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

8:00am **CM3-2-WeM-1 Accelerated Discovery of the Processing Genome for Nickel Superalloys***, Andrea Hodge [ahodge@usc.edu],* University of Southern California, USA **INVITED**

The creation and implementation of novel materials relies on the interconnected *processing-microstructure-property-performance* lifecycle. Specifically, we focus on building a data-driven testbed for *processing-microstructure* relationships capable of unraveling the complex synthesis of multi-phase, heterogeneous nanostructured materials (HNMs). To achieve this, we have launched a novel processing platform, Data-driven Recursive AI-powered Generator of Optimized Nanostructured Superalloys (DRAGONS), that will utilize predictive models to infer microstructure features based on provided processing parameters (DRAGONS-Predict) and prescribe processing parameters required to achieve a desired microstructure through inverse design (DRAGONS-Prescribe). Experimentally, nanotwinned (NT) Inconel alloys were synthesized via magnetron sputtering and subjected to an aging treatment that ultimately induced a transformation from a highly NT structure to a heterogeneous nanostructured material with a unique and complex gradient grain topology. In this presentation, the microstructure of distinct domains with variable grain size, precipitate formation, and morphologies will be discussed and connected to accelerated materials discovery using combinatorial and high throughput characterization techniques.

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.

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