of binary PtAu and CuAg films for use as metal contacts. First, we describe a high-throughput, X-ray reflectivity (XRR) analysis method that rapidly determines the density of >100 unique, combinatorial films produced in a given deposition. Traditionally, complex fitting procedures are applied to XRR to estimate the critical angle (angle at or below which total reflection occurs), which can then be used to calculate the film density. This study demonstrates an alternative method – using an indirect surrogate angle θ_s (instead of θ_c) that is numerically calculated (without any curve-fitting) as the minima in the first derivative of the acquired XRR profiles. It was found that density values estimated using θ_s and adjusted with a systematic offset were in agreement with the traditional curve-fitting method, with typical average error peaking at < 2% and reduced hands-on analysis time by ~95%. Second, we describe progress toward automated, ex-situ measurement of combinatorial film stress using a wafer curvature mapping approach. Employing a k-Space Co. ThermalScan instrument, we rapidly interrogate the curvature of >100 individual substrate pieces coated uniquely in a single deposition. We determine the residual stress of the various films using Stoney's equation and demonstrate extensions to automated measurements of thermal expansion coefficient. Altogether, the gathered information augments an extensive combinatorial library providing opportunities to pinpoint relevant process-structure-property relationships for improved, reliable thin film performance.

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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-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 (~1.8×10^5 $\Omega \cdot cm^2$) 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 (~$4–5 \times 10^4$ $\Omega \cdot cm^2$) 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

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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

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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.

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