Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM4-1-MoM

Simulations, Machine Learning and Data Science for Materials Design and Discovery I

Moderators: Ferenc Tasnadi, Linköping University, Davide G. Sangiovanni, Linköping University, Sweden

10:00am **CM4-1-MoM-1 Crystal Symmetry Determination in Electron Diffraction Using Machine Learning**, ***Kevin Kaufmann,*** Oerlikon Metco, USA **INVITED**

The recent adoption by the general public of artificial intelligence (AI) tools such as ChatGPT has reinvigorated research into AI applied to material science.Deep learning, a subset of AI, allows computer systems to autonomously learn patterns in data and construct efficient decision rules for tasks including classification, regression, or segmentation.In material analysis, these tools have primarily been applied to techniques requiring analysis of data collected in the form of images. Electron backscatter diffraction (EBSD) is one such technique benefitting from these recent efforts to improve material analysis by leveraging deep neural networks.Within the last decade, advancements in EBSD equipment have enabled the capture of high-definition diffraction patterns at rates exceeding 3,000 Hz.This creates significant opportunities for increasing the amount of information that can be ascertained from a sample, as well as opens the door for training data intensive deep neural networks.

Deep neural network-based classification of the diffraction patterns is motivated by Hough-based EBSD's susceptibility to structural misclassification; a failure mode that modern EBSD can encounter even when the researcher has complete knowledge of the sample prior to beginning analysis.While several methods to improve phase-differentiation have been proposed, each still requires pre-selection of phases and additional data (e.g. chemistry or simulated diffraction patterns) to be available.In contrast, deep neural network-based methods have demonstrated effective phase differentiation and identification of phases to the space group level without the need for further information.The deep learning approach to EBSD diffraction pattern analysis is capable of these more advanced analyses because it uses all information in the image when assessing a diffraction pattern, whereas traditional Hough-based EBSD pattern analysis discards a significant amount of information.

To promote adoption of AI tools, it must be determined if and when it is prone to error.To test the ideal operating conditions, the deep neural network model is trained using diffraction patterns captured with a fixed geometry and SEM settings, and a parametric study is performed to develop an understanding of model performance as several of the most common EBSD operating conditions are varied. Each time one parameter is varied, the diffraction patterns are re-collected, and the CNN used to reassess the space group identification.Ultimately, the model is found to retain a high classification accuracy even with significant changes to the diffraction conditions.

10:40am **CM4-1-MoM-3 Perturbation Analysis and Solutions to the One-Dimensional Cahn-Hilliard Equation in Thin Films**, ***Rahul Basu,*** 71 Nagavarpalyam, India

This paper presents an analytical investigation of phase separation dynamics in thin films using the one-dimensional Cahn-Hilliard equation. The main focus is on the development of perturbation solutions for Greens functions under various boundary conditions, specifically periodic, Neumann, and Dirichlet. The derived solutions provide insight into the behavior of concentration profiles, essential for understanding the phase separation process in technologically relevant thin film materials.

Thin films are widely used in various technological applications, including microelectronics and energy storage. The phase separation within these films is critical to their performance and properties. The one-dimensional Cahn-Hilliard equation serves as a fundamental model for studying the evolution of concentration profiles during phase separation. This paper aims to explore the dynamics of phase separation under different boundary conditions by deriving similarity transform and perturbation solutions to the Cahn-Hilliard equation.

Starting with the 1D Cahn Hilliard equations, Perturbation expansions are applied to the Green function solution and then evaluated for various boundary conditions. Alloys evaluated were Cu-Ni and Pd-Si.

Results showed differences for the diffferent Boundasry consditions and material parameters involved. The small perturbation parameter is chosen to be k the interface parameter. in the CH equation.

The results are hoped to ber useful in designing surface thin films, using inputs like thermal diffusivity M and the interface parameter appearing in the CH equation .

11:00am **CM4-1-MoM-4 Predicting Segregation Behaviour in Polycrystalline Materials: A Case Study of P in Fe**, *Amin Reiners-Sakic, Christoph Dösinger, Alexander Reichmann, Ronald Schnitzer, Lorenz Romaner,* ***David Holec,*** Montanuniversität Leoben, Austria

The segregation of solutes to grain boundaries has a significant impact on material behaviour, particularly with regard to its mechanical properties and microstructural evolution. Computational tools have previously been employed to investigate this phenomenon, although the majority of studies are limited to coincidence site lattice (CSL) symmetrical boundaries. A methodology incorporating geometries associated with general grain boundaries, as observed in polycrystals, has recently been employed to investigate the substitutional segregation of phosphorus in iron. In this study, we further develop this approach to include interstitial sites. The model of polycrystalline bcc Fe comprises approximately $7x10^5$ atoms distributed across 12 grains of ~8 nm^3 total volume. Of these, approximately $1x10^5$ are substitutional segregation sites. In addition, approximately 1.2 million interstitial sites have been identified. The full segregation spectra for all of the aforementioned sites have been investigated using interatomic potentials in conjunction with state-of-the-art machine-learning techniques. The results demonstrate that phosphorus segregates to both site types, with a lower mean segregation energy for substitutional sites in comparison to interstitial sites. However, due to the higher number of interstitial sites, the total number of sites with comparable segregation energies to substitutional sites is significantly greater. By incorporating both segregation distributions, we can accurately predict P enrichment at different concentrations and temperatures, in agreement with experimental data. To validate this approach, we applied it also to Ni and H, showing that Ni segregates, albeit moderately, only to substitutional sites, while H segregates exclusively to interstitial sites, in line with existing literature.

11:20am **CM4-1-MoM-5 Tunable Interface Stress in Cu/W Nanomultilayers**, ***Yang Hu,*** *Giacomo Lorenzin, Jeyun Yeom,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; Manura Liyanage, William A. Curtin,* EPFL, Switzerland*; Lars P.H. Jeurgens, Jolanta Janczak-Rusch, Claudia Cancellieri, Vladyslav Turlo,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Controlling the intrinsic stresses developed during the growth of nanomultilayers (NMLs) is critical for their performance and applications. In Cu/W NMLs, a transition from positive to negative interface stresses has been observed under varying film deposition conditions, yet the underlying mechanisms driving this transition remain unresolved. The sign of experimentally measured interface stress has long been debated, highlighting the complexity of interface phenomena in NMLs.To address this, we employed atomistic simulations using a state-of-the-art neural network potential to uncover the strong influence of intermixing and metastable phase formation at Cu/W interfaces on interface stress. These simulations provide a direct link between interface chemistry and stress, a connection that is challenging to establish experimentally due to the difficulty of characterizing interfacial structures and compositions at atomic resolution for the Cu/W system.The insights gained from this work offer a deeper understanding of the interplay between interface structure, stress, and deposition conditions, paving the way for the rational design of NML coatings with tunable stress states. This approach enables the optimization of the thermomechanical stability and multifunctional properties of NMLs, advancing their applications in fields such as flexible electronics, energy storage, and protective coatings. Our findings also underscore the power of advanced computational methods in guiding materials design and addressing long-standing challenges in interface engineering.

11:40am **CM4-1-MoM-6 Understanding the Effects of Underlayer Materials on Electron Beam Resists Through the Use of Monte Carlo Simulations and the Development of a New Simulation Tool**, ***David Castillo Lozada,*** *Toby Thomassen, Scott Lewis, Axel Scherer, Guy De Rose,* California Institute of Technology, USA*; Luisa Bozano, Kevin Gu,* Applied Materials, USA

The ability to write structures at the nanoscale using lithography underpins all modern society. The electronic devices we take for granted contain integrated circuits, the key component being the field-effect transistors

(FETs). They have reduced in size by a factor of two every two years for over fifty years, following “Moore’s Law”. This size reduction is dependent on the continuous development of materials and techniques that produce better line resolution. The technical program aimed to apply a simulation tool called Excalibur to materials and processing problems critical to Applied Materials Inc. The Excalibur simulation suite can model the behavior of electrons and ions in the range of 100 keV to 3.6 eV. This software allows rapid prototyping of the next-generation resists for electron beam lithography (EBL) and ion beam lithography (IBL) for the semiconductor industry. Although Excalibur currently does not simulate extreme ultraviolet (EUV) radiation, we propose that it can provide a first-order analysis and prediction of EUV based on e-beam behavior. This project provides evidence that such prediction can be well modeled using the Excalibur tool. We also provide an alternative simulation, which we call Merlin, that aims to be more accurate and faster than its predecessor.

Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM4-2-MoA
Simulations, Machine Learning and Data Science for Materials Design and Discovery II

Moderators: Davide G. Sangiovanni, Linköping University, Sweden, Ferenc Tasnadi, Linköping University

1:40pm **CM4-2-MoA-1 Computational Approach to Probing Hydrogen in Atomic Layer-Deposited Barrier Coatings***, Vladyslav Turlo,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland **INVITED**

The energy transition of our society requires an improved fundamental understanding of the chemical interaction of H with oxide materials, such as oxide membranes for H-purification, oxides for photocatalytic water splitting, and passivated oxides on steel. In particular, the effect of H impurities on the barrier properties of oxide layers grown by Atomic Layer Deposition (ALD) is of great scientific and technological interest, since hydrogen permeation barriers fabricated by ALD are broadly applied to address specific challenges for transport, handling, and storage of H, as well as for electronics, catalysis and gas sensing. However, resolving tiny changes in local chemical bonding states and structure of e.g. amorphous alumina oxides, as induced by H impurities originating from the ALD deposition process, still poses huge challenges for modern analytical tools up to date.

Here, the effect of hydrogen on the local chemical bonding states and structures of amorphous ALD alumina films is disclosed by predicting Auger parameter shifts, as measured by XPS/HAXPES, using a combination of atomistic and electrostatic modeling. First of all, it is demonstrated that a conventional melt quenching simulation procedure is not applicable for generating representative amorphous oxide structures with different H contents and densities, as observed in the experiment. Instead, a novel approach is proposed for simulating amorphous H-containing oxide structures by annealing reconstructed, highly defective crystalline hydroxide structures using a universal machine learning interatomic potential. As such, excellent agreement between the density, structure, and H-content was obtained between theory and experiment. Moreover, measured Auger parameter shifts for Al as a function of the H-content were accurately predicted by assuming all H atoms to be present in the form of hydroxyl ligands in the randomly interconnected 4-fold, 5-fold, and 6-fold nearest-coordination spheres of Al (by O). Combined atomistic and electrostatic modeling shows in detail how measured Auger shifts depend on the complex correlations between local coordination, bond lengths, bond angles, and ligand type(s) around the core-ionized atom, which equally applies to amorphous and crystalline compounds.

This work enables the computational design of new barrier coatings for hydrogen economy, providing a comprehensive computational characterization framework able to interpret even the tiniest Auger parameter chemical shifts obtained from experimental XPS/HAXPES techniques.

2:20pm **CM4-2-MoA-3 Conditions for the Preparation of Maximum-Quality Crystalline ZnO by Molecular Dynamics Simulations of the Atom-by-Atom Film Growth***, Jiri Houska, Kamila Hantova,* University of West Bohemia, Czechia

Crystalline zinc oxide thin films are important due to a combination of optical transparency, electrical conductivity and piezoelectric and pyroelectric properties. These functional properties largely depend on perfection of the crystalline structure. Reproducing the growth of thin films by molecular-dynamics (MD) simulations is very useful for the disentanglement of processes and phenomena which take place in parallel in the experiment and can yield a lot of atomic-scale information which is difficult to access experimentally. After introducing MD simulations in general, classical MD based on a reactive force field is used to study the atom-by-atom growth of ZnO_x films on a crystalline template. The effect of kinetic energy of fast atoms (E_{fast}) and fraction of fast atoms (f_{fast}) at varied elemental ratio (x = [O]/[Zn]) is analyzed in a wide range. Following the visual inspection, the crystallinity is quantified in terms of network ring statistics.

Simulations with fixed f_{fast} = 100% revealed that the highest crystal quality was obtained at x = 1.03 (not at the intuitive ratio x = 1.00) and E_{fast} = 3-12 eV with a maximum at E_{fast} = 10 eV. When only a low E_{fast} = 1 eV is available, even higher x = 1.10 leads to the relatively best results. Simulations with varied f_{fast} and fixed E_{fast} = 10 eV revealed that the crystallinity at $f_{fast} \geq 50\%$ is saturated. The ratio x = 1.03 is optimum at all these f_{fast} values and it is followed by x = 1.05 which also leads to higher crystal quality than x = 1.00. However, the ratio x = 1.10 is for the present energy distribution functions too high, not only in terms of growth rate which decreases with increasing x, but also in terms of crystal quality.

First, the results provide a quantitative insight into the role of individual deposition parameters. Second, the results explain available experimental data (for example, the dependence of the mobility of free charge carriers on the pulse-averaged target power density expresses the same character as the dependence of network ring statistics on E_{fast}). Third, the results facilitate a further improvement of the film properties. For example, it is important that the recommended E_{fast} is comparable to achievable positions of maxima of energy distribution functions during reactive HiPIMS.

2:40pm **CM4-2-MoA-4 Effect of the Presence of Oxygen on Hydrogen Adsorption on BCC Fe Surface: A Density Functional Theory Study Combined with Molecular Dynamics Simulations***, Zixiong Wei, Fei Shuang, Poulumi Dey,* Delft University of Technology, Netherlands

Hydrogen is one of the most promising candidates for the replacement of current carbon-based energy sources. It is one of the most potential candidates of sustainable energy produced in an eco-friendly manner. However, the use of hydrogen as an energy source is severely restricted by its damaging effect on mechanical properties of materials widely known as Hydrogen Embrittlement (HE). It is, thus, urgently needed to develop new HE resistant alloys or re-design the existing alloys for safe and efficient hydrogen storage and transportation. In this regard, Density Functional Theory (DFT) based approach is particularly important for obtaining atomistic insights into hydrogen interaction with surfaces to ensure less uptake of hydrogen by the material e.g. steels. Within this study, DFT is employed to obtain atomistic insights into hydrogen adsorption on different surfaces of bcc-Fe in the presence of oxygen. At the initial stage, we investigate the adsorption of oxygen on different surfaces of bcc-Fe using DFT following which we study the adsorption of hydrogen on Fe surface in the presence of the oxygen. At the next stage, we employed Molecular Dynamics (MD) simulations to study hydrogen diffusion into the bulk of bcc Fe from the surface in the presence of oxygen atoms on the surface. Our combined DFT-MD study thus offers atomistic insights into how surface oxygen atoms influence hydrogen intake into bcc Fe.

3:00pm **CM4-2-MoA-5 Machine Learning Prediction of Work Functions for No, No_2, Co, Co_2, and H_2S Gas Molecules Adsorbed on $Znga_2O_4$(111) Surfaces***, Po-Liang Liu, Hsiang-Yu Hsieh, Chao-Cheng Shen,* National Chung Hsing University, Taiwan

Zinc gallium oxide is a metal oxide gas sensing layer with exceptional thermal and chemical stability, capable of detecting gases such as NO, NO_2, CO, CO_2, and H_2S. The work function of Zinc gallium oxide can be assessed through first-principles calculations based on Density Functional Theory, which allows for the prediction of the sensor's sensitivity. Although Density Functional Theory provides accurate computational results, its high computational cost and time requirements limit its applicability for large-scale surface screening. This study used a database based on a density functional theory-based zinc gallium oxide sensor model. We developed an automated workflow using Python programming to extract crystal structure features as input for the machine learning model. The processed and filtered input features were employed to predict the work function of the sensor model, achieving a mean absolute percentage error below 6% in the prediction results. This study presents a trained machine-learning model interface that allows users to input crystal structure files for the rapid and accurate evaluation of the work function of Zinc gallium oxide sensors.

3:20pm **CM4-2-MoA-6 Ml-Assisted Atomistic Modeling of Transition Metal Diborides: Mechanical Response and Phase-Dependent Phenomena***, Shuyao Lin,* TU Wien, Institute of Materials Science and Technology, Austria*; Davide Sangiovanni, Lars Hultman,* Linköping Univ., IFM, Thin Film Physics Div., Sweden*; Paul Mayrhofer, Nikola Koutna,* TU Wien, Institute of Materials Science and Technology, Austria

Transition metal diborides (TMB_2) represent materials with ultra-high hardness and melting points but limited resistance to crack propagation. Understanding the thermodynamic stability of typical TMB_2 polymorph structures (α, ω, and γ) at finite temperatures as well as the phase-dependence of mechanical and fracture properties has been challenging due to non-trivial synthesis and structural similarity of the phase polymorphs, complicating their detection. This work presents uniform shear and tensile strain simulations of defect-free Group IV-VII TMB_2 ceramics using *ab initio* molecular dynamics as well as molecular dynamics

powered by machine-learning interatomic potentials (MLIP), trained in the moment tensor potential framework. Studied materials include TiB_2 (Group IV), TaB_2 (Group V), WB_2 (Group VI), and ReB_2 (Group VII), covering the α, ω, and γ polymorphs. Among our main results is a robust workflow for training transferable MLIPs. These MLIPs are suitable for atomic-to-nanoscale MD simulations, allowing to understand deformation and fracture mechanisms of each TMB_2, and extending the insights into phase transformation mechanisms under shear deformation. By demonstrating the outstanding mechanical performance of TMB_2:s in extreme environments, our predictions clearly underpin their huge application potential in protective coatings and high-temperature engineering. To deepen our understanding of fracture behavior, we additionally perform Mode-I fracture simulations allowing to quantitatively assess fracture toughness (K_{IC}) using pre-cracked models. The results are discussed in light of relevant experimental data, including high-resolution transmission electron microscopy analysis of nanoindentation experiments on TiB_2 thin films.

4:00pm **CM4-2-MoA-8 Computational Modeling of Nanoelectronics and Emerging Materials*, Chao-Cheng Kaun,*** Academia Sinica, Taiwan **INVITED**

Using first-principles calculations, we investigate electronic transport through carbon-, oxide- and transition metal dichalcogenide (TMD)-based nanojunctions for nanoelectronic applications. Effects of biasing, defecting, contacting and quantum interfering are addressed. We study noncollinear interlayer exchange coupling in magnetic trilayers for spintronic application. Effects of spacing are uncovered. We also study the efficiencies of hybrid-protected perovskite quantum dot films for LED backlighting and hydrogen evolution reaction in oxides for sustainable-energy applications. Effects of polymer-adsorbing and material-configuring are highlighted. Moreover, we explore the plasmonic properties of complex transition metal nitrides for photonic applications.

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

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

Moderators: Barbara Putz, Empa Thun, Aparna Saksena, MPI für Eisenforschung GMBH, Germany

8:40am **CM1-1-ThM-3 Analysis of Deuterium by Atom Probe Tomography (Apt) - D in V Films and Fe/V Multi-Layered Films**, ***Ryota Gemma,*** Tokai University, Japan*; Talaat Al-Kassab, Astrid Pundt,* University of Göttingen, Germany **INVITED**

In this presentation, we will present the results of deuterium distribution and quantitative analysis by atom probe tomography (APT) in single-layered V or Fe/V multi-layered films. While V is a hydrogen-absorbing metal, Fe hardly dissolves hydrogen (H). Therefore, in Fe/V multi-layered films, almost all of the H atoms are supposed to be in the V layer, and the H distribution should show a clear contrast at the Fe/V interface. This is also the case for deuterium (D). D has a lower diffusion coefficient than H. Hence, a surface segregation of D during the APT analysis can be suppressed, enabling to visualize original D position in the host metal lattice. Furthermore, D can be distinguished from background hydrogen in the APT analysis chamber. By using a portable chamber to prevent the sample from being exposed to oxygen, we were able to measure the D concentration in V or Fe/V films over a wide concentration range. We compared the D concentration measured by APT with the compared with the results of measurements of the hydrogen concentration dependence of electromotive force (EMF) for similar samples, it was found that the average D concentration in the sample could be correctly evaluated using APT.

9:20am **CM1-1-ThM-5 Monitoring Thin Film Battery Electrodes via in-Situ/in-Operando Ellipsometry**, ***Máté Füredi,*** Semilab Semiconductor Physics Laboratory Co. Ltd., Hungary*; Jialin Gu, Adam Lovett,* University College London, UK*; Bálint Fodor, András Marton,* Semilab Semiconductor Physics Laboratory Co. Ltd., Hungary*; Stefan Guldin,* Technical University of Munich, Germany*; Thomas Miller,* University College London, UK

The electrochemical energy storage behavior of nano- and microscale (thin- and thick-film) electrodes displays unique characteristics that provide crucial insights into various charge storage mechanisms, essential for the optimal design of commercial battery applications. Additionally, these films are applicable for constructing microbatteries for miniature electronic devices (such as sensors). Critically, material chemistry, crystallinity, and nanostructure significantly influence active charge transfer mechanisms in these systems, generally classified as electrochemical double layer capacitive, pseudocapacitive, or battery-type behaviors. In lithium-ion batteries specifically, the charge storage mechanism involves the (de)/intercalation of lithium ions in active electrode materials, such as silicon, graphite, or transition-metal oxides.

By optically monitoring thin-film electrodes under electrochemical charge/discharge, a range of time-resolved structural data can be obtained. This work elaborates on this by integrating operando spectroscopic ellipsometric data acquisition. Ellipsometry, highly sensitive to thin films, offers an advantage by effectively excluding any electrolyte side-reactions from measurement, thus providing accurate, real-time data on the evolving structure of lithiated electrodes across charging states. Additionally, ellipsometry tracks thickness changes, enabling precise monitoring of degradation mechanisms.

This work demonstrates (on the example of transition-metal oxide thin-film electrodes) how ellipsometry can reveal intercalation processes, diffusion limitations, and pseudocapacitive contributions. This is further correlated with the complementing electrochemical data. The considerations of this work are furthermore broadly applicable to other thin-film electrode materials.

10:20am **CM1-1-ThM-8 RBS Study of PiTi and NiTi Multilayer Thin Film for Hydrogen Generation and Water Splitting**, *Enos Nemukula,* University of Venda, South Africa*; Christopher Mtshali,* iThemba laboratoty, South Africa*;* ***Fhulufhelo Nemangwele,*** University of Venda, South Africa

In this study, thin film samples of Pd-Ti and Ni-Ti systems were prepared using an electron beam evaporator under a vacuum pressure of 10^{-6} torr on Si<100>, borosilicate glass, and pure Ti substrates. The absorption of hydrogen, carbon, and oxygen into the thin films was followed by conducting an in-situ real-time Rutherford backscattering (RBS) investigation. RBS confirmed no spontaneous interdiffusion of atoms between the layers during the deposition. The layers were approximately ~30×10^{15} atoms/cm^2 (10 nm), and ~433×10^{15} atoms/cm^2 (150 nm) for Pd, and Ti layers in the Pd-Ti system, respectively while Ni layer was ~31×10^{15} atoms/cm^2 (10.3 nm). The in-situ real-time RBS was performed by linear temperature ramping from room temperature to a maximum temperature of 600 °C at a constant ramping rate of 7 °C per minute. The results showed an interfacial reaction, indicating an unstable system at higher temperatures. Elastic recoil detection analysis (ERDA) revealed an increase in hydrogen absorption of up to 5 at% from the residual gases inside the scattering chamber at a vacuum of 1×10^{-6} mbar. Increased oxygen peaks indicated enhanced absorption of this element from the residual gases inside the scattering chamber. These results suggest that this system has potential applications in hydrogen absorption.

10:40am **CM1-1-ThM-9 Exploring the Benefits of Automated, Redox Reactions in XPS Analysis**, ***James Lallo,*** Thermo Fisher Scientific, UK, USA*; Robin Simpson, Paul Mack, Tim Nunney,* Thermo Fisher Scientific, UK

This presentation investigates the benefits of automated, in-situ redox reactions for the purpose of producing well controlled oxide growth on the surface of various sample types. The driving force behind using such a procedure is in the potential for generating a sequence of spectra from a progressively chemically-modified surface to remove ambiguities that can lead to misinterpretation, thus aiding in faster understanding of the unmodified surface. Our study presents XPS results from coupled stepwise oxidation/reduction of surfaces, to aid in resolving such ambiguities across a wide array of materials. We use gas-phase oxidation agents to control the redox states of a specimen, leveraging the logarithmic growth of oxide thickness. This oxidation is implemented using vacuum ultraviolet light (VUV) and the generation of ozone and gas-phase hydroxide free radicals close to the surface of the specimens within the entry-lock of the Thermo Scientific Nexsa surface analysis instrument. This work focusses on the benefits of automating this process to ascertain the potential merits of including it into a standard operating procedure for XPS analysis.

11:00am **CM1-1-ThM-10 Hydrofluoric (HF) Acid Corrosion Study of Corrosion Resistant Alloys Used in Semi-Conductor Etching Process Equipment**, ***Donald Williams,*** *Kayvon Savadkouei, Brian Chung, Brad Drake, Patrick Lowery, Andrey Krayev, Eddy Robinson,* Horiba Instruments Inc., USA

Corrosion studies require the use of complementary analytical techniques, as each method provides results based on the interaction of the investigated material with a probing medium [1]. Obtaining elemental, molecular, and crystal/grain structure information at different spot sizes and probing depths is crucial, particularly for elements that are challenging to observe simultaneously, such as hydrogen and fluorine.

In this study, the dissolution of gaseous phase anhydrous hydrogen fluoride and diffusion of fluorine into various metal superalloys were monitored by analyzing changes in concentration, depth, and diffusion rate using Glow Discharge Optical Emission Spectroscopy (GD-OES). A representative area of ultra-high purity (UHP) 316L (composition compliant with SEMI standard F20) and Inconel® 600 alloys were rapidly sputtered to obtain fast elemental depth profiles with nanometer resolution [2].Atomic Force Microscopy (AFM) provides complementary data with relevance to corrosion studies, ranging from the subtle effects of surface passivation uniformity on the measured surface potential and conductivity of the material to the simple evolution of the surface topography with progression of corrosion (even in the earliest stages) [3].

The corrosion test samples are representative of alloys used in semiconductor manufacturing equipment, where improved alloy durability and the prevention of leaching of corrosion byproducts is critical. The goal is to understand the prevalent corrosion mechanisms in these common semiconductor alloys in order to find ways to increase equipment longevity and minimize contamination to the semiconductor manufacturing processes.

References:

1. Compendium of Surface & Interface Analysis, Springer
2. Review: What Can Glow Discharge Optical Emission Spectroscopy (GD-OES) Technique Tell Us about Perovskite Solar Cells? Small Methods 2022, 2200633
3. Review: Application of AFM-Based Techniques in Studies of Corrosion and Corrosion Inhibition of Metallic Alloys. Corrosion and Materials Degradation 2020, 1, 345–372; doi:10.3390/cmd1030017

11:20am **CM1-1-ThM-11 Numerical Ellipsometry: Artificial Intelligence Based Real-Time, in Situ Process Control for Absorbing Metal Films Depositing on Known Transparent Substrates***, **Frank Urban**, David Barton,* Florida International University, USA

Ellipsometry can provide the optical properties and thickness of a thin film depositing on a known substrate, including transparent substrates, in real time using commercially available *in situ* instrumentation. The desired film parameters are related to visible light reflection measurements through Maxwells equations, wavelength, and geometry. A number of different methods have been developed for obtaining the desired parameters given a reflection or multiple reflections. One category of methods is iterative least squares curve fitting, frequently the Levenberg-Marquardt method. An emerging method is that of artificial intelligence (AI) employing artificial neural networks. One of the primary advantages of the AI method is speed. It can be a thousand times faster than the pre-existing curve fitting methods. The work here demonstrates the use of such an Artificial Intelligence method to enable real-time, *in situ* monitoring of thin film growth. Examples will be given using a single angle of incidence and three angles of incidence for comparison. Thin absorbing films (up to 45 nm) will be given using a multilayer perceptron configuration consisting of either 4 or 12 input and 4 output neurons with two hidden layers of 80 neurons each. Solutions are performed at each wavelength independently and do not rely on fitting functions. The design, training and use of a number of neural networks will be presented.

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

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

Moderators: Matteo Ghidelli, CNRS, France, David Holec, Montanuniversität Leoben, Austria

8:00am **CM2-1-ThM-1 Nano-Mechanical Characterization and Modeling of Plasticity in Metallic Materials***, **Takahito Ohmura**,* Kyushu University/NIMS, Japan **INVITED**

Plastic deformation behavior is characterized through nano-mechanical testing in a small scale associated with microstructures including inter-phase and grain boundary in metallic materials. Deformation behavior was evaluated for Fe-Si bicrystal with different grain boundary plane with S9{221} and S9{114}1). The resistance to a slip transfer at the grain boundary depends on a combination of crystallographic orientation and dislocation character. Plasticity initiation behavior was characterized for ferrite-cementite interface with different coherency in a pearlitic steel2). The critical stress for the plasticity initiation is lower for a semi-coherent interface than that for an incoherent one, suggesting a potential reason for the continuous yielding phenomenon in macroscopic stress-strain curve of the steel with semi-coherent interface. Transmission Electron Microscope (TEM) in-situ straining was applied to reveal dislocation-grain boundary interactions. In the case of ultra-fine grain steel, dislocations in grain interior can sink at the grain boundary with no remarkable pile-up3). This behavior indicates a dislocation density dominancy for the extra-hardening in the UFG steel. Dislocation-Dislocation interaction was also captured through TEM in-situ straining4). The dislocation reaction forms a stable grain boundary, which could be an elementally step of grain refining during severe plastic deformation. The critical stress for a slip transfer was estimated for □3 boundary of pure Al5). The mechanism of the slip transfer can be modeled in a simple dislocation reaction generating a grain boundary dislocation. Deformation mechanisms of plasticity initiation and subsequent behavior were modeled through stochastic analysis based on a pop-in phenomenon on a loading segment obtained from nanoindentation measurement6). The critical stress for the plasticity initiation shows Gaussian like distribution function, indicating a thermally-activated process including a nucleation of shear loop dislocation at defect-free region. In the subsequent stage, the loading curve shows intermittent plasticity, and the probability function for the event magnitude shows power-law type, suggesting a catastrophic phenomenon with a fractal dimension such as dislocation avalanche.

References

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5. S. Ii, T. Enami, T. Ohmura, S. Tsurekawa, Scripta Mater., 221, (2022) 114953.

8:40am **CM2-1-ThM-3 Accelerating Workflows for High-Throughput Nanoindentation***, **Eric Hintsala**, Kevin Schmalbach, Douglas Stauffer,* Bruker Nano Surfaces, USA

Heterogenous microstructures are commonly employed across a wide range of applications as a tool for materials scientist to engineer the bulk properties, which can be seen in composite materials, multi-phase alloys or even surface treatments and coatings. Sometimes, property distributions can also arise due to processing history, with laser-based techniques with micro-scale heat affected zones being of particular interest recently.In most cases these structures are nano- to microscale in size, so to isolate mechanical properties from individual regions high-throughput nanoindentation-based techniqueshave become increasingly popular.

Two recent advances in nanoindentation mapping are highlighted here. First, the indentation depth controls the finest spacing that can be utilized without affectingthe subsequent nearby indentations and thereby defines the resolution of a nanoindentation map. Displacement control is particularly important when mapping samples with highly variable hardness. To address this, recent enhancements for the HysitronTI 990 TriboIndenter(Bruker, USA) allows for trigger points to be used to switch segments and feedback control all within one test.This enables ahigh-throughput workflow where translation between positions is followed by approach,surface detection, and a displacement-controlled indent. This mode workswith both high load and low load transducers for addressing a large range of depths and spacings.

Secondly,relating the measured mechanical properties to local structure and composition is also essential for materials development.This can be done by switching instruments from the nanoindenter to the SEM, but this is time consuming and generally necessitatesuse of fiducial markers. To facilitate this process,theHysitron PI 89 Auto (Bruker, USA) in situ SEM indenter utilizes a rotation-tilt stage to move the sample between 3 distinct positions: Indentation position, top-down SEM and EDS position, and 70°tilted EBSD position. The accompanying software enables the same sample region to be co-located in all 3 positions easily, such that regions of interest from an EBSD or EDS map can be directly targeted for indentation testing.

9:00am **CM2-1-ThM-4 Understanding the Fracture Behavior, Interface Characteristics of Micro and Nanocrystalline Diamond Laminates Through Flexural Studies***, **Krishna Sarath Kumar Busi**,* Technical University Darmstadt, Germany*; Tim Fuggerer,* University of Erlangen-Nuremberg, Germany*; Sebastian Bruns,* Technical University Darmstadt, Germany*; Timo Fromm, Stefan M Rosiwal,* University of Erlangen-Nuremberg, Germany*; Karsten Durst,* Technical University Darmstadt, Germany

Diamond metallic laminates (DML) have been demonstrated to exhibit an improved toughening mechanism by modifying the crack driving force with alternate hard and ductile layers [1]. These laminates were produced from free-standing diamond foils using HFCVD, exhibiting distinct crystalline morphologies microcrystalline (conventional) and nanocrystalline integrated with metallic layers deposited through PVD. A systematic investigation was set up to understand the mechanical behavior, interface characteristics of these multilayer system through macro 3PB and micro cantilever flexural studies. Nanocrystalline diamond foils exhibited better toughness, and their fracture sensitivity was analyzed by recording continuous stiffness change with respect to crack propagation for notched cantilevers using nanoindentation. Significant delamination was observed in nanocrystalline laminate (nDML) exhibiting weak interfacial strength between diamond and metal layers. Suitable analytical laminate models were effectively applied to investigate shear stress distribution, critical cracking events and the extent of delamination. Additionally, A 2D model of FEM with cohesive interactions was designed in same experimental scenarios (3-point bending, micro cantilever bending) to understand the diamond-metal interfacial properties, showed strong alignment with the analytical models and offered valuable insights to optimize the overall design of the laminate.

Keywords: Laminates, nanoindentation, toughness, fracture, bending, FEM.

References:

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[2] Timo Fromm et. al (2022), Bioinspired damage tolerant diamond-metal laminates by alternating CVD and PVD processes, Materials & Design, Volume 213,2022,110315, ISSN 0264-1275.

9:20am **CM2-1-ThM-5 Deposition of Hierarchical Ti/Ti_2AlC Metal/MAX Multilayered Nanolaminates and Investigating their Mechanical Properties and Deformation Mechanisms***, **Amruta Vaghela,*** Iowa State University, USA*; Skye Supakul,* Pacific Northwest National Laboratory, USA*; Kevin Jacob, Sid Pathak,* Iowa State University, USA

We report the challenges (e.g. the diffusion and formation of MAX phase) with the high temperature synthesis of a hierarchical metal/MAX phase multilayered nanolaminate (MMN) where the interface between metal and MAX phase layers are in direct competition with the internal interfaces within the MAX layers. Using a combinatorial physical vapor deposition (PVD) and atomic layer deposition (ALD) system, we report our first successful deposition of a Ti/ $Ti_{n+1}AlC_n$ (n=1 or 2) MMN where thin Al_2O_3 diffusion barrier layers inhibits interlayer diffusion and enables the multilayered architecture to be retained. The mechanical properties of the MMN system show impressive indentation hardness (12.75±0.33GPa), micro-pillar instability stresses (8.1±0.2GPa), and instability strains (8.3±0.4%) compared to a rule-of-mixtures approximation of the hardness and yield strength of the system. Post compression TEM analysis is also being conducted to gain insight on the deformation mechanisms at play in these hierarchical MMN systems.

9:40am **CM2-1-ThM-6 Effect of Fe Addition on the Structural, Mechanical and Electrical Properties of $(ZrCu)_{1-x}Fe_x$ Thin Film Metallic Glass***, **Evgeniy Boltynjuk,*** *Yulia Ivanisenko,* KIT, Germany*; Marco Ezequiel, Francesco Bignoli, Damien Faurie, Philippe Djemia, Matteo Ghidelli,* CNRS, France*; Horst Hahn,* Oklahoma State University, USA

Thin film metallic glasses (TFMGs) have emerged as a promising class of materials for applications in the field of flexible electronics, owing to their large deformability, metallic-like electrical conductivity, and low or even negative temperature coefficient of resistivity. However, despite these advantages, the properties of TFMGs require improvement to expand their range of applications. In this study, we focus on $(ZrCu)_{1-x}Fe_x$ system, as the properties of the ZrCu system have been investigated across a broad range of compositions, while the addition of Fe can potentially improve its glass forming ability and thermal stability. Specifically, we will discuss experimental results and *ab initio* calculations on the effect of Fe addition on mechanical and electrical properties, with a focus on clarifying the relationship between these properties and atomic structure and local ordering.

$(Zr_{34}Cu_{66})_{1-x}Fe_x$ TFMGs were synthesized by magnetron sputtering varying the Fe content from 0 up to 76 at.%. All obtained samples, up to the highest Fe content (76 at. %), have an amorphous structure, indicating a high glass forming ability. The electrical resistivity shows a monotonic decrease with increasing Fe content, reducing from 192.4 down to 113.8 μΩ × cm. At the same time, tensile tests on polymeric substrate show a reduction in crack onset strain (COS) from ~ 2.2 down to 1.6% in the range of Fe concentrations from 0 to 54 at.%. For higher Fe concentrations COS shows inverse trend, reaching ~ 2.0% at 76 at.% Fe. Thus, TFMG containing 76 at.% of Fe shows COS value comparable to that of the ZrCu, while achieving a 1.7-fold decrease in electrical resistivity.

Transmission electron microscopy and atom probe tomography reveal structural modifications, mapping the evolution of local ordering and atomic arrangements. By correlating our experimental findings with *ab initio* calculations, we establish a clear relationship between the modification of atomic order and performance of $(ZrCu)_{1-x}Fe_x$ TFMGs. This correlation not only enhances our understanding of TFMGs but also provides a solid foundation for their potential applications in flexible electronics, guiding future research in optimizing TFMGs for advanced technological uses.

10:20am **CM2-1-ThM-8 Mechanical Properties of Thin Films Studied using 4D-STEM***, **Christoph Gammer,*** Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria*; Alice Lassnig,* Montanuniversität Leoben, Leoben, Austria*; Lukas Schretter, Simon Fellner,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria*; Jürgen Eckert,* Montanuniversität Leoben, Leoben, Austria **INVITED**

The mechanical behavior of thin films is highly dependent on their microstructure Micromechanical testing can be used to study small-scale mechanical properties. Modern thin film systems are becoming increasingly complex and their overall mechanical properties are influenced by strong variations in the local elastic and plastic response. Therefore, to understand their deformation behavior the local nanoscale stress distribution during loading has to be considered. The overall load-displacement curve is not sufficient. Recently, we have demonstrated that 4D-STEM allows to perform strain mapping at the nanometer scale during continuous *in situ* deformation in the TEM. In the present talk we will present recent advances demonstrating how 4D-STEM can be used to understand the deformation mechanisms in single-crystalline, nanocrystalline and amorphous thin films.

11:00am **CM2-1-ThM-10 Investigating the Interplay between Biaxial Multicracking of Nanometric Thin Films and Their Magnetic Properties: A Nuanced Separation of Magnetoelastic and Magnetostatic Effects***, Hatem Ben Mahmoud, **Damien Faurie,*** Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France*; Pierre-Olivier Renault, Pierre Godard,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France*; Dominique Thiaudière, Philippe Joly, Christian Mocuta,* Soleil Synchrotron, France*; Eloi Haltz, Noël Girodon-Boulandet, Fatih Zighem,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France

The magnetoelectronic systems of the future will be designed to adapt to complex geometries. Flexible electronics have seen rapid growth, offering promising applications in areas such as confined environments and flexible displays [1]. These systems rely on polymers, which are lighter and more cost-effective than silicon. Understanding the interplay between mechanical strain and magnetic properties is essential [2]: at low strains, magnetic anisotropy is key, while at higher strains, microscopic damage (e.g., fragmentation and decohesion) becomes critical [3].

However, the relationship between thin film fragmentation and magnetic properties [4], especially under biaxial tension, remains poorly studied. This thesis aims to fill this gap through novel experimental techniques and studies on model systems. We investigated flexible magnetic systems using in situ methods, applying significant mechanical strain (up to 10%) while simultaneously probing their magnetic properties. A magneto-optical Kerr effect (MOKE) magnetometer was developed at the DiffAbs beamline of the Soleil synchrotron. Our research focuses on the distribution of stress (before and during cracking) and its impact on the magnetic response, along with the underlying mechanisms.

Two main mechanisms are identified: first, stresses generated during mechanical loading can induce a strong magnetoelastic field that alters the magnetic response; second, magnetostatic fields between fragments separated by cracks can contribute to coercivity during magnetization cycles. However, these effects have yet to be fully quantified. To address this, we studied magnetization cycles under large deformations in Ni80Fe20 films (with negligible magnetoelastic contribution), of varying thickness, with or without W layers of different thicknesses to modify fragment size. We demonstrate that the magnetostatic contribution is closely linked to the aspect ratio (diameter/thickness) of the fragments. This study, compared with research on Co layers, clearly distinguishes between geometric (magnetostatic) effects and stress-induced (magnetoelastic) effects.

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11:20am **CM2-1-ThM-11 Cross-Sectional Nanoindentation Mapping of Sputtered Inconel 725 Films***, **Ikponmwosa Iyinbor,*** Mork Family Department of Chemical Engineering and Materials Science, University of Southern California., USA*; Jin Wang,* Institute of Energy Materials and Devices, Microstructure and Properties of Materials (IMD-1), Forschungszentrum Jülich GmbH., Germany*; Ruth Schwaiger,* Institute of Energy Materials and Devices, Microstructure and Properties of Materials (IMD-1), Forschungszentrum Juelich GmbH., Germany*; Andrea Hodge,* Mork Family Department of Chemical Engineering and Materials Science, University of Southern California., USA

Heterogeneous nanostructured materials (HNMs) offer significant potential for overcoming the strength-ductility trade-off observed in conventional homogeneous nanostructured materials. Recently, we have demonstrated the influence of heterogeneous stress distribution on the development of

unique nanostructured features in sputtered nanotwinned Inconel 725 thick films after undergoing heat treatment. A gradient microstructure with three distinct nanodomains featuring a nanocrystalline equiaxed region, a nanotwinned region with carbides, and a region featuring abnormal recrystallization wherein abnormally large grains, delta-phase precipitates, and rafted structures were observed. This unique combination of nanodomains is expected to contribute distinct responses to mechanical deformation behavior.

In this work, two different HNMs of 8 µm and 20 µm film thicknesses were synthesized and heat treated. A nanoindentation mapping technique using a Femto-Tool NMT04 in-situ SEM nanoindenter was performed in order to generate high-spatial resolution hardness and elastic modulus property maps. The nanoindentation maps show a good correlation to the observed heterogeneous microstructure, revealing trends that provide an understanding of the local deformation behavior of these HNMs. Understanding the contribution of each nanodomain to the overall deformation behavior of the films enables the optimization of design and fabrication strategies to provide a superior combination of properties.

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

Accelerated Thin Film Development: High-throughput Synthesis, Automated Characterization and Data Analysis I

Moderators: Davi Marcelo Febba, NREL, Sebastian Siol, Empa

8:00am **CM3-1-ThM-1 Combinatorial Screening of Quaternary Piezoelectric Nitrides, Enabled by HiPIMS**, ***Nathan Rodkey***, *Jyotish Patidar, Federica Messi, Sebastian Siol,* EMPA (Swiss Federal Laboratories for Materials Science and Technology), Switzerland

Increasing demand for data and the surge of AI technologies is escalating the needs of telecommunication devices. RF filters are a limiting factor in this regard, where improvements in bandwidth and selectivity are needed. Advanced RF filters rely on piezo thin films like AlN, valued for its linear response and strong electromechanical coupling, with Sc doping enhancing its d_{33} and overall performance. While AlScN is considered state-of-the-art, many proposed dopants (e.g. B, Y, La) could further improve its properties. High-throughput experiments are instrumental in exploring quaternary or multinary materials, but few studies examine combinatorial screening of piezoelectric materials. This is because piezoelectric materials are difficult to screen effectively, as their device properties strongly depend on the c-axis texture of the film. During combinatorial gradient deposition the shallow deposition angles and static substrate can cause significant grain tilt towards the dominant source, convoluting composition and texture gradients. In high-power impulse magnetron sputtering (HiPIMS), additional energy can be introduced to arriving species by synchronizing a substrate bias to arriving metal ions. This improves the adatom mobility of species, removing grain tilt, and resulting in highly textured films without substrate rotation. In this work, we use AlScYN as an example material to demonstrate how HiPIMS enables effective device screening of piezoelectric properties.

Before the use of HiPIMS, DCMS screening is used to assess solubility limits in the quaternary phase space. This is typically done using X-ray diffraction mapping while applying the disappearing phase method. However, in combinatorial screening of materials this method loses effectiveness, as precipitates can be tilted out of the diffraction plane. Consequently, we use the peak shift of the (0001) plane to track discontinuities from Vegard's law and identify precipitation. Despite the larger ionic radius of Y, the combined solubility of Y and Sc increases, reaching a maximum of ~50%. For context, the solubility limit of AlScN is ~40%. Materials libraries were then made using metal-ion synchronized HiPIMS. The libraries are highly textured, with rocking curve FWHMs of <2°. Following this, the coupling (k) and clamped d_{33} coefficients of these libraries were mapped, showing their dependence on the combined Sc and Y contents. Importantly, d_{33} coefficients were mapped using a double beam laser interferometer (DBLI) for improved accuracy.

8:20am **CM3-1-ThM-2 High-Throughput Experiments Informed by High-Throughput Theory Reveal Zintl Phosphides as a New Family of High-Performance Semiconductors**, ***Sage Bauers***, 15013 Denver West parkway, USA **INVITED**

The discovery of a new structural class of semiconductor is a rare occurrence. For example, in the case of solar absorption, nearly all relevant semiconductors can broadly be described as materials derived from the tetrahedrally-coordinated diamond structure (e.g., Si, III-Vs, II-VIs, chalcopyrites, kesterites). This is part of the reason that new high-performing materials, such as perovskites, which are made up of octahedral bonding motifs, garner so much interest and help generate new materials design concepts. Using high-throughput computational workflows, we recently discovered that several AM_2P_2 (*A* = Ca, Ba, Sr and *M* = Cd, Zn) compounds possess the requisite intrinsic materials properties for high optoelectronic performance, including solar-spectrum matched band gaps, strong optical absorption, and benign intrinsic defects, leading to long photoexcited carrier lifetimes. This family of compounds, which exhibits a mixed octahedral + tetrahedral bonding motif, has been known for several decades but the optoelectronic properties had been almost entirely unexplored.

Using a combinatorial synthesis approach based on a hybrid PVD/CVD method, we recently prepared the first thin films of Zintl phosphides $CaZn_2P_2$ and $SrZn_2P_2$. By combinatorial sputtering from metallic targets in the presence of PH_3 at low temperature, we prepare films across the ternary composition space. Growths at higher temperatures result in much narrower compositional spreads pinned around the AM_2P_2 composition, indicating an adsorption-controlled growth regime can be realized. Mapping measurements including x-ray fluorescence, x-ray diffraction, UV-vis spectroscopy, photoluminescence, and Raman spectroscopy are used to probe the properties of the zintl phosphide films. To establish the photoactivity and semiconducting nature of the AM_2P_2materials, minority carrier lifetimes and electronic properties were measured via time resolved microwave conductivity, transient absorption, and van der Pauw/Hall effect. To summarize the characterization of $CaZn_2P_2$ as an example, we observe high optical absorption of ~10^4 cm^{-1} at the ~1.95 eV direct transition, near band edge optical emission, and a photoexcited carrier lifetime of up to 30 ns at a fluence of 2 10^{13} cm^{-2}. Films are intrinsic, but p-dopable with +1 elements such as Na (*A* site dopant) or Cu (*M* site dopant). Such performance metrics are usually not observed in inorganic solar absorber materials until well into their development, highlighting the value of coupling high-throughput theory, high-throughput experiments, and targeted experiments toward new functional materials.

9:00am **CM3-1-ThM-4 High-Throughput Nanoindentation Methodology for Combinatorial Thin Film Material Libraries**, ***Andre Bohn***, University Of Southern California, USA; *Adie Alwen, Andrea Maria Hodge,* University of Southern California, USA

Combinatorial and high-throughput (CHT) methods offer an accelerated pathway for the discovery and development of novel materials with wide ranging biological, electronic, and structural applications. One common approach to accelerate synthesis is the deposition of large compositionally graded thin film arrays with hundreds of distinct samples, often referred to as thin film material libraries. High-throughput characterization techniques are then employed to quickly assess processing-structure-property relationships, which generates large datasets for machine learning models and screens for promising next-generation materials. For assessing mechanical behavior in these libraries, nanoindentation is particularly suitable due to the ease of automation, minimal sample preparation requirements, and compatibility with thin films. However, despite the widespread use of this technique in CHT research, many inconsistencies between reported methodologies in literature can be identified. This work presents a CuNi alloy library to identify how to improve data reliability while minimizing experimental times and costs. Emphasis is given to optimizing the number of indents per sample and the distribution of samples tested. By improving method standardization, both efficiency and reproducibility of combinatorial studies can be enhanced, thus expanding the value of material libraries to the scientific community.

9:20am **CM3-1-ThM-5 Empowering Manufacturers with Low-Temperature Plasma: A Novel Approach to Real-Time Thin Film Metrology**, ***Peter Rudd***, 8000 Edgewater Dr, USA

Thin films, or micro- and nano-scale materials with unique functional properties, enable many clean energy industries, such as lithium-ion batteries, solar cells, and carbon conversion. Minimal-waste manufacturing of high-performance thin films will be vital for achieving society's net-zero carbon emission goals. Because existing thin film sensors cannot operate within most sections of manufacturing lines, manufacturers often complete hundreds of processing steps before they can test (a small portion of) their products and detect problems. Current thin-film manufacturing thus often yields many low-quality products, or off-spec products that must be discarded.

SirenOpt has developed a real-time low-temperature plasma-based thin film metrology sensor. The sensor is compact, can be integrated within existing manufacturing lines, and can collect multiple thin film property measurements (such as thickness with a precision of 1/10th of a nanometer, density, resistivity, chemical composition, and contaminate identification) in parallel and in real-time, thus allowing for the collection of critical manufacturing data that is otherwise unobtainable. SirenOpt is currently applying the sensor to industrial thin film coating processes such as Lithium-ion battery electrodes, where this flexible sensor can be used to accelerate R&D and process optimization, improve quality control, and enable real-time process control.

9:40am **CM3-1-ThM-6 Streamlining Inorganic Thin-Film Data Management with the High-Throughput Experimental Materials Database (HTEM)***, Davi Febba,* ***Nicholas Wunder****, Hilary Egan, Max Gallant, Andriy Zakutayev,* National Renewable Energy Laboratory, USA

Artificial intelligence (AI) is ushering in a new era of progress in materials science, where self-driving laboratories and autonomous instruments are performing experimental research that was once the exclusive domain of humans. Central to this paradigm shift is effective data management, as AI-driven laboratories make decisions based on the data they collect. Ensuring that materials science data is Findable, Accessible, Interoperable, and Reusable (FAIR) is crucial for accelerating materials discovery, as it facilitates seamless integration of diverse datasets and enhances collaboration across research teams.

In this presentation, we will discuss NREL's Research Data Infrastructure (RDI) [1], which catalogs experimental data from inorganic thin-film experiments at NREL and underpins the High-Throughput Experimental Materials Database (HTEM-DB) (https://htem.nrel.gov/) [2]. The HTEM-DB stores comprehensive information about synthesis conditions, chemical composition, crystal structure, and optoelectronic properties of materials, making the data readily accessible and reusable for the research community.

Will also present recent advancements in the HTEM's extract-transform-load (ETL) pipeline. These advancements not only allow for large-scale AI analysis of X-ray diffraction (XRD) patterns [3] but also enable the containerization of applications and instruments, making the database more modular and maintainable. Enabled by the recently developed Hybrid Environment Resources and Operations (HERO), these improvements help to lower the barriers to accessing NREL's computational resources, data analysis, and visualization capabilities. By facilitating both AI integration and modular design, HERO empowers scientists to share their research and collaborate with external partners through interactive applications.

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[2] Scientific Data 5, 180053, 2018
[3] PEARC '24, 39, 1-5, 2024

10:20am **CM3-1-ThM-8 A Python-Based Approach to Sputter Deposition Simulations in Combinatorial Materials Science***, Felix Thelen, Rico Zehl, Jan Lukas Bürgel,* Ruhr University Bochum, Germany*; Diederik Depla,* Ghent University, Belgium*; Alfred Ludwig,* Ruhr University Bochum, Germany

In combinatorial materials science, magnetron sputtering plays a key role for the exploration of future high-performance materials due to its capability to produce well-defined, continuous compositional gradients in form of thin-film libraries. Its scalability from laboratory settings to industrial applications, relatively high deposition rates, and compatibility with a wide range of materials make it an effective choice for combinatorial synthesis [1]. However, achieving precise control over the deposition profile and compositional distribution often requires multiple preliminary experiments to optimize process parameters - an approach that can be time- and resource-intensive.

Aiming to predict those properties, several analytical and numerical simulations were reported in literature over the past decade [2-4]. However, only the magnetron sputter deposition model SIMTRA [4] was made publicly available. Based on the Monte Carlo approach, it allows to simulate the deposition profile of a single magnetron source, while taking into account the dimensions of the components through a graphical user interface.

In order to make this tool more suitable for the application in combinatorial materials science, the command line version of the SIMTRA application was wrapped in a Python environment, enabling the definition of sputter chambers through code and executing the time-consuming Monte Carlo calculations through user defined scripts. This approach also enables parallel simulation of multiple magnetrons by using multi-threading, decreasing simulation times significantly, especially when simulating co-sputtering systems with 5-8 cathodes. The accuracy of SIMTRA and the capabilities of the Python wrapper are demonstrated by comparing the compositions predicted by simulation and measured by energy-dispersive X-ray spectroscopy of seven materials libraries in the system Ni-Pd-Pt-Ru.

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10:40am **CM3-1-ThM-9 Discovery and Development of Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion***, Ian Sharp,* Walter Schottky Institut, Technische Universität München, Germany **INVITED**

Transition metal nitride semiconductors are rapidly emerging as a promising class of materials for advanced optoelectronic and energy conversion applications. Compared to oxides, nitrides offer narrower bandgaps, stronger bond covalency, and improved carrier transport properties that make them well suited for harvesting sunlight in photovoltaic and photoelectrochemical systems. Despite this considerable promise, far fewer nitrides than oxides have been experimentally investigated due to their synthetic complexity and a broad range of new compounds remain to be explored. Furthermore, synthesis challenges have led to poorly controlled defect and impurity properties within this class of materials. In this work, we overcome these limitations using reactive co-sputtering to synthesize thin film nitride semiconductors with controlled compositions, exploring both dopants and new compounds in the Ti-Ta-N, Zr-Ta-N, and Hf-Ta-N composition spaces. Starting with orthorhombic Ta_3N_5, which stands as the best performing photoanode material within this class, we investigate the critical roles of native and impurity defects on carrier transport and recombination, showing that substitutional Ti and Zr doping with rationally optimized concentrations can be used to improve photoconversion efficiencies. While high Ti contents in Ta_3N_5 lead to the precipitation of a secondary TiN phase, different behavior is observed for the case of Hf and Zr. In particular, solid solutions with broadly tunable compositions across the Hf-Ta-N-(O) and Zr-Ta-N-(O) composition spaces are investigated, leading to bandgap-tunable compounds that exhibit remarkably large refractive indices suitable for photonics applications. Moreover, deposition of a stoichiometric 1:1 Zr:Ta ratio leads to formation of a new ternary nitride compound, bixbyite-type $ZrTaN_3$, that it is a strong visible light absorber, functioning as an active photoanode material. Complementary DFT calculations indicate a direct bandgap that is tunable based on cation site occupancy. Thus, this material offers exciting prospects not only for solar energy conversion but also for optoelectronics applications. Overall, these results highlight the promise of both established and new transition metal nitride semiconductors for solar energy harvesting, as well as the importance of precise composition engineering to tune optoelectronic and charge transport characteristics. Considering the compositional complexities of these compounds, exploration and optimization can be dramatically accelerated through use of gradient sputtering and rapid characterization approaches.

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

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

Moderators: Damien Faurie, Université Sorbonne Paris Nord, Barbara Putz, Empa Thun, Aparna Saksena, MPI für Eisenforschung GMBH, Germany

1:20pm **CM1-2-ThA-1 Crystalline-Amorphous Interface Fracture Explored Across Different Length Scales**, ***Alice Lassnig***, Montanuniversitat Leoben, Austria; *Michael Meindlhumer,* Montanuniversität Leoben, Austria; *Stanislav Zak,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria; *Megan Cordill, Christoph Gammer,* Austrian Academy of Sciences, Austria; *Andrew Minor,* Lawrence Berkeley Lab, USA **INVITED**

Interfaces separating bi- and multilayered thin film structures, are susceptible to premature failure due to the challenge of bridging distinct physical properties of adjacent materials. Thus, the reliability of these interfaces significantly influences the overall lifespan of such structures. Consequently, a thorough investigation of their reliability and a comprehensive understanding of the underlying failure mechanisms are essential for enhancing novel material composites and combinations.

In this study, we investigate the fracture behavior of model crystalline-amorphous interfaces, specifically focusing on Cu thin films delaminating from bulk glass substrates and nanocrystalline Cu – amorphous CuZr multilayers. Utilizing advanced characterization techniques, we aim to study the delamination behavior, interface adhesion, and fracture under static and cyclic loading of such structures using advanced experimental techniques spanning both the meso-scale and nanoscale, incorporating in situ transmission electron microscopy for a detailed exploration of these phenomena.

2:00pm **CM1-2-ThA-3 Tailoring Structure and Mechanical Properties of TiZrHfTa Refractory Alloy Thin Films**, ***Gregory Abadias***, *Hocine Slimani,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France; *Pietro Vecchietti,* Politecnico Milano, Italy; *Meriadeg Chalopin,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France; *Ferenc Tasnádi,* Linköping University, IFM, Sweden; *Matteo Ghidelli, Philippe Djemia,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France

Complex concentrated alloys (CCAs), including medium- and high-entropy alloys, offer attractive thermomechanical properties which make them promising candidates for various technologies such as corrosion resistant or radiation tolerant structural materials. Among the various CCAs, alloys with multi-principal refractory elements (RCCA) have drawn significant attention for hydrogen (H) storage applications [1-3] due to their ability to reversibly absorb H in the form of metal hydrides. However, up to now, studies on RCCA for H storage have only focused on bulk materials, with limited attention to thin film counterparts, which could be considered as model materials enabling an easy tailor of composition, phase and microstructural features (grain size, porosity or texture), providing valuable insights on the mechanisms of hydride formation and dissolution in RCCAs.

In this work, $(TiZrHf)_{100-x}Ta_x$ thin films, with thickness up to 700 nm and Ta content ranging from 0 to 60 at.%, were synthesized by co-sputtering deposition. The phase composition, crystal structure, morphology and elemental composition was determined using a combination of analytical techniques (XRD, SEM/TEM, EDS), while the intrinsic stress was measured *in situ* during deposition by wafer curvature method. The mechanical properties of the films were assessed by nanoindentation and opto-acoustics (Brillouin light scattering and picosecond laser ultrasonics) methods. By tuning the Ta content, different phases were stabilized in these quaternary alloys, from hcp to bcc and amorphous. These structural changes are accompanied by variation in growth morphology (evolving from nanocolumns to vein-like patterns), stress reduction and a progressive softening of hardness, shear and elastic modulus with increasing Ta content. The experimental findings are discussed and compared with results obtained from atomistic models of random alloys and amorphous phases, using *ab initio* molecular dynamics simulations combined with machine-learned interatomic potentials, as well as relevant data from the existing literature [4].

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2:20pm **CM1-2-ThA-4 Exploring Mechanical Properties of Thin Films Through Synchrotron X-Ray Diffraction, Digital Image Correlation and Electrical Resistivity Measurements**, ***Pierre-Olivier Renault***, University of Poitiers, France **INVITED**

Mechanical behavior of thin films deposited on polymeric substrates was investigated under in-situ controlled tensile biaxial loading conditions. The study employed synchrotron X-ray diffraction (XRD), digital image correlation (DIC) techniques, and electrical resistivity measurements. The combination of X-ray diffraction and digital image correlation provides classical stress-strain curves.

The three complementary measurement techniques allow for a comprehensive analysis of the deformation characteristics of each component of the thin film. This approach helps to identify and distinguish the various deformation regimes that arise during mechanical loading. Beyond the yield stress, distinct mechanical behaviors are observed in the stress-strain curves, which can be attributed to plasticity and fracture phenomena. These behaviors are identified as characteristic signatures of material failure modes.

Additionally, the experimental setup offers the capability to assess whether deformations are fully transmitted through the interfaces between the thin film and the substrate, providing also insight into the interaction between different layers in a multilayer coating.

After describing the experimental setup, examples of the mechanical behaviors observed in metallic bilayer or trilayer systems and, oxide-metal films deposited on polyimide substrates will be presented. These examples illustrate the range of deformation responses that can arise in such multilayer systems. Differences in the mechanical behavior of films are shown to be influenced by factors such as type of interface or the presence of residual stresses in the as-deposited films, as well as variations in film thickness and grain size. These factors play a key role in determining the overall mechanical performance of the thin film systems.

3:00pm **CM1-2-ThA-6 A Combined X-ray Microdiffraction and Micromechanical Testing Approach for Direct Measurement of Thin Film Elastic Constants**, ***Rainer Hahn***, CDL-SEC, TU Wien, Austria; *Rebecca Janknecht,* Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland; *Nikola Koutná,* Institute of Materials Science and Technology, TU Wien, Austria; *Anna Hirle,* CDL-SEC, TU Wien, Austria; *Anton Davydok,* Helmholtz-Zentrum Hereon, Germany; *Klaus Boebel,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein; *Szilárd Kolozsvári, Peter Polcik,* Plansee Composite Materials GmbH, Germany; *Christina Krywka,* Helmholtz-Zentrum Hereon, Germany; *Paul H. Mayrhofer,* Institute of Materials Science and Technology, TU Wien, Austria; *Helmut Riedl,* CDL-SEC, TU Wien, Austria

The direct measurement of elastic constants for thin films is not yet a routine procedure and presents a number of significant technical and analytical challenges when compared to the analysis of bulk materials. Ab initio density functional theory calculations can provide a theoretical basis for understanding the properties of materials. However, discrepancies between model systems and real-world properties persist, primarily due to a lack of available experimental data for newly emerging material systems. Furthermore, computationally affordable models are typically constrained to defect-free single crystals, thereby excluding microstructural effects that exert a pronounced influence on the material's behavior.

This study addresses this gap by proposing a novel experimental approach to measure direction-dependent elastic constants, combining synchrotron microdiffraction and micropillar compression. The approach was tested on a polycrystalline face-centered cubic TiN thin film, where linear elastic failure prevails. An advanced in-situ testing environment has been established to enable the continuous recording of the load-displacement of the indenter, while simultaneously collecting the material's deformation response to uniform uniaxial compression. This dynamic approach permits the evaluation of the orientation-dependent elastic strain components and the macroscopic uniaxial compressive stresses, each over time, thereby enabling a differential analysis to assess the elastic and X-ray elastic constants.

The excellent agreement between experimental and ab initio data serves to corroborate the here-proposed robust method for direct elastic constant measurements, which is of crucial importance for advancements in thin film material testing.

3:20pm **CM1-2-ThA-7 Real-Time Particle Detection for Enhanced Coating Deposition Processes**, ***Constant Boris Rieille***, *Sylvain LeCoultre,* Berner Fachhochschule BFH, Switzerland

Industries in photonics, optics, and semiconductors are increasingly challenged by particles emitted during PVD/ALD deposition processes. As device miniaturization advances, stricter requirements on defect size and particles inclusions make effective control essential to ensure product conformity.

Currently, these industries rely on preventive maintenance schedules that do not account for unexpected particle emissions or variations in machine usage. When particles appear, repeated maintenance is required due to the lack of a system to detect or locate their source. Integrating a real-time particles sensor into machines would transform this approach by enabling predictive monitoring, reducing downtime, and improving operational efficiency.

This session will deliver key insights into particle emissions during PVD deposition, explore market trends, and present business cases for the PVD/ALD market.

4:00pm **CM1-2-ThA-9 Real-Time Monitoring of Sputter Deposition Process: Application in the Context of Ag-Based Low-Emissive Coatings**, ***Rémi Lazzari,*** CNRS/Sorbonne Université, France **INVITED**

The challenge of green-house gas reduction pushes towards a better thermal insulation of housing. In this context, glass industry strives to decrease the infra-red radiative transfer across windows while keeping transparency. In the so-called low-E or solar control glazings, the functionality is provided by a complex stack of layers deposited by magnetron sputtering in which the active component is a ~10 nm thick Ag film encapsulated in between ZnO dielectric layers. Because of its noble character, Ag follows intrinsically a Volmer-Weber growth mode and is prone to dewetting upon thermal treatments such as windows tempering. Thus, there is tremendous need of understanding and control of its out-of-equilibrium growth process.

In this context, this presentation will illustrate the interest of combining real-time measurements (UV-vis spectroscopy[1,2]; stress measurement via wafer curvature and digital image correlation[3]; film resistivity) with *in situ* photoemission spectroscopy to have a full overview on the Ag growth mechanism. Among others, the impact of sputtering deposition parameters and of gas additives on stress build-up and relaxation, on film percolation and on Ag chemistry will be discussed[4-6]. The second part of the talk will show the contribution of model experiments in understanding the epitaxy at Ag/ZnO interface[7], the reactivity[8] and band alignment[9] at metal/ZnO interfaces as seen by *in situ* hard x-ray photoemission and the various contributions to Ag film resistivity[7].

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4:40pm **CM1-2-ThA-11 A Combination of Real-Time Diagnostics Probing the Impact of N_2 on Ag Thin Film Growth**, ***Michal Kaminski,*** KIT, Germany*; Gregory Abadias, David Babonneau,* Institute Pprime, France*; Alessandro Coati, Yves Garreau,* Synchrotron SOLEIL, France*; Anny Michel,* Institute Pprime, France*; Anton Plech,* KIT, Germany*; Andrea Resta,* Synchrotron SOLEIL, France*; Karan Solanki,* Institute Pprime, France*; Alina Vlad,* Synchrotron SOLEIL, France*; Baerbel Krause,* KIT, Germany

Silver thin films are used in a number of applications (e.g., transparent and conductive electrodes and plasmonic devices) which require a continuous layer with thickness below a few nanometers. However, Ag films grown by magnetron sputtering have the tendency to form 3D-structures on weakly interacting substrates, what prevents their application as transparent and conductive layers. It is reported that the use of gas additives (particularly N_2 [1]) allows for obtaining a continuous layer at earlier deposition stage.

A thorough understanding of the nanoscale mechanisms of thin film formation requires real-time techniques [2]. In particular the widely used *ex situ* diagnostics can provide misleading information, as the structure of the thin film can evolve even under high vacuum conditions. We employ a simultaneous combination of real-time grazing incidence small-angle x-ray scattering (GISAXS), grazing incidence diffraction (GID), and substrate curvature measurements to get information about polycrystalline thin film evolution during growth. In particular, GISAXS reveals changes in nanoscale morphology, GID gives insight into the crystallinity of thin films, and substrate curvature measurements provide information about the average intrinsic stress. With our methodology we can study the interdependence between stress state, thin film structure and morphology, using the quantitative information obtained from the scattering techniques. Since the influence of the substrate curvature can be crucial for grazing incidence condition x-ray techniques, we show that in the curvature regime encountered in our experiment the effect on GISAXS is negligible.

Using the information from all three techniques, we will discuss the impact of nitrogen additive on all growth stages (from initial stages of island nucleation, growth, and coalescence, up to formation of percolated and continuous films), including the relaxation of the film during growth interruptions.

Acknowledgements: The work is performed within the frame of the ANR-DFG project IRMA (491224986).

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Advanced Characterization, Modelling and Data Science for Coatings and Thin Films
Room Town & Country C - Session CM2-2-ThA

Advanced Mechanical Testing of Surfaces, Thin Films, Coatings and Small Volumes II

Moderators: Thomas Edwards, NIMS, Matteo Ghidelli, CNRS, France

1:20pm **CM2-2-ThA-1 Influence of Applied Deformation on Magnetic Properties of Ferromagnetic $Ni_{60}Fe_{40}$ Thin Films Deposited on Polymeric Substrate**, ***Alejandro Toledano Povedano,*** Institut Pprime - CNRS - ENSMA - Université de Poitiers, France*; Dominique Thiaudière,* Synchrotron SOLEIL, France*; Pierre Godard,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France*; Eloi Haltz,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France*; Damien Faurie, Fatih Zighem,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France*; Anny Michel, Pierre-Olivier Renault,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France

Metallic ferromagnetic thin films are key components in devices including sensors, data storage, and signal processing systems. With the rise of flexible electronics, understanding the relationship between magnetic properties and mechanical deformations in the low and high strain regimes is critical. These deformations induce homogeneous elastic strains as well as strain heterogeneities due to crystalline defects and cracks, impacting the magnetic properties of films through magneto-striction and dipolar interactions. This study focuses on how mechanical strain and controlled crack propagation affect the magnetic properties of thin films on polymer substrates. The research aims to reveal the relationship between controlled microstructural changes (residual stress, film thickness) and magnetic properties, from initial strain to crack onset and subsequent propagation. These insights are critical for developing flexible magnetic devices that

maintain performance under mechanical stress. To investigate these effects, a multi-scale approach has been caried out thanks to a unique setup developed at Synchrotron SOLEIL (DiffAbs beamline). It combines four techniques to study, in situ, the crystalline and magnetic properties of the sample subjected to equibiaxial or sequenced uniaxial tensile testing: X-ray diffraction to monitor the local lattice strain, digital image correlation to measure macroscopic distortions, electrical resistivity to reveal the crack onset and Magneto-Optical Kerr Effect to track the evolution of magnetic reversal. Ni60Fe40 thin films with varying thicknesses (20 and 200nm) have been deposited by ion beam sputtering on flexible polymer substrates and characterised under strain with this setup. Deformation tests of Kapton/Mo/Ni60Fe40 systems highlight the important role of the magnetoelastic field, induced by the difference of the in-plane stress components, for multi-cracking dynamics. The study also examined different film thicknesses to determine whether these variations were linked to fragmentation effects or magnetoplasticity. These findings show how crack density (which varies with thickness) influences the material's magneto-mechanical properties.The hysteresis loops initially show a square shape. As applied deformation increases, the loops change and exhibit features typical of a direction that resists magnetization, attributed to the negative magnetostrictive coefficient of Ni60Fe40. Beyond the maximum of the lattice strain, the loops appear to return to a square shape.

1:40pm **CM2-2-ThA-2 The Local Electrical Fingerprint of Deformation and Growth -Induced Defects in Alloys***, **Hanna Bishara**,* Tel Aviv University, Israel **INVITED**

A microstructural defect, whether spontaneously or intentionally induced, impacts the electrical properties of its surroundings. Defects dominate the electrical behavior of materials only when they become sufficiently dense. Therefore, capturing the defect's electrical characteristics is usually performed on a macroscopic scale, leading to averaging over multiple defect's types. This prevents studying the structure-properties relations in defects. This talk provides advanced electrical characterization methods of individual defects on surface and within the volume of bulk and thin film alloys.

The presentation initially introduces an experimental procedure to measure the local electrical resistivity of defect segments - with high sensitivity and spatial resolution *in-situ* scanning electron microscopy (SEM). The studied defects, i.e. pure and segregated grain boundaries (GBs), dislocations, stacking faults, and phase boundaries are either growth-controlled or deformation-induced. The segments are chemically and structurally characterized by electron backscatter diffraction (EBSD), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), and atom probe tomography (APT), in addition to molecular dynamics (MD) simulations.

In the context of grain boundaries (GBs), we report that the GB resistivity spans over a spectrum of values, depending on the boundary's excess volume. The resistivity values might increase by an order of magnitude due to segregation effects in metallic systems. However, segregation-influenced complexions are found to boost the electrical conductivity of semi-metallic materials. Additionally, the talk relates to the formation and electrical characterization of near-surface dislocations in brittle Heusler alloys.

Revealing the contribution of different GB types to electrical resistivity would pave the path for predicting the electrical degradation of materials upon controlled mechanical deformation. In addition, it allows a novel defect engineering to optimize the performance of conductors and functional alloys.

2:20pm **CM2-2-ThA-4 On the Effect of Thin Film Residual Stress on the Crack Propagation Resistance of ALD Coated Nano-Ceramics***, Edoardo Rossi,* Università degli studi Roma tre, Dipartimento di ingegneria Civile, Informatica e delle Tecnologie Aeronautiche., Italy*;* ***Marco Sebastiani,*** Università degli studi Roma Tre, Dipartimento di Ingegneria Civile, Informatica e delle Tecnologie Aeronautiche, Italy

The present work aims at investigating the effects of Atomic Layer Deposition (ALD) coatings on 3D printed ceramic micro-pillars, which were produced by Two-photon polymerization-direct Laser Writing (TPP-DLW). With a uniform 50 nm layer of Al_2O_3 under varying processing conditions (Plasma Enhanced-ALD at 200 °C, Thermal ALD at 200 °C, and 350 °C), the study first evaluated how these coatings influenced the retainment of fracture toughness through the splitting of glassy carbon (GC) pillars across a spectrum of Relative Humidity levels (below 5% and above 60%). Then, incorporating spatially resolved stress measurements through Focused Ion Beam (FIB) ring-core analysis, the specific interface effects of the coatings on the crack propagation process were investigated. A corresponding investigation of lithographically produced fused quartz micro-pillars treated with the same ALD parameters provided a comparative foundation to gauge the coatings' effectiveness in enhancing the composite fracture toughness.

Additionally, the research detailed how the found residual stresses within the ALD coatings, significantly varying depending on the deposition temperature, are critical for the understanding of crack initiation and propagation mechanisms, suggesting that the observed reduction in fracture toughness, when compared to undefective, uncoated pillars under similar humid conditions, might be attributed to premature crack tip opening.

The research clarified these interplayed dynamics with the coating's stresses through the silica system's response to ALD coatings, significantly improving the baseline crack resistance. Indeed, uncoated silica experience an approximate 134% increase in fracture toughness for a 50 nm deposition at 200 °C, while a 100 nm coating at 300 °C resulted in around a 165% enhancement. This illustrates how interface engineering (deposition temperature and induced stresses from ALD coatings) can fine-tune fracture toughness in 3D TPP micro-ceramics, depending highly on the substrate material and surface defects (likely missing in lithography silica structures).

2:40pm **CM2-2-ThA-5 Micromechanical Testing of Ceramic Coatings for Nuclear Applications up to 1000°C***, **Dong (Lilly) Liu**,* University of Oxford, UK **INVITED**

Multi-layered ceramic coatings, such as SiC and PyC, have been used to encapsulate spherical nuclear fuel kernels for use in the next generation of nuclear fission reactors. These coatings are typically between 30 µm to 100 µm thick and will subject to harsh environments such as elevated operation temperatures and neutron radiation during service. It is important to acquire local mechanical properties of these individual coating layers as well as the interfacial strength between the coatings for better understanding of their structural integrity and to support performance modelling. In this work, nanoindentation tests were carried out on SiC and PyC coatings over a range of temperatures from ambient to 1000°C with and without in-situ SEM imaging. The change of modulus and hardness as a function of temperature will be presented and the challenges associated with the high-temperature tests will be discussed. In addition, micro-cantilever bending method was utilized to evaluate the interfacial strength between the SiC and PyC coatings. During the coating deposition process (chemical vapour deposition), residual stresses were generated in the coatings and affected the local properties. Therefore, the residual stresses in each coating layer were characterised by focussed-ion-beam digital image correlation (FIB-DIC) method on unirradiated and neutron irradiated coatings where the magnitude of residual stresses are further modified due to radiation induced dimensional changes. The local mechanical properties and residual stresses measured are correlated with the coating deposition process, radiation damage and 3D microstructure generated using FIB tomography based on conventional Ga+ FIB and Plasms FIB.

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

Accelerated Thin Film Development: High-throughput Synthesis, Automated Characterization and Data Analysis II

Moderators: Davi Marcelo Febba, NREL, Sebastian Siol, Empa

1:20pm **CM3-2-ThA-1 Feature Selection and High-Throughput Synthesis: Can They Be Used to Predict Adsorption Energies on Multinary Materials?***, **Hannah-Noa Barad**,* Bar-Ilan University, Israel **INVITED**

Electro-reduction of CO_2 to sustainable fuels and value-added chemicals is one of the most promising paths for closing the anthropogenic CO_2 cycle. The catalyst, the main component of the electrochemical CO_2 reduction reaction (CO_2RR), is used to reduce CO_2 dissociation activation energy. Metal and metal oxide catalysts have been studied as catalysts for CO_2RR, yet selectivity towards desired products remains elusive. To overcome this issue, discovery of new materials with more components (*e.g.*, ternary, or quaternary materials), is paramount. These multinary materials, have the potential to improve the selectivity and activity toward a desired product, due to synergistic effects between the elements. However, the exploration space is enormous and needs to be decreased. An important descriptor for realizing the reaction mechanism leading to a specific product by a given catalyst is the adsorption energy of the rection intermediates, like *CO. Yet,

adsorption energies on these new and complex materials have not been studied systematically.

Here, we present the development of a machine learning model for the prediction of adsorption energies of materials. Our model is based on a simple description of the adsorption environment by choosing very basic features, and more intricate structural features, like orbital field matrix.[1] We also apply the moments theorem for the density of states (DOS)[2] to depict our materials in terms of closed paths in their lattices, from which we obtain features relating to the adsorption site. We also use high-throughput synthesis and characterization methods to try and obtain more experimental data points on new multinary materials to enhance out dataset. These methods will support prediction of adsorption energies of multinary materials to discover new highly active and selective CO_2RR catalysts.

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2:00pm **CM3-2-ThA-3 Development of Cu, Ni-Co-Doped $Bi_2Te_{2.7}Se_{0.3}$ for Thermoelectric Energy Generation Using Pulsed Laser Deposition**, ***Yakubu Sani Wudil***, King Fahd University of Petroleum and Minerals, Saudi Arabia

This work reports the preparation of ternary Cu/Ni/$Bi_2Te_{2.7}Se_{0.3}$ nanocomposite thin films via pulsed laser deposition. For comparison, pure $Bi_2Te_{2.7}Se_{0.3}$ (BTS) and binary Cu/$Bi_2Te_{2.7}Se_{0.3}$ and Ni/$Bi_2Te_{2.7}Se_{0.3}$ nanocomposites were also synthesized. Morphological characterizations revealed the presence of abundant grains typical of the BTS sample. Energy-dispersive spectroscopy confirmed trace amounts of Cu and Ni within the films, while X-ray photoelectron spectroscopy indicated that both metals were present as unoxidized metallic atoms, free from telluride formation. Structural analyses using X-ray diffraction and Raman spectroscopy showed peaks consistent with the pure BTS structure, suggesting that the dopants were primarily located at the grain boundaries within the BTS matrix. The ternary nanocomposites were prepared using a specialized configuration at three different Cu/Ni concentrations. The highest room temperature thermoelectric figure of merit (ZT) of 0.97 was achieved at the optimal doping concentration (BTS-2Cu/Ni), attributed to a simultaneous increase in power factor (2988 $\mu W/mK^2$) and a decrease in thermal conductivity (0.93 W/mK). The enhanced thermoelectric power factor resulted from the selective filtering of low-energy charge carriers, which improved the Seebeck coefficient. Additionally, the introduction of Cu and Ni into the nanocomposites created abundant grain boundaries that scattered phonons, reducing intrinsic lattice thermal conductivity and thereby enhancing the ZT value.

2:20pm **CM3-2-ThA-4 Autonomous Experiments for Thin Films and Solid Materials**, ***Taro Hitosugi***, The University of Tokyo, Japan **INVITED**

Integrating machine learning, robotics, and big data analysis into established research methodologies can significantly accelerate materials science research. Many studies have already demonstrated the potential of autonomous (self-driving) experiments in materials science [1, 2]. The rapid advancement of digital technologies is changing the way we conduct research.

Here, we discuss the status and prospects of data- and robot-driven materials research using autonomous experiments. We have developed an autonomous experimental system for thin-film materials. We constructed a system that automates sample handling, thin-film deposition, optimization of growth conditions, and data management. By using Bayesian optimization in conjunction with robots, our approach facilitates high-throughput experiments and generates comprehensive datasets that cover many aspects of materials (X-ray diffraction, Raman spectroscopy, scanning electron microscopy, optical transmittance measurement, electronic conductivity measurement). We tuned the hyperparameter for Bayesian optimization using the domain knowledge of chemistry; the number of trials to reach the global optimum is reduced.

The system demonstrated the synthesis and optimization of the electrical resistance in Nb-doped TiO_2 thin films [5]. Moreover, this autonomous approach has enabled the discovery of new ionic conductors [6]. We discuss the potential impact of this technology in accelerating materials science research, particularly in solid materials.

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[3] Tuning of Bayesian optimization for materials synthesis: simulation of the one-dimensional case, R. Nakayama, T. Hitosugi *et al.*, STAM Methods 2, 119-128 (2022).

[4] Tuning Bayesian optimization for materials synthesis: simulating two- and three-dimensional cases, H. Xu, R. Nakayama, T. Hitosugi *et al.*, STAM Methods 3, 2210251 (2023).

[5] Autonomous materials synthesis by machine learning and robotics. R. Shimizu, T. Hitosugi *et al.*, APL Mater. 8111110 (2020).

[6] Autonomous exploration of an unexpected electrode material for lithium batteries. S. Kobayashi, R. Shimizu, Y. Ando, T. Hitosugi, ACS Materials Lett. 5, 2711–2717 (2023).

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

CM-ThP-1 How to Predict the Deposition Rate During Reactive Sputtering Using an One-Volume Reference Resource?, ***Diederik Depla***, Ghent University, Belgium

A longstanding challenge in reactive magnetron sputtering is the quantitative prediction of the deposition rate, which is primarily determined by the partial metal sputtering yield from the oxide layer formed on the target surface during poisoning. The first step in addressing this issue is to determine the total sputtering yield of the oxide. This has been accomplished by refining a published semi-empirical model. This model has been applied to fit an extensive set of oxide sputtering yield data from the literature, comprising 65 datasets for 21 different materials. The fitting process establishes a relationship between the surface binding energies of metal and oxygen atoms and the cohesive energy of the oxide. The calculated partial sputtering yield of metal from a poisoned target is then compared with previously published experimental data on the metal sputtering yield during reactive magnetron sputtering. While both yields are linearly correlated, the magnetron-based sputtering yields are approximately eight times lower than the model predictions. This reduction in yield is attributed to the formation of an oxygen-rich surface layer, a hypothesis supported by binary collision approximation Monte Carlo simulations. However, these simulations do not fully capture the mechanism, as a more detailed description of the surface oxygen origin is needed. Despite this limitation, the experimental correlation provides a practical strategy for predicting deposition rates during reactive magnetron sputtering in fully poisoned mode. As demonstrated, the oxide sputtering yield can be calculated using standard data sources, and the empirical correlation between the sputtering yields enables a reliable estimate of the metal partial sputtering yield in poisoned mode, thus allowing for an accurate estimation of the deposition rate.

D. Depla, Note on the low deposition rate during reactive magnetron sputtering, Vacuum 228 (2024) 113546

D. Depla, J. Van Bever, Calculation of oxide sputter yields Vacuum 222 (2024) 112994

CM-ThP-2 Deep Insertion Induced Fracture in Soft Solids, ***MUTHUKUMAR MARIAPPAN***, Department of Mechanical Engineering, IISc Bangalore, India

Deep insertion of sharp objects like a needle into soft tissues is a common procedure in the medical domain for delivering drugs, biopsies and other medical interventions. It is inevitable to avoid tissue damage during needle insertion which sometimes leads to catastrophic outcomes. Opaqueness and inhomogeneity of the tissues make it difficult to observe the underlying damage mechanisms. In this context, it is essential to understand the underlying mechanisms of the formation of various cracks, crack nucleation and crack propagation in soft tissue-mimicking materials during deep penetration to minimise tissue damage. In this talk, we discuss the fracture behaviour of soft tissue-mimicking gels during deep penetration of a sharp needle. For the first time, we observed nearly periodic, stable, and well-controlled 3-D cone cracks inside the soft gel during deep penetration. We show that the stress field around the needle tip is responsible for the symmetry and periodicity of the cone cracks. These results provide a better understanding of the fracture processes in soft and brittle materials and open a promising perspective in needle designs and the control of tissue damages during surgical operations.

CM-ThP-3 Temperature-Dependent Oxidation Mechanisms of Binary Nitride Compounds: A Molecular Dynamics Approach, *Sara Fazeli,* MS4ALL, France*; Edern Menou,* ***Marjorie Cavarroc,*** SAFRAN, France*; Pascal Brault,* MS4ALL / GREMI, France

Binary nitride (XN) compounds represent an important class of advanced ceramic materials, increasingly recognized for their suitability in high-temperature applications such as aerospace components, turbine blades, and protective coatings. Transition metal nitrides such as titanium nitride (TiN) and zirconium nitride (ZrN) are especially noted for their outstanding hardness and resistance to corrosion. In addition, nitrides of non-transition metals, including carbon nitride (CN), silicon nitride (SiN), and boron nitride (BN), function as essential refractory materials due to their high stability under extreme temperatures and durability in harsh environments. The oxidation behavior of binary nitride materials is often a crucial factor in selecting materials for high-temperature use, as the oxidation resistance of a given XN phase depends on its capacity to form a stable, passivating oxide layer. It is worth noting that a distinct change in the oxidation mechanism is observed at high temperatures, which is attributed to phase transformations in the oxidation products. The insights gained from the oxidation behavior will facilitate the more efficient design and rapid discovery of XN phases that maintain optimal performance in oxidizing environments at elevated temperatures. In this study, we perform ReaxFF and COMB3-molecular dynamics (MD) simulations of the oxidation of binary nitride compounds XN (X = B, C, Si, Ti, and Zr) at four different temperatures (900 K, 1300 K, 1500 K, and 1700 K) to elucidate the mechanism of the oxidation states in the oxide layer.

At the lowest temperature, oxygen chemisorption occurred on the binary compounds without significant surface oxidation. In contrast, at higher temperatures, the amount of O_2 adsorbed increased steadily, particularly for transition metal nitrides. High oxygen coverage at elevated temperatures may lead to structural reconstructions of the surface. This study provides valuable insights into the oxidation mechanisms, helping researchers identify strategies to form stable, protective oxide layers, which enhance corrosion resistance and broaden the industrial applications of high-temperature materials, paving the way for the development of other binary nitride compounds.

CM-ThP-4 Simulating Mode-I Crack Opening Process in Transition Metal Diborides via Machine-Learning Interatomic Potentials, ***Shuyao Lin***, TU Wien, Institute of Materials Science and Technology, Austria*; Zhuo Chen, Zaoli Zhang,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria*; Lars Hultman,* Linköping Univ., IFM, Thin Film Physics Div., Sweden*; Paul Mayrhofer, Nikola Koutna,* TU Wien, Institute of Materials Science and Technology, Austria*; Davide Sangiovanni,* Linköping Univ., IFM, Thin Film Physics Div., Sweden

The critical stress-intensity factor K_{IC} and fracture strength σ_f define the fracture resistance of brittle ceramics. However, their experimental measurement is challenging and provides limited atomic-scale insight into crack tip behavior. In this work, we overcome these limitations by offering atomic-scale information on crack growth while evaluating fracture toughnesses and fracture strengths via machine-learning-assisted simulations. Transition metal diborides (TMB_2:s) serve as a case study, with a focus on understanding the Mode-I crack opening response across six distinct orientations within 2 different phases (α and ω). Molecular statics and dynamics calculations were used to systematically test model sizes and thicknesses, ensuring efficient simulations and accurate extrapolation of macroscale mechanical properties via constitutive scaling laws. By incorporating the phase-dependent and anisotropic mechanical properties of the α-phase TMB_2:s, the observed phenomena, as revealed through strain distribution and bond distances, align closely with those well-studied ceramics such as nitrides, offering insights into the fracture mechanisms within realistic deformation environments via atomistic level perspective. Furthermore, while α- and ω-WB_2 exhibits minimal phase dependence in deformation plasticity strength, as supported by both theoretical and experimental results, the fracture strength, as determined through the defective model, demonstrates a significant variation. The results show that the K_{IC} varies across different orientations and phases within the group IV, V, and VII TMB_2:s, correlating with their respective tensile and shear strengths.

CM-ThP-5 Simulation Study on Color Modulation of Diamond Substrates via Localized Surface Plasmon Resonance Effects Induced by Metal Nanoparticles, ***Tsung-Jen Wu***, *Sheng-Rong Song, Wen-Shan Chen,* National Taiwan University, Taiwan*; Wen Lin,* National Taipei University of Technology, Taiwan*; Shao-Chin Tseng,* National Synchrotron Radiation Research Center, Taiwan

This study employs the Finite-Difference Time-Domain method to simulate the Localized Surface Plasmon Resonance effects induced by gold, silver, and copper nanoparticles on diamond substrates, aiming to recreate the rare pink, yellow, and blue hues observed in certain diamonds. The simulation results reveal that gold nanoparticles impart a pinkish hue to the diamond, silver nanoparticles produce a yellow tint, and copper nanoparticles create a blue shade. These color variations are significantly influenced by the size and arrangement of the nanoparticles, with optimized configurations enhancing the color effects in synergy with the diamond's crystalline structure.The findings of this study provide an innovative and cost-effective approach for the jewelry industry to manufacture colored diamond coatings and serve as a valuable reference

for thin-film and coating technologies in applications involving optical components and sensors.

CM-ThP-6 Correlative XPS & SEM Analysis for NMC and Na-Ion Battery Cathode Material Surface Composition, ***James Lallo***, Thermo Fisher Scientific, UK, USA; *Nannan Shi, Albert Ge,* Thermo Fisher Scientific, UK, China; *Tim Nunney,* Thermo Fisher Scientific, UK

Advanced energy storage has become increasingly vital in many fields, from transportation, to defence, to everyday connectivity. This has led to a growing market demand and development for lithium-ion battery storage solutions.High-tech products such as smartphones, tablets, drones, and electric vehicles all rely on compact, powerful energy storage, with lithium-ion batteries being an essential component. Lithium battery primarily consist of cathode, anode, electrolyte, and separator materials. In lithium battery material research, how to comprehensively characterize and analyse battery materials, and how to use this characterization information to further improve battery material performance has become the focus of current researchers.This poster uses LiNixCoyMn(1-x-y)O2 (NCM)/LiCoO2 [NMC] composite cathode and Sodium Ion Fe/Mg cathode materials as examples. We employee a combination of Scanning Electron Microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS) characterization techniques to conduct a comprehensive analysis of the composite cathode materials. This approach yields rich sample information, helping researchers quickly evaluate and study any battery cathode materials.

The workflow combines scanning electron microscopy (SEM) [Thermo Scientific AXIA Chemisem] and X-ray photoelectron spectroscopy (XPS) [Thermo Scientific Nexsa G2 & ESCALAB QXi] into a correlated process, enabling the same regions of interest to be investigated; providing both high-resolution imaging and surface analysis from the same positions, even when collected using separate tools.

While SEM can easily visualize 2D materials, these layers are typically too thin to be easily characterized with the analytics commonly present on the microscope such as energy dispersive X-ray (EDX) analysis. XPS, meanwhile, cannot easily resolve surface structures at the required resolution, but can clearly detect what material is present at the surface, and quantify any chemical changes that might have occurred. XPS instrumentation typically also incorporates additional analytical techniques, such as an in-situ Raman spectrometer that is coincident with the XPS analysis position, which can be used to obtain further information.

CM-ThP-7 Optimizing Combinatorial Materials Discovery with Active Learning: A Case Study in the Quaternary System Ni-Pd-Pt-Ru for the Oxygen Evolution Reaction, ***Felix Thelen***, *Rico Zehl, Ridha Zerdoumi, Jan Lukas Bürgel, Wolfgang Schuhmann, Alfred Ludwig,* Ruhr University Bochum, Germany

Steering through the multidimensional search space of compositionally complex solid solutions towards desired materials properties makes the use of efficient research methods mandatory [1]. Combinatorial materials science offers rapid fabrication, e.g. magnetron sputtering, and high-throughput characterization methods. Still, improvements to materials exploration cycles are necessary, since combinatorial methods are also suffering from the curse of dimensionality. At the scale of multinary systems, planning follow-up experiments based on already acquired data is economically feasible only through the use of machine learning techniques [2].

In this study, we comprehensively explored the quaternary composition space of Ni-Pd-Pt-Ru for electrocatalytic applications with a streamlined discovery workflow. Enabling a fast synthesis, the fabrication of the materials libraries was performed by magnetron co-sputtering, and all libraries were subsequently characterized by energy-dispersive X-ray spectroscopy and X-ray diffraction. Guiding through the composition space, an active learning algorithm was used in an optimization cycle, which balances exploration and exploitation through the expected improvement acquisition function. The libraries were characterized electrochemically by an automated electrochemical scanning droplet cell setup [3] for the oxygen evolution reaction.

Six materials libraries were enough to find the global activity optimum in the system. The findings of six additional libraries are used to validate the activity trend. Our approach illustrates the potential of ML-driven optimization frameworks in accelerating the identification of promising multinary materials and underscors the value of integrating ML with high-throughput synthesis and characterization techniques in modern materials science.

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CM-ThP-8 High-Throughput Aging Studies of Vapor-Deposited Perovskite Thin-Films Using Precise Automated Characterization and Machine Learning-Assisted Analysis, *Alexander Wieczorek,* ***Sebastian Siol***, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

High-throughput experimentation (HTE) is increasingly being employed to accelerate metal halide perovskite (MHP) semiconductor thin-film development.[1] As of now, most approaches focus on solution-based deposition methods. To address the need for scalable and fabrication approaches, vapor-based deposition methods are gaining popularity.[2] However, durability concerns remain a major obstacle for large-scale deployment.[3] This motivates high-throughput stability studies of vapor-deposited MHP thin films. Combinatorial materials science is perfectly suited to address this challenge, specifically for time-consuming degradation studies where parallelization of experiments is key.[4] Using vapor deposition techniques, large parameter spaces can be covered on single substrates, whereas automated characterization and data analysis facilitate rapid properties screening.[5]

In this work, we present a comprehensive workflow for the aging of thin-film MHPs which includes structural, optical and chemical characterization.[6] To mitigate ambient degradation during characterization or transfers, we employ a complete inert-gas workflow. Furthermore, we perform a rapid *in-situ* screening of the transmission and reflectance under accelerated aging conditions. The samples are exposed to 85 °C and 1 kW m^{-2} white light bias, probing intrinsic material degradation in an accelerated fashion. With a temperature variation of ±1 °C and light intensity variation of <2% across combinatorial libraries, meaningful combinatorial stability screening is enabled. Automated characterizations of the structural properties yield deep insights into the aging process, extending and validating insights from changes in the optical transmission. We further demonstrate how these data sets can be used to better understand changes in the optical properties for highly scattering thin-films using machine learning assisted analysis. Furthermore, the workflow can be combined with high-throughput surface characterization techniques that our group previously demonstrated as a novel tool for accelerated materials discovery and optimization.

As a case study, we investigate the effect of residual precursors on the stability of two-step deposited MHP thin films grown on vapor-deposited templates. This workflow further allows to screen compositional spaces of libraries grown from completely vapor-based deposition methods.

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CM-ThP-9 Advanced Depth Profiling of Thin Films Using Angle-Resolved XPS/HAXPES, ***Jennifer Mann***, *Norb Biderman, Kateryna Artyushkova,* Physical Electronics, USA

X-ray photoelectron spectroscopy (XPS) is a powerful technique for non-destructive analysis of the chemical composition of thin layers and interfaces. Angle-resolved XPS (AR-XPS) has traditionally been used with Al Kα (1486.6 eV) X-ray beams to determine non-destructively determine layer thicknesses up to 5-10 nm below the surface. Recent advancements in AR-XPS, including the integration of Cr Kα (5414.8 eV) hard X-ray photoelectron

spectroscopy (HAXPES), have extended capability to 15-30 nm below the surface.

PHI's *Strata*PHI analysis software has been developed to reconstruct quantitative, non-destructive depth profiles from angle-dependent and single-angle photoelectron spectra. The latest version of *Strata*PHI combines Al Kα and Cr Kα XPS and HAXPES data within a single depth profile, enhancing the analytical information extracted from various depths.

Modern microelectronics devices contain thin films with different properties and purposes. Chips are often comprised of conducting films that form the interconnect layers as well as dielectric films that provide electrical insulation. In multilayer stacks, buried interfaces and subsurface layers are often beyond the analysis depth of traditional XPS. The information depth enabled by combined XPS and Cr Kα HAXPES is particularly useful for analyzing these types of materials.

This poster will discuss the principles behind AR-XPS and HAXPES, the new features of *Strata*PHI, and show some recent applications of the combination of these advanced methods to non-destructively probe thin films relevant to microelectronics.

CM-ThP-10 Numerical Ellipsometry: Artificial Intelligence Based Real-Time, in Situ Process Control for Virtual Substrates Including Multiple Unknown Layers, ***Frank Urban,*** 7980 SW 144th St, USA*; David Barton,* Florida International University, USA

Ellipsometry can be used to determine the optical properties and thickness of a thin film depositing on a known substrate based on light reflecting from the surface.This approach has the advantage of being able to be used in situ during the growth of the film with commercially available equipment to pass the light in and out of the deposition chamber. Nevertheless, a serious challenge in practice is that the material structure underlying the growing film commonly is composed of multiple layers. In these cases, very accurate knowledge of all of the underlying structure is required in order to obtain accurate results. Another challenge is that it the computation takes significant time using pre-existing iterative solution methods such as Levenberg Marquardt. The work here demonstrates the use of an Artificial Intelligence (AI) method suitable for real-time growth in which the underlying structure is complicated. This method is based upon previous development using five separate reflections simultaneously to solve for the underlying reflection coefficients at the same time the film parameters are being determined. The method is sufficiently fast that multiple groups of five measurements can be analyzed during the growth to confirm results and to examine the vertical homogeneity of the film being deposited. Examples will be given using a single angle of incidence. Thin absorbing films (up to 45 nm) will be given using a multilayer perceptron configuration consisting of 10 input neurons and 10 output neurons with two hidden layers of 80 neurons each. Solutions are performed at each wavelength independently and do not rely on fitting functions. The design, training and use of a number of neural networks will be presented.

CM-ThP-11 A Computational DFT Investigation of γ-CuI as an HTM for Perovskite Solar Cells, ***Salma Naimi,*** Green Energy Park (IRESEN/UM6P), Benguerir, Morocco/ Mohammed V university, Rabat, Morocco

Perovskite solar cells (PSCs) are recognized for their high efficiency and potential for low-cost production. However, the use of organic Hole Transporting Materials (HTMs) in these cells poses challenges due to their high cost and tendency to degrade the perovskite layer over time, threatening the commercial viability of PSCs.

In this study, we employed first-principles calculations based on Density Functional Theory (DFT), utilizing both the Generalized Gradient Approximation (GGA) and GGA + Hubbard correction, to evaluate the potential of γ-CuI as a cost-effective HTM. Initial investigations involved a comprehensive geometry optimization to ensure structural stability, followed by an analysis of elastic and mechanical properties, which confirmed the material's compatibility with flexible PSCs [1].

The electronic and optical properties of γ-CuI were explored, revealing a low extinction coefficient and high refractive index across the infrared and visible spectra. Notably, γ-CuI demonstrated minimal reflectivity and absorption in key spectral regions, highlighting its potential to reduce optical losses in PSCs [1].

These findings position γ-CuI as a promising and economically viable HTM, offering significant advantages for the next generation of perovskite solar cells.

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CM-ThP-12 Role of Gold-Doped Zno Nanoparticles to Degrade Dr-31 Dye as a Photocatalyst, ***Manik Rakhra,*** Lovely Professional University, Jalandhar, India

Water contamination is a significant issue in the modern day, caused by the textile dyingbusiness, and it has a detrimental impact on living organisms. We report on the manufacture ofgold-doped ZnO nanospheres using a simple heat treatment approach, and the use of ZnOnanoparticles as photocatalysts for the degradation of methyl orange dye. To increase thisdegrading activity, Au was utilized as a modifier, and their temperature quenching effect wasnoticed. One of the most efficient electron grabbers in the conduction band is au ion. Thestructural, morphological, optical, electrical, and photo catalytic characteristics of thesynthesized nanocatalysts were determined. These nanoparticles have a grain size of 45-75 nm.Photocatalytic activity was investigated using UV Vis spectra, and a significant absorption peakabout 482 nm was discovered. With increasing frequency, the dielectric constant and frequencyof the produced nanoparticles drop. The kinetic analysis yields a rate constant of 0.0165 min -1 forNano sphere-like particles. At a concentration of 1% Au, the produced nanoparticles degrade thedye completely in 150 minutes when exposed to UV light.

CM-ThP-13 The Application of Environmentally Friendly and Sustainable Corrosion Inhibitor for Carbon Steel in Petroleum Fields, ***Omotayo Sanni,*** University of Pretoria, South Africa*; Ren Jianwei,* university of pretoria, South Africa

In industrial sectors that deal with metallic materials, corrosion is a major problem. Steel corrosion causes significant economic losses in the oil and gas industry when oil wells are acidized. One common solution to this problem is the use of organic molecules as corrosion inhibitors. Therefore, the goal of this study was to determine the feasibility of using inexpensive, environmentally friendly, and organic compound from agricultural waste to reduce the rate of corrosion of carbon steel in an acidic environment that contains 1 M HCl. This research aims to investigate the potential use of agricultural waste as an inhibitory agent that can be reused for a variety of applications. Additionally, the extraction process in this work is done using water extraction. The compound was tested as a mitigator for the destruction of carbon steel in a 1 M HCl solution, and its composition was verified using a variety of spectroscopic techniques. Scanning electron microscopy-energy dispersive X-ray analysis (SEM-EDX) was used to investigate the surface of some corroded carbon steel samples in addition to electrochemical potentiodynamic polarization, impedance spectroscopy, and gravimetry studies. The data indicated that the addition of the waste compound inhibits the destruction of carbon steel by lowering the corrosion current density (iorr) and the double-layer capacitance (cdl). Tafel polarization data confirmed that the studied compound acted as a mixed inhibitor. The values of the cathodic Tafel slope (bc), are found to be near to each other demonstrating that the adsorbed chemicals did not modify the mechanism of hydrogen evolution. The spontaneity of the adsorption process is explained by the negative values of ΔG°ads.

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