Monday Morning, April 20, 2026

Plenary Lecture
Room Town & Country A - Session PL-MoM

Plenary Lecture

Moderator: Sandra E. Rodil, Universidad Nacional Autónoma de México

8:00am **PL-MoM-1 Welcome and Opening Remarks***,*

8:20am **PL-MoM-2 Nano-Engineered Materials: Heterostructures and Composites***, **Pulickel M. Ajayan [ajayan@rice.edu]**,* Rice University, USA **INVITED**

The last three decades have seen spectacular discoveries and developments in the field of nanotechnology. This talk will focus on some of these developments, particularly related to the opportunities and challenges in designing and controllably synthesizing functional nano-engineered materials. The talk will discuss several classes of materials, for example, carbon based and boron-nitrogen-carbon based materials, two-dimensional materials such as transition metal di-chalcogenides and their heterostructures, defect engineered materials and single-atom catalysts, interface controlled polymer nanocomposites and spark plasma sintered ceramic composites. I will also consider the impact of bottom-up engineering on the design of material systems relevant to many areas of applications. Several aspects including synthesis, chemical manipulation and hybridization will be discussed to address the opportunities that are available in creating novel nanoengineered materials.

Protective and High-temperature Coatings
Room Palm 3-4 - Session MA1-1-MoM

Coatings for High Temperatures and Harsh Environment Applications I

Moderators: Sabine Faulhaber, University of California, San Diego, USA, **Francisco Javier Perez Trujillo**, Universidad Complutense de Madrid, Spain

10:00am **MA1-1-MoM-1 Improving the Lifetime and Efficiency of Next Gen Aircraft Turbine Engines with PVD***, **Thibault Maerten [thibault.maerten@oerlikon.com]**,* Oerlikon Balzers Coating AG, France

Aircraft engine operating conditions continue to push the limits of material capabilities, which requires robust, multifunctional, and durable coating solutions for turbine hot-sectioncomponents. These turbines are mainly made from metallic components that are protected by thermal barrier coatings (TBCs). A TBC system is usually formed by a top ceramic layer deposited onto a bond layer over the substrate. MCrAlY (where M = Ni, Co, Fe or combinations of these metals) coatings are widely used as bond-coat material on blades and vanes due to their good resistance against oxidation and corrosion at high temperature. MCrAlY coatings are typically applied through thermal spray, electroplating and CVD methods. However, with ever-increasing turbine combustion temperatures, rotation speed for the sake of increased efficiency, the classic deposition methods are approaching their functional limits.

Significant developments over the last decade have made Physical Vapor Deposition (PVD) technologies increasingly compelling for MCrAlY coating deposition. PVD MCrAlY coatings exhibit high deposition rate, excellent surface adhesion, high density, and exceptional uniformity on complex geometries such as airfoils. Additionally, PVD MCrAlY coatings show a significantly lower surface roughness (Ra = 3-4 µm), which can be further smoothed by post-treatment, benefiting the application of EB-PVD TBCs.

With these significant advantages, PVD MCrAlY coatings produced by cathodic arc offer new opportunities for next gen aircraft engines development. In this talk, we aim to present several case studies involving replacement by PVD of traditional methods to produce MCrAlY. The coating properties (microstructure, composition, thickness distribution) and resulted performances (fatigue debit, oxidation and corrosion resistance) will be presented and compared.

10:20am **MA1-1-MoM-2 Mechanisms of Solid Particle Erosion in Aerospace Materials and Protective Coatings***, **Stephen Brown [stephen.brown@polymtl.ca]**[1], Etienne Bousser, Benjamin Milan-Ramos,* Polytechnique Montréal, Canada*; Juan Manuel Mendez,* MDS Coating Technologies, Canada*; Marjorie Cavarroc-Weimer,* Safran Tech, France*; Ludvik Martinu, Jolanta Ewa Klemberg-Sapieha,* Polytechnique Montréal, Canada

Solid particle erosion (SPE) is a tribological process involving material removal by repeated impacts of high-velocity particles. Despite years of research, fundamental mechanisms governing SPE remain poorly understood, particularly those concerning the erosion of metals at 90° impingement and the deformation of protective coatings in the elasto-plastic erosion regime. This work presents a detailed erosion study of bare Ti-6Al-4V and protective TiAlN-based coatings under varied particle velocity (50-120 m/s), impingement angle (15°-90°), and particle type/size (Al_2O_3, crushed glass 50-140 µm). Beyond standard metrics such as scar depth and volume loss rates, the eroded surfaces were extensively characterized by Plasma Focused Ion Beam cross-sectioning (PFIB), Electron Backscatter Diffraction (EBSD), Transmission Electron Microscopy (TEM) of eroded lamellae with Selected Area Diffraction, Transmission Kikuchi Diffraction (TKD), and nanoindentation mapping.

For Ti-6Al-4V, full erosion tests were compared to single particle impacts; both approaches showed cloudy microstructures indicative of severe local strain near impact sites, confirmed by TEM to be nanocrystalline. The affected depth did not exceed 7 µm, and nanoindentation revealed an 11% hardness increase. Extensive particle embedment occurred during multi-impact tests, yet damage morphology and affected depth were near-identical to single impacts, challenging cumulative wear models and suggesting that the 90° erosion of Ti-6Al-4V can be represented as the sum of individual impacts.

TiAlN coatings deposited via cylindrical magnetron sputtering exhibited architecture-dependent failure. Monolithic TiAlN initially degraded by nano-chipping, along with plastic deformation of the columnar structures 100-200 nm into the subsurface. This was followed by catastrophic adhesive failure after the coating thins beyond a certain threshold. A multilayer TiAlN/TiAl system exhibit a similar but distinct failure mode: cracks propagated along TiAl interlayers, promoting local delamination of the overlying TiAlN. In essence the same threshold-type failure occurs, however, the TiAl interlayers decrease the TiAlN layer thickness and thus the distance to the nearest interface. The result is progressive layer-by-layer material removal rather than bulk spallation, offering insight into how architecture governs erosion resistance.

10:40am **MA1-1-MoM-3 Microstructure and Oxidation of PVD Coatings on TiAl and Ni Superalloys for High-Temperature Applications***, **Radosław Swadźba [radoslaw.swadzba@git.lukasiewicz.gov.pl]**,* Łukasiewicz Research Network - Uppersilesian Institute of Technology, Poland **INVITED**

Modern aircraft engines operate at increasingly higher temperatures to improve thermal efficiency and reduce fuel consumption. These extreme conditions place severe oxidation and corrosion demands on structural materials such as TiAl intermetallics and Ni-based superalloys. Although these alloys combine excellent strength-to-weight ratios with good high-temperature mechanical properties, their long-term performance depends strongly on effective surface protection. The development of advanced oxidation-resistant coatings is therefore essential for enabling higher operating temperatures and extending the lifetime of next-generation aeroengine components.

This talk presents recent work on the development, microstructural design, and oxidation behaviour of protective coatings produced by the Closed Hollow Cathode Physical Vapor Deposition (CHC-PVD) method on TiAl and Ni-based substrates. The CHC-PVD process offers high plasma ionization, allowing deposition of thick, adherent, and compositionally complex coatings with tailored architectures.

The coating systems investigated include Ti–Al–Cr alloys modified with Si and Y, MAX phase coatings (Ti_2AlC and Cr_2AlC) on γ-TiAl, and MCrAl-type coatings on Ni-based superalloys. Detailed characterization was performed using High-Resolution Transmission Electron Microscopy (HRTEM), Scanning Transmission Electron Microscopy (STEM), and high-temperature X-ray diffraction (HT-XRD) to study both as-deposited coatings and their phase evolution during heat treatment. These advanced techniques made it possible to reveal nanolaminate microstructures, analyze interfaces, and examine thermally grown oxides in detail.

High-temperature oxidation studies under isothermal and cyclic conditions revealed clear differences in performance among the investigated coatings. The degradation modes, along with the formation and evolution of protective alumina scales, were examined in detail using HRTEM and STEM to establish correlations between microstructure, composition, and oxidation behavior.

The results highlight the potential of the CHC-PVD technique for producing advanced high-temperature coatings with optimized microstructures and oxidation behavior, contributing to the development of durable, lightweight materials for future aircraft engines.

11:20am **MA1-1-MoM-5 Predictive Analytics of Aluminide Diffusion Coatings Using Machine Learning to Forecast Their Aging and Service Life***, **Vladislav Kolarik [vladislav.kolarik@ict.fraunhofer.de]**, Maria del Mar Juez Lorenzo,* Fraunhofer Institute for Chemical Technology ICT, Germany*; Pavel Praks, Renata Praksová,* IT4Innovations National Supercomputing Center, VSB - Technical University of Ostrava, Czechia

Aluminide diffusion coatings offer a reliable and economical way to protect steel from high-temperature corrosion in harsh environments. These coatings can be applied as aluminum slurries using various deposition methods, including spraying or brushing, and are subsequently heat-treated to form the diffusion layer. Predictive analytics using machine learning offers great potential to forecast the aging behavior and lifetime of the coating under operating conditions. Machine learning predictions rely solely on historic data and do not require physical models to describe dependencies. This is especially advantageous for systems influenced by multiple parameters, as machine learning can identify patterns and relationships that humans cannot. Regression-based predictive models, such as Symbolic Regression or decision-tree algorithms like CatBoost and XGBoost, have proven to be suitable.

Two key variables were identified for describing the service life of an aluminum diffusion coating: (1) the ratio of the inner Fe_3Al layer to the total

[1] **Graduate Student Award Finalist**

coating thickness, and (2) the aluminum concentration in the Fe_3Al layer. The first variable indicates a milestone in the coating's service life, occurring when the ratio equals 1. At this point the diffusion coating evolves into a single aluminum-poor layer. The aluminum concentration in this single layer reflects the amount of aluminum remaining in the coating, which is essential for forming a protective alumina layer. The input parameters, time, temperature, atmosphere, overall coating thickness, thicknesses of the partial layers, number of the partial layers, type of slurry etc., were collected from our previous research as well as from literature. The transition to a single-layer coating was forecasted to occur after 28,000 hours at 650°C in air, following a time law close to parabolic, indicating that diffusion dominates the process. The aluminum content remains in the range of 25 at% over 100,000 hours, indicating that Fe_3Al will still be present.

The research shows that machine learning is very effective in analyzing complex material systems affected by multiple parameters, where understanding the relationships and importance of these parameters is difficult using conventional physical modeling approaches.

11:40am **MA1-1-MoM-6 Tailored Formation of Intermetallic Phases in Nanolayered Metallic Systems***, **Vincent Ott [vincent.ott@kit.edu]**, Sven Ulrich, Michael Stüber,* Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany

The temperature induced formation and stability of phases in nanoscale multilayer thin films are strongly affected by confinement effects and interface-controlled kinetics. As the characteristic dimensions of the layers are reduced, the thermodynamic driving forces and atomic mobility change, leading to distinct size-dependent phase formation behavior during heat treatment. In metallic multilayers, this often results in a modified or entirely suppressed sequence of equilibrium phase transformations. Using the Ru/Al model system and its ternary extensions with Hf, Cr, and Cu, we demonstrate that decreasing the individual layer thicknesses can kinetically inhibit the formation of equilibrium phases while promoting the preferential stabilization of the crystallographically simple cubic B2 structure. This enables the controlled synthesis of metastable intermetallic alloys beyond the thermodynamic equilibrium regime. The phase evolution was monitored in-situ by high-temperature X-ray diffraction (HT-XRD), while complementary electron microscopy and atom probe tomography (APT) provided insight into the resulting nanoscale structure and chemical distribution. The general validity of this kinetic stabilization concept is further illustrated by the Fe–Ti system, in which the B2 FeTi phase can be selectively formed at comparable nanometer-scale periodicities. These findings highlight the potential of nanoscale layering to engineer novel metastable phases with tailored structural and functional properties.

Functional Thin Films and Surfaces
Room Palm 5-6 - Session MB3-MoM

Low-dimensional Materials and Structures

Moderator: Kostas Sarakinos, University of Helsinki, Finland

10:00am **MB3-MoM-1 Shape and Symmetry Engineering in Transition Metal Dichalcogenide Nanoribbons for Light Harvesting***, Ganesh Ghimire, **Stela Canulescu [stec@dtu.dk]**,* Technical University of Denmark, Denmark **INVITED**

In this talk, I will discuss how controlling shape and symmetry at the nanoscale can fundamentally change how transition-metal dichalcogenides (TMDs) interact with light. By tailoring these materials into nanoribbon architectures, we can induce local symmetry breaking, tune excitonic behavior, and open new pathways for light harvesting and nonlinear optical response.

I will begin by introducing our alkali-assisted CVD approach for growing highly crystalline MoS_2 nanoribbons.[1,2] These nanoribbons can extend to tens of microns in length and naturally form monolayer–multilayer junctions within a single structure. This built-in structural gradient creates regions that either preserve or break inversion symmetry. As a result, we observe strong second harmonic generation and distinct excitonic emission localized at the nanoribbon edges. These symmetry-driven optical characteristics directly translate into improved device performance: individual nanoribbon photodetectors exhibit responsivities among the highest reported for TMD-based nanoscale photodetectors.

I will then expand the discussion to the bulk photovoltaic effect (BPVE), a mechanism that enables photocurrent generation in non-centrosymmetric crystals without the need for p–n junctions. I will show how engineered asymmetry in 3R-stacked MoS_2 and lithographically defined WS_2 nanoribbons leads to strong nonlinear optical response and shift-current generation. The resulting devices display large short-circuit current densities and measurable open-circuit voltages, underscoring the potential of symmetry-driven photovoltaic operation.

Overall, I will highlight how **nanoscale shape and symmetry engineering** serve as powerful design principles for next-generation optoelectronic and energy-conversion technologies. By deliberately breaking symmetry—through strain, stacking control, and dimensional confinement—we can create TMD architectures that harvest light more efficiently and exhibit enhanced nonlinear optical behavior. These findings position TMD nanoribbons as versatile building blocks for future light conversion, sensing, and photovoltaic applications.

References:

1. Ghimire, G. *et al.* Molybdenum Disulfide Nanoribbons with Enhanced Edge Nonlinear Response and Photoresponsivity. *Adv. Mat.* 35, (2023).

2. Miakota, D. I., Ghimire, G., Ulaganathan, R., Rodriguez, M. & Canulescu, S. A novel two-step route to unidirectional growth of multilayer MoS_2 nanoribbons. *Appl Surf Sci*. 619, (2023)

10:40am **MB3-MoM-3 Discovery of Goldene Comprising Single-atom Layer Gold; Prospects for Novel Noble Metallenes***, **Lars Hultman [lars.hultman@strategiska.se]**,* Linköping University, IFM, Thin Film Physics Division, Sweden **INVITED**

The quest to make monolayer gold has hitherto been limited to a few atomic layers stabilized on or inside another material. The bonding nature of metals is the root cause to gold's tendency to take 3D shapes during all kinds of synthesis, like vapor-phase deposition or precipitation from solutions.

Through an innovative scheme, single-atom-thick 2D gold[1)], named *goldene*, has been exfoliated by wet-chemically etching away Ti_3C_2 layers from Ti_3AuC_2 nano-laminated MAX-phase[2), 3)] ceramic initially formed by substituting the Si layer in Ti_3SiC_2thin films with Au[3)]. The driving force for such exchange substitution lies in the eutectic nature of the Au-Si phase diagram. Etching-free the goldene sheets is made using a diluted form of the Murakami's reagent[5)]. Surfactant schemes are applied to hinder *goldene* sheets from coalescing with each other in water suspension.

Goldene is observed by scanning transmission electron microscopy. A tendency for curling and agglomeration of*goldene* is observed, whereas *ab initio* molecular dynamics simulation shows that flat atomic layers are inherently stable. X-ray photoelectron spectroscopy reveals an Au 4f binding energy increase of 0.88 eV. Prospects for preparing *goldene* from a series of carbide and nitride MAX phases are also presented.Proposed applications for *goldene* include sensors and photocatalyst for water splitting during solar energy harvesting. The use of Au resources would be minimized due to the ultimate surface-area-to-volume ratio for *goldene*.

Isolated three-atomic-layer Au sheets – trilayer *goldene* – was recently reported by us by selectively removing the Ti_4C_3 sheets from $Ti_4Au_3C_3$, formed by Au-intercalated Ti_4SiC_3 thin films.[6)] Finally, this presentation will discuss ways to realize other noble-metal *metallenes*[7)] from thin-film or bulk-powder templates.

1. *Nature Synthesis*, **3** (April 16, 2024) 744-751

2. *MAX phases* are inherently nanolaminated hexagonal ternary metal carbides and/or nitrides with a general formula $M_{n+1}AX_n$, where M is a transition metal, A is a group 13-16 element, X is carbon and/or nitrogen, and n = 1, 2, 3,...
3. Review: M. Dahlqvist, M.W. Barsoum, J. Rosen, *Materials Today* **72** (2024) Jan/Feb, p. 1 https://doi.org/10.1016/j.mattod.2023.11.010

4. H. Fashandi, M. Dahlqvist, J. Lu, J. Palisaitis, S. Simak, I. Abrikosov, J. Rosen, L. Hultman, M.Andersson, A.Lloyd-Spetz, P.Eklund *Nature Materials* **16** (2017) 814

5. Potassium ferricyanide is combined with potassium hydroxide (or sodium hydroxide) and water to formulate Murakami's etchant.

6. Y. Shi, [...], L. Hultman*Sci. Advances***11**, eadt7999 (2025) 28 March 2025

S. Kashiwaya, Y. Shi, J. Rosen, L, Hultman, *2D Materials* **12** (2025) 033001

11:20am **MB3-MoM-5 Nanoporous TiO2 Thin Films by Helium-Assisted Sputtering for Noble-Metal-Free Hydrogen Sensing***, **Stanislav Haviar [haviar@ntis.zcu.cz]**, Akash Kumar, Tomáš Kozák, Petr Zeman,* University of West Bohemia in Pilsen, Czechia

A large portion of magnetron-sputtered film applications targets the fabrication of highly compact, dense films. Textbook knowledge of thin-film growth delineates process windows that lead to "low-quality," non-compact morphologies. However, there are use cases where higher porosity or other forms of nanostructuring are advantageous—for example, when a large reactive surface area is desired. In this work, we discuss a modification of classical reactive sputtering in an Ar/O_2 mixture by introducing helium gas. Subsequently, we evaluate the resulting materials assembled as conductometric hydrogen gas sensors.

Titanium oxide films were deposited by conventional DC reactive sputtering, where helium replaced part of the Ar/O_2 working-gas mixture. The substoichiometric as-deposited films were post-annealed to achieve stable TiO_2. The introduction of helium promotes the formation of distinctive morphological features, which increase film porosity, as observed by electron microscopy.

We analyze the mechanisms involving reflected fast neutrals underpinning the emergence of nanoporous structures, supported by SEM imaging as well as structural characterization via XRD and Raman spectroscopy. We describe the evolution of the microstructure with annealing temperature and identify key processing parameters required to obtain porous yet stable films.

The application potential is then assessed by employing the films as conductometric hydrogen sensors. Films prepared by He-assisted sputtering show a several-fold increase in sensitivity to hydrogen without the addition of any noble metals.

Overall, controlled nanostructuring of thin films represents a promising route to engineer novel materials for gas sensing, and He-assisted deposition is one such approach.

Surface Engineering of Biomaterials, Devices and Regenerative Materials: Health, Food, and Agriculture Applications

Room Palm 1-2 - Session MD1-1-MoM

Coatings and Surfaces for Medical Devices: Mechanical, Corrosion, Tribocorrosion, and Surface Processing I

Moderators: Jean Geringer, Ecole Nationale Superieure des Mines, France, **Mathew T. Mathew**, University of Illinois College of Medicine at Rockford and Rush University Medical Center, USA

10:00am **MD1-1-MoM-1 NaOh Etching and Oxygen Plasma Treatments on Surface Characteristics and Their Potential to Activate Micro-Arc Oxidized TiO_2 Biomedical Coatings***, **Paulo Noronha Lisboa-Filho [paulo.lisboa@unesp.br]**,* UNESP, Brazil **INVITED**

Activation treatments such as NaOH etching or O_2 plasma can play an essential role in surface conjugation of titanium with biomolecules, providing a better interaction at the bone-implant interface. However, their application on complex titanium dioxide (TiO_2) surfaces is still not explored. In this contribution, bioactive and porous TiO_2 coatings produced by micro-arc oxidation (MAO) were treated with NaOH etching or O_2 plasma and then placed in contact with a reactive isocyanate test compound to evaluate the potential of molecule conjugation. Results suggested that O_2 plasma treatment has only changed the surface chemistry of the coating through carbon contaminants removal, plasma-driven oxidation and generation of functional OH species, including reactive carboxyl groups. This chemical modification by plasma has made the surface superhydrophilic. After NaOH etching, the coating became rougher and also superhydrophilic, containing titanate structures doped with sodium and calcium on its surface and inside the inner pores. Upon reaction with butyl isocyanate, the O_2 plasma-treated surfaces seem to better provide molecule conjugation, introducing characteristic conjugation bonds, and also making MAO coatings more hydrophobic due to the surface-terminated methyl chains from isocyanate. This proof-of-concept study has demonstrated the promising grafting potential given by O_2 plasma on complex TiO_2 surfaces.

10:40am **MD1-1-MoM-3 Influence of Microstructures on the Corrosion Behavior of Cobalt-Chromium Alloys Under Different Ortho Joint Conditions***, **Mathew T. Mathew [mtmathew@uic.edu]**, Avirup Sinha, Sujoy Ghosh, Maansi Thapa, Remya Ramachandran, Nicki Ta,* University of Illinois at Chicago, USA

Cobalt-Chromium-Molybdenum (CoCrMo) alloys have been used in various biomedical applications, including hip and knee implants, making them highly essential in orthopedics. A major concern regarding these implants is their long-term corrosion resistance, as corrosion can have a negative impact on patient health. Corrosion resistance is impacted by a variety of factors, such as the alloy's microstructure and the environmental conditions that can affect the release of metal ions. In this study, two different microstructures of CoCrMo were tested including homogeneous and banded samples. Each microstructure was tested under three different conditions: normal, inflammatory, and infectious. To stimulate these environments, 30 g/L protein was used for normal conditions, 0.5 mM hydrogen peroxide for inflammation, and 15 µg/L LPS for infectious conditions. To test the long term effects of these conditions, 24 hour corrosion experiments were performed using a three-electrode electrochemical set up. The electrochemical testing protocol included the sequence of open circuit potential, potentiostatic run, electrochemical impedance spectroscopy, and cyclic polarization. For banded samples the experiments were run at a constant potential of -0.7V and for homogeneous samples, it was run at -0.68V. The banded structure exhibited higher current values than the homogeneous structure, indicating that CoCrMo alloys with a homogeneous microstructure have greater corrosion resistance. Furthermore, among normal, inflammatory, and infectious conditions, the inflammatory condition resulted in the greatest alloy loss (µg) for both banded and homogeneous structures. Specifically, the banded structure showed a loss of 37.53 µg, while the homogenous structure exhibited a loss of 5.69 µg, indicating inflammatory conditions have the least corrosion resistance.

11:00am **MD1-1-MoM-4 Synergistic Fretting–Corrosion Mechanisms in DLC Coatings***, **Tomasz Liskiewicz [T.Liskiewicz@mmu.ac.uk]**,* Manchester Metropolitan University, UK*; Samuel McMaster,* Anglia Ruskin University, UK*; Michael Bryant,* University of Birmingham, UK*; Thawhid Khan,* University of Sheffield, UK*; Yu Yan,* University of Science and Technology Beijing, China*; Ben Beake,* Micro Materials Ltd, UK **INVITED**

This study investigates the synergistic interactions between fretting wear and electrochemical crevice corrosion in diamond-like carbon (DLC) coating systems on AISI 316L substrate under physiologically representative conditions. Particular emphasis is placed on understanding how albumin influences fretting–corrosion mechanisms, given their critical role in many engineering and biomedical environments. A combined experimental methodology is employed, integrating micro-mechanical characterisation (instrumented indentation and scratch testing) with fretting experiments employing in-situ electrochemical characterisation to assess coating durability, damage initiation, and interfacial degradation. Electrochemical techniques, including open-circuit potential monitoring, potentiodynamic polarisation, and electrochemical impedance spectroscopy, are applied in situ during fretting to capture the evolving interaction between mechanical and electrochemical degradation processes.

Fretting was replicated by applying micro-motion to the Al2O3 ball relative to the coated plate under a dead weight normal load. A maximum Hertzian contact pressure of 800 MPa was used for the tests, at a fretting displacement amplitude of 100 µm, giving a gross slip fretting regime. Each fretting test lasted 60 minutes resulting in 3600 cycles at a frequency of 1 Hz. Detailed surface and subsurface analyses using scanning electron microscopy, focused ion beam cross-sectioning, and energy-dispersive X-ray spectroscopy reveal progressive coating damage involving micro-cracking, interfacial delamination, and tribologically induced graphitisation of the DLC layer. Results demonstrate that fretting accelerates corrosion through mechanical disruption of the coating–substrate interface, while corrosion promotes further fretting damage via under-film attack and crack propagation, establishing a genuine fretting-corrosion synergy.

A mechanistic model is proposed in which mechanical defect initiation, electrochemical attack, and debris generation act in a feedback loop, driving progressive coating degradation. These insights highlight the importance of considering protein–surface interactions and combined degradation modes when designing DLC coatings for demanding fretting–corrosion service conditions in biomedical and engineering applications.

11:40am **MD1-1-MoM-6 Mechanisms of Fretting Corrosion in Titanium-based Biomedical Modular Implant Interfaces***, **Avirup Sinha [asinha38@uic.edu]**,* University of Illinois - Chicago, USA

Fretting corrosion is observed at modular junctions under load, where micro-motions lead to material loss and release of metallic ions or debris. Depending on applied load and displacement amplitude, fretting progresses through partial slip, mixed, and gross slip regime. In this study, fretting corrosion behavior was investigated under two contact configurations: metal on metal (Ti-6Al-4V on Ti-6Al-4V) and metal on ceramic (Ti-6Al-4V on ZrO2) in Bovin Calf Serum (BCS). BCS used in the experiment reflect two conditions: normal and infectious. Experiments were performed using 83 N normal load with a displacement amplitude of 5 µm at 1 Hz. Electrochemical protocols include sequential measurements of open circuit potential (OCP), potentiostatic (PS), and electrochemical impedance spectroscopy (EIS) which are synchronized with fretting motion. The test condition includes 10.9 mm diameter mirror polished disk and a 3 mm diameter pin with 20 ml of electrolyte used for each trial.This approach allows systematic evaluation of how contact pair and electrolyte chemistry influences the synergistic effects of wear and corrosion. The results are expected to advance the understanding of fretting corrosion in modular implants and support the design of materials and interfaces with improved in-vivo durability.

Plasma and Vapor Deposition Processes
Room Town & Country A - Session PP1-1-MoM
PVD Coatings and Technologies I

Moderator: Christian Kalscheuer, IOT, RWTH Aachen, Germany

10:00am **PP1-1-MoM-1 Optimizing Sputter-Deposited MoS2 Coatings: Insights from Monte Carlo Simulations and In-Situ Plasma Diagnostics***, **Alexander Mings [ajmings@sandia.gov]**, Steven Larson, Kyle Doorman, Tomas Babuska, John Curry, Remi Dingreville, David Adams,* Sandia National Laboratories, USA

Sputter-deposited molybdenum disulfide (MoS_2) coatings are widely utilized in aerospace applications, primarily due to their exceptional reliability and ultralow friction in vacuum environments. However, the unique structure of MoS_2 often leads to high porosity in sputtered coatings which can significantly compromise wear life and accelerate film oxidation. To address these challenges, engineers typically engage in costly process development, varying deposition parameters to maximize film density with limited available heuristics. This process development is also equipment specific and must be repeated when a process needs to be transferred.

This study explores how the kinetic energy of species impacting the substrate during the growth of MoS_2 films influences their porosity. We employ Monte Carlo simulations using both SRIM (Stopping and Range of Ions in Matter) and SIMTRA (Simulating the Transport of Atoms from the Source to the Substrate) to analyze the contributions of both sputtered atoms and backscattered neutrals. By correlating these findings with nanoindentation hardness, we gain insights into how deposition dynamics affect coating porosity. Additionally, we compare the simulation results to in-situ measurements made with a Retarding Field Energy Analyzer (RFEA) positioned at the substrate. Our findings reveal the energy flux necessary to produce dense coatings, which can be used in combination with a RFEA to provide essential feedback for process development. This approach has the potential to both greatly accelerate process transfer and enhance the film performance of existing MoS_2 processes.

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10:20am **PP1-1-MoM-2 HiPIMS and Digitalization: Increasing Efficiency in Machining***, **Stephan Bolz [stephan.bolz@cemecon.de]**, Biljana Mesic, Oliver Lemmer, Christoph Feig,* CemeCon AG, Germany

The presentation "HiPIMS and Digitalization: Increasing Efficiency in Machining" shows how modern digitalization and innovative coating technologies accelerate the development of HiPIMS coatings for cutting tools.

The focus is on using a HiPIMS coating system “CC800 HiPIMS,” for which a digital twin model exists that captures and analyzes large amounts of data.

Machine data are first collected via an OPC-UA interface, persisted in a database, and then transferred into the digital twin. This allows simulation results to be quickly integrated into process development. Consequently, only a few validation experiments are needed, saving time and resources. The simulation-optimized HiPIMS process parameters enable the deposition of coatings that are denser and harder than ever before. These were tested on cutting tools and achieved better results than previous layers.

Overall, the talk demonstrates how the combination of HiPIMS technology and digitalization increases efficiency in coating development, improves product quality, and strengthens competitiveness in high-performance machining.

10:40am **PP1-1-MoM-3 From Poisoned Targets to Healthy Models: The Quest for Parameters***, **Diederik Depla [Diederik.Depla@ugent.be]**,* Ghent University, Belgium **INVITED**

The conceptual simplicity of reactive magnetron sputtering facilitates the description of global trends in process curves characteristic of reactive magnetron sputtering. However, achieving a quantitative description of these trends through simulations remains far more challenging, as the critical bottleneck of every modelling effort lies in the determination of accurate input parameters. Following a brief introduction to the RSD model, this paper provides an overview of several experimental methodologies designed to extract the parameters essential for its implementation. A central parameter in any thin-film deposition technique is the deposition rate. While its determination in metallic mode is relatively straightforward, the task becomes substantially more complex in poisoned mode due to the limited availability of sputter yield data for oxides. Our experiments reveal that in poisoned mode sputter yields exhibit a pronounced dependence on process conditions. Monte Carlo simulations, moreover, uncover a remarkable material-independent correlation between reported partial yields for oxides and experimentally measured yields in poisoned mode. Another crucial quantity, the ion-induced electron yield, can only be reliably determined experimentally, even for metals. By employing empirical scaling laws, however, it becomes feasible to estimate these yields under poisoned-mode conditions. The strong influence of chemisorption on the electron yield explains the discharge voltage behaviour in metallic mode. The influence of chemisorption on target poisoning emerges as the next major challenge, particularly as a novel strategy to control the reactive sputtering process exposes discrepancies between the current formulation of the model and experimental observations. Nevertheless, this measuring strategy provides compelling evidence that the RSD model’s prediction of double hysteresis behaviour is fundamentally correct.

11:20am **PP1-1-MoM-5 Advanced YSZ Coatings Deposited by Magnetron Sputtering for High-Temperature Applications***, **Imene Toumi [imene.toumi@utt.fr]**,* Université de Technologie de Troyes, France*; Sofiane Achache,* Université de technologie de Troyes, France*; Akram Alhussein, Benoit Panicaud,* Université de Technologie de Troyes, France

Thermal barrier coatings (TBCs) are essential for extending the lifetime and efficiency of components exposed to extreme thermal environments, particularly in aerospace and energy systems [1-2]. Yttria-stabilized zirconia (YSZ) remains the benchmark topcoat material due to its low thermal conductivity, high fracture toughness, and outstanding thermal stability [1-4]. The performance of these coatings is strongly governed by the stabilization of the metastable tetragonal phase, which depends on both yttria content and deposition conditions [5].

In this study, YSZ thin films were deposited by dual-target reactive magnetron sputtering (Zr + Y) under an Ar/O_2 atmosphere. A parametric analysis was conducted to evaluate the effects of oxygen flow rate, substrate position, scanning amplitude, and yttrium doping level (expressed as Y_2O_3 content) on film growth, chemical composition, and crystalline structure.

Physicochemical and mechanical characterizations were performed using X-ray diffraction (XRD), energy-dispersive spectroscopy (EDS), scanning electron microscopy (SEM), and nanoindentation. The optimal yttria content (Y_2O_3) was found to be ≈ 2.9 mol%, ensuring stable tetragonal phase formation.

Furthermore, the thermal stability of the prepared coatings was assessed through annealing cycles at 500 °C, 750 °C, and 1200 °C. The study aims to evaluate the stability of the tetragonal phase at elevated temperatures and to investigate the microstructural evolution of YSZ thin films.

This work establishes a multi-parameter optimization strategy for YSZ thin films, contributing to the design of next-generation TBCs with improved structural integrity and reliability in harsh service conditions.

11:40am **PP1-1-MoM-6 Measurement of Residual Stress and Evaluation of Stored Energy Relief Efficiency for TiN/Ti/TiN/Ti Coatings with Different TiN/Ti Thickness Ratios***, Yi-Cheng Yang [richardyang329@gmail.com],* Department of Engineering and System Science National Tsing Hua University, Taiwan

Transition metal nitride (TMeN) coatings deposited by physical vapor deposition (PVD) are often subjected to high residual stress, which may induce delamination and failure of coatings. Introducing a metal interlayer between the coating and substrate is one of the common approach to relieve residual stress. In our previous studies, we proposed an energy-balance model to quantitatively evaluate the energy relief efficiencies of ZrN/Ti, ZrN/Zr [1] and TiN/Ti [2] coatings. With the growing demands for multilayer structures, optimizing the thickness ratio between coating and the metal interlayer for the effective relief of stress and stored energy has become essential in improving coating performance. Therefore, this study aims to evaluate the thickness ratio between coating and interlayer using TiN/Ti/TiN/Ti as a model system. Quadlayer coatings with different TiN/Ti thickness ratios were deposited on Si substrates using DC unbalanced magnetron sputtering. Residual stress was measured by both laser curvature measurement and the average X-ray strain methods. Subsequently, the stored elastic energies of the coatings with different architectures were calculated. Using the previously proposed energy-balance model, the energy relief efficiencies of specimens with various TiN/Ti thickness ratios could be estimated. Accordingly, the effect of TiN/Ti thickness ratios on stress and energy relief could be accessed. Based on the results, the previous energy-balance model can be extended from bilayer to quadlayer coatings.

Keywords: Energy relief, energy-balance model, quadlayer coatings, average X-ray strain methods

Topical Symposium on Sustainable Surface Engineering
Room Town & Country B - Session TS1-1-MoM
Coatings for Batteries and Hydrogen Applications I

Moderators: Chen-Hao Wang, National Taiwan University of Science and Technology, Taiwan , **Martin Welters**, KCS Europe GmbH, Germany, **Fan-Bean Wu**, National United University, Taiwan

10:40am **TS1-1-MoM-3 Hydrogen Technology – Which Role Play Thin Films on the Performance and Sustainability?***, Christina Scheu [scheu@mpie.de],* Max-Planck-Institut for Sustainable Materials, Germany **INVITED**

Hydrogen technology is an important route to an environmental friendly economy. It includes the generation of green hydrogen via (photo)electrochemical cells, the efficient storage and transport of hydrogen in (often) metallic gas tanks and pipelines and the usage in fuel cells to power trucks and cars. Thin films play a crucial role in transitioning from conventional power systems to this value-added chain. In the presentation, different examples will be given to demonstrate the necessity of thin film development for hydrogen technology. For example, hydrogen is stored and transported often in expensive steel containers and pipelines, but a protective coating made by e.g. Al_2O_3 on cheaper steels can sufficiently prevent hydrogen ingress. In photoelectrochemical cells, thin absorber thin films (often only a few tens of nanometer thick) allow to absorb a high amount of visible light and generate electron – hole pairs which are used to split water into hydrogen and oxygen. Typical examples for excellent absorber thin films are based on Sn doped Fe_2O_3 or $BiVO_4$, but further development is needed to make them even more efficient. Thin films are also used in fuel cells, not only as corrosion protector for the metallic flow field where hydrogen and oxygen are distributed, but also in the protection of catalyst and support material to prevent their degradation. An important role is also the development of novel catalyst for fuel cells or electrolyzer with excellent longevity by investigating thin film model catalyst where the impact of the chemical composition and crystal structure can be systematically evaluated. In all the examples, defects such as grain boundaries or stacking faults within the thin film are crucial for the performance and lifetime, and they need to be analysed down to the atomic scale. In our work we use aberration corrected (scanning) transmission electron microscopy and atom probe tomography to get insights in the thin film structure and defects.

Acknowledgment: The author is grateful to all the colleagues and co-workers who contributed to the different aspects of the hydrogen technology projects and to financial support from the German Science Foundation (DFG) within the CRC 1625 and the Federal Ministry for Economic Affairs and Climate Protection (BMWK) within the project PAULL1/2.

11:20am **TS1-1-MoM-5 PVD-synthesized Nitrides as Hydrogen Barrier Coatings***, Phillip Rückeshäuser [phillip.rueckeshaeuser@tuwien.ac.at],* TU Wien, Austria*; Szilard Kolozsvari, Peter Polcik,* Plansee Composite Materials GmbH, Germany*; Timea Stelzig,* Oerlikon AM Europe GmbH, Germany*; Konrad Fadenberger,* Oerlikon Balzers Coating Germany GmbH, Germany*; Klaus Boebel,* Oerlikon Balzers, Liechtenstein*; Tomasz Wojcik, Helmut Riedl,* TU Wien, Austria

Hydrogen-based energy systems require materials that are resilient to the reactive nature of hydrogen. This is important due to phenomena such as hydrogen embrittlement and corrosive attacks, which are common in fuel cells and electrolyzers. One potential solution to mitigate material deterioration is the use of physical vapor deposition (PVD) synthesized hydrogen-resistant barrier coatings on exposed surfaces.

Currently, investigations into hydrogen permeation for bulk materials are primarily conducted using either pressurized or electrochemical testing methods. The electrochemical method, while offering advantages such as versatility and simplicity, is mostly applied to bulk materials and seldom used for thin film materials. Therefore, it is important to establish electrochemical permeation testing methods for coating materials as well. In this study we investigated the hydrogen permeation characteristics of the well-known coating systems TiN and CrN deposited on unalloyed ferritic steel substrates via sputter deposition and cathodic arc evaporation. These samples were electrochemically charged in a Devanathan-Stachursky permeation cell and parameters like diffusion coefficients, hydrogen fluxes and permeation reduction factors have been determined. Additionally, these results were correlated with the coating's microstructure, obtained from scanning and transmission electron microscope and linear sweep voltammetry.

Our results indicate that both the deposition process and coating morphology significantly influence the permeation characteristics of the material. These findings on well-known nitride-based material systems could assist in engineering hydrogen barrier coatings for various future applications.

11:40am **TS1-1-MoM-6 Low-Temperature Sintering of $Li_7La_3Zr_2O_{12}$ (LLZO) Electrolyte Coatings by the Sol Impregnation Method for All Solid-State Lithium-Ion Batteries***, Yen-Yu Chen [yychen@mail.npust.edu.tw], Guang-Yi Yao, Shao-Chien Tai,* National Pingtung University of Science and Technology, Taiwan

All solid-state lithium-ion batteries (ASSLIBs) have attracted attention from academics and industries due to the safety issues and high efficiencies. Among kinds of the electrolyte materials for ASSLIBs, the oxide-based electrolytes show high electrical conductivities and electrochemical stabilities and are one of the potential materials for the solid electrolyte of ASSLIB. $Li_7La_3Zr_2O_{12}$ (LLZO) is one of the oxide-based electrolyte materials and was developed in our previous investigation. After sintering at 1100℃ for 12 h, significant interdiffusion between the LLZO electrolyte coatings and the LCO cathode was observed, and second phases were also formed between the LLZO coatings and LCO substrates that inhibited the electrical performance of LLZO-based ASSLIBs. In this study, we try to reduce the sintering temperature to less than 1000℃ to prevent the over-diffusion between LLZO coatings and LCO-based substrates. A sol impregnation method was taken to fill the pores in the pre-sintered LLZO coatings and densify the coating samples at a temperature lower than 1000℃. Several techniques were taken to analyze the LLZO coating samples, including crystalline phases by X-ray diffraction (XRD), the microstructures by scanning electron microscopy (SEM), the elemental distribution mapping by scanning transmission electron microscopy (STEM), and electrical performance analysis by electrochemical impedance spectrum (EIS). The results show that by the LiOH sol impregnation, the densities of the LLZO coating layers can be significantly increased after sintering at 1000℃ for 12 h, as well as the electrical performance of the semi-cells. The details of the interface diffusion phenomena between LLZO coatings and LCO substrates after low-temperature sintering will be shown in the presentation.

12:00pm **TS1-1-MoM-7 Nitride and Amorphous/Crystalline Multilayers as Hydrogen Permeation Barriers***, Balint Istvan Hajas* ***[balint.hajas@tuwien.ac.at]***[1]*,* TU Wien, Institute of Materials Science and Technology, Austria*; Vincenc Nemanič, Marko Žumer, Ardita Kurtishaj Hamzaj,* Jožef Stefan Institute, Slovenia*; Alexander Kirnbauer, Tomasz Wojcik,* TU Wien, Institute of Materials Science and Technology, Austria*; Szilard Kolozsvari,* Plansee Composite Materials GmbH, Germany*; Paul Heinz Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria

Hydrogen permeation presents a key obstacle to the deployment of hydrogen-based energy systems, necessitating robust coatings that act as permeation barriers. In this study, we investigate nitride-based monolithic and multilayer (ML) coatings deposited by magnetron sputtering as hydrogen permeation barriers (HPBs). Coating systems including TiN, (Ti,Al)N, MoN/TaN, and Si–B–C–N–O, as well as TiN/AlN and Si–B–C–N–O/TiN MLs, were synthesized and characterized by XRD, SEM, TEM, and nanoindentation. Their efficiency as HPB was evaluated on films deposited on Eurofer 97 substrates using the gaseous hydrogen permeation method at 400°C.

Monolithic crystalline coatings exhibited limited barrier properties, with TiN reaching a PRF of ~190 and (Ti,Al)N failing due to microstructural defects induced by high deposition bias. Crystalline MLs demonstrated that coherent fcc–fcc interfaces in TiN/AlN with a bilayer ratio Γ = 2:1 (2 nm TiN and 1 nm AlN) effectively suppress permeation by combining nearly epitaxial interfaces with interruptions of columnar growth, which block fast diffusion pathways, leading to a PRF above 20,000. In contrast, thicker AlN layers relaxed into hcp-AlN, disrupting coherency and providing diffusion paths. The MoN/TaN system showed only moderate resistance (PRF ~50). Amorphous Si–B–C–N–O already exhibited excellent barrier performance (PRF >1000) by eliminating grain and specifically column boundaries, which was further improved through the incorporation of TiN. In particular, the $\Gamma_{Si–B–C–N–O/TiN}$ = 2:3 multilayer reached PRF values of ~5300 by embedding crystalline TiN within amorphous Si–B–C–N–O layers, yielding a dense, columnar-free architecture without continuous diffusion channels. These findings underscore that hydrogen permeation resistance can be maximized either by coherent interface stabilization or by amorphous/crystalline alternation, highlighting interface engineering and microstructural control as decisive design principles for next-generation energy technologies.

[1] **Graduate Student Award Finalist**

Keynote Lectures
Room Town & Country A - Session KYL1-MoKYL

Keynote Lecture I

Moderator: Sandra E. Rodil, Universidad Nacional Autónoma de México

1:00pm **KYL1-MoKYL-1 HiPIMS with Cathode Reversal -- Physics and Applications***,* ***David N. Ruzic [druzic@illinois.edu]****, Tag Choi, Nicholas Connolly,* University of Illinois at Urbana-Champaign, USA **INVITED**

This talk covers the physics behind, and applications of a high-power impulse magnetron sputtering (HiPIMS) deposition system which allows for the potential of the cathode to be reversed at the end of magnetron pulse.Results from a system which allows for detailed waveform control was first published [1], commercialized [2] and patented [3] at Illinois and has been the subject of numerous investigations. Reversing the cathode potential at the end of a high-power impulse magnetron sputtering (HIPIMS) pulse first turns the magnetron into a Hall-thruster expelling ions and plasma, and then raises the plasma potential allowing the control of the ion energy during the kick to within one eV -- even on insulating substrates. In addition, we will show that the ratio of target ions to gas ions can be controlled by changing the angle of the target with respect to the workpiece. Time-resolved Langmuir probes have been used as a function of position to show how the electron energy distribution evolves from a Maxwellian during the main negative pulse, to a Druyvesteyn during the delay before reversal, and to sub-Druyvesteyn during the positive pulse. The commutation of the potential to the workpiece happens on the micro-second timescale and the attendant dV/dx heats the local electron population leading to enhanced ionization and therefore higher deposition rates. By running the appropriate waveform, a PVD tool can be used as an etcher.These abilities open a wide range of applications for such devices from the ability to make conformal super-conducting films, corrosion barriers for bipolar fuel cell plates, more efficient CIGS solar cells, reduced-stress coatings and room-temperature high-hardness TiN thin films.

[1] Wu B, Haehnlein I, Shchelkanov I, McLain J, Patel D, Uhlig J, Jurczyk B, Leng Y and Ruzic D N, “Cu films prepared by bipolar pulsed high power impulse magnetron sputtering” *Vacuum* **150** 216–21 (2018)

[2] Starfire Industries LLC http://starfireindustries.com

[3] US Patents #11,069,515 B2 and #12,211,680 B2

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Protective and High-temperature Coatings
Room Palm 3-4 - Session MA1-2-MoA

Coatings for High Temperatures and Harsh Environment Applications II

Moderators: Vladislav Kolarik, Fraunhofer Institute for Chemical Technology ICT, Germany, **Fernando Pedraza**, La Rochelle University, Laboratory LaSIE, France

1:40pm **MA1-2-MoA-1 Synergistic Effects of Ta and Si Alloying on the Longterm Oxidation and Hot Corrosion Resistance of Ti–Al–N Coatings**, ***Anna Hirle [anna.hirle@tuwien.ac.at]***, *Rainer Hahn, Oliver E. Hudak, Philip Kutrowatz, Tomasz Wojcik,* Christian Doppler Laboratory for Surface Engineering of High-performance Components, TU Wien, Vienna, Austria; *Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials GmbH, Lechbruck am See, Germany; *Anders.O Eriksson, Carmen Jerg, Klaus Boebel,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Balzers, Liechtenstein; *Helmut Riedl,* Christian Doppler Laboratory for Surface Engineering of High-performance Components, TU Wien, Vienna, Austria; Institute of Materials Science and Technology, TU Wien, Vienna, Austria

$Ti_{1-x}Al_xN$ is one of the most used coating materials applied in various applications, including i.e. machining and forming tools but also components, due to its excellent thermomechanical properties. However, as operating temperatures rise, new strategies are needed. Alloying $Ti_{1-x}Al_xN$ with Ta or Si shows promise. In more detail, the incorporation of Ta shifts the onset of the spinodal decomposition towards higher temperatures. Furthermore, the formation of the unfavoured anatase phase during oxidation is suppressed and the rutile phase is stabilised [1,2]. Adding Si enhances the thermal stability and oxidation resistance, while concomitantly leading to the formation of a nanocomposite microstructure [3]. Recent research explores combined alloying with Ta and Si to improve both oxidation resistance and mechanical performance. [4,5]. Compared with $Ti_{1-x}Al_xN$ coatings – which fully oxidize at 1000 °C (15 h, synthetic air) – $Ti_{1-x-y-z}Al_xTa_ySi_zN$ thin films form oxide scales below 1 µm [5].

Furthermore, $Ti_{1-x-y-z}Al_xTa_ySi_zN$ coatings exhibit excellent mechanical properties, making them promising candidates for high temperature applications [4].

The present study investigates a series of $Ti_{1-x-y-z}Al_xTa_ySi_zN$ coatings deposited by cathodic arc evaporation using an industrial-scale Oerlikon Balzers INNOVA 1.0 system. Two distinct target compositions were utilised, along with varying deposition parameters. Long-term oxidation experiments were conducted in a conventional furnace at temperatures of 850 °C for durations of 24 h up to 500 h. After the oxidation processes, we conducted an analysis using X-ray diffraction (XRD), focused ion beam (FIB) techniques, and transmission electron microscopy (TEM). Additionally, we performed low-temperature hot corrosion (LTHC) experiments at 700 °C with a hot gas corrosion testing rig, varying the concentrations of SO_2.

In summary, the study demonstrates that $Ti_{1-x-y-z}Al_xTa_ySi_zN$ coatings exhibit extremely low oxidation kinetics, suggesting long-term stability well beyond 500 hours, alongside excellent resistance to hot gas corrosion environments. Based on these results, cathodic arc-evaporated Ti-Al-N-based coating materials are also promising candidates for protective applications in the aviation and power generation sectors.

[1] R. Hollerweger et al., Surf. Coat. Technol. 257 (2014) 78–86.
[2] C.M. Koller et al., Surf. Coat. Technol. 259 (2014) 599–607.
[3] Z.R. Liu et al., J. Alloys Compd. 917 (2022) 165483.
[4] A.R. Shugurov et al., Vacuum. 216 (2023) 112422.
[5] X. Sun et al., Surf. Coat. Technol. 461 (2023) 129428.

2:00pm **MA1-2-MoA-2 Fabrication, Characterisation and Tribological Testing of Magnetron Sputtered Cr Coated Zr Alloy Cladding for Enhanced Accident Tolerance in Light Water Reactors**, *Thais Netto,* Manchester Metropolitan University, Brazil; *Adele Evans,* Manchester Metropolitan University, UK; *David Goddard, Jack Cooper,* United Kingdom National Nuclear Laboratory, UK; ***Peter Kelly [peter.kelly@mmu.ac.uk]***, Manchester Metropolitan University, UK

Research into accident-tolerant fuels (ATFs) for light water reactors (LWRs) has focused on improving the safety of zirconium alloy fuel rod claddings and one of the more developed approaches is the use of chromium coatings deposited onto the claddings. In addition to performing in oxidising conditions, normal operation also causes fretting wear on the fuel rod surface, which requires tribological improvements.

The aim of this work, therefore, is to produce Cr coatings using the magnetron sputtering technique for Zr alloy nuclear fuel rod cladding material to enhance oxidation and mechanical resistance. The coatings were characterised, as a function of deposition conditions, in terms of their morphology, topography, hardness, reciprocating and fretting wear resistance, scratch test performance and oxidation resistance in autoclave and air oxidation tests.All the coatings provided excellent oxidation protection, in comparison to the uncoated samples. Mechanical testing indicated contrasting results with coatings with higher hardness showing enhanced wear protection, but lower coating hardnesses provided better scratch test performance and reduced fretting wear.

Scale up of these experiments has progressed from small flat coupons, through short (<20cm) rods, to full length (4m) fuel rods.

2:20pm **MA1-2-MoA-3 Second Phase-Driven Surface Engineering Strategies for Corrosion and Oxidation Protection of Mg–8Al–4Ca Alloy***, Yueh-Lien Lee [yuehlien@ntu.edu.tw],* National Taiwan University, Taiwan **INVITED**

This study elucidates how second phases, particularly the β-Al-Ca intermetallic, influence the behavior and corrosion performance of the non-flammable Mg–8Al–4Ca alloy during cerium conversion coating and micro-arc oxidation (MAO) treatments. Scanning Kelvin probe force microscopy (SKPFM) and transmission electron microscopy (TEM) analyses reveal that the β phase exhibits a lower Volta potential and higher electrochemical activity than the α-Mg matrix, serving as a micro-galvanic anode that accelerates localized corrosion and hydrogen evolution. During the cerium conversion process, this activity disrupts film uniformity; however, a simple deionized-water pretreatment dissolves the exposed β phase into $Al(OH)_3$, promoting homogeneous Ce deposition with enhanced coating integrity and corrosion resistance. In MAO processing, the distribution and conductivity of β phases strongly affect discharge behavior and coating development. At low voltages, localized discharges near β regions lead to thinner and non-uniform films, while higher voltages facilitate the formation of Mg–Ca-rich silicate/oxide phases that improve corrosion resistance but hinder further thickening. Selective removal of surface β phases prior to MAO yields thicker and more uniform coatings. These findings clarify the mechanistic link between second-phase characteristics and coating evolution, providing effective strategies to engineer durable protection for non-flammable magnesium alloys.

3:00pm **MA1-2-MoA-5 Development of High-Temperature Ceramic Bond Coats for Environmental Barrier Coatings***, **Rebekah Webster [rebekah.webster@nasa.gov]**, Benjamin Kowalski, Bryan Harder,* NASA Glenn Research Center, USA

Environmental barrier coatings (EBCs) have enabled the use of silicon carbide (SiC)-based ceramic matrix composites (CMCs) in gas turbine engines by protecting the underlying CMC from corrosive combustion species such as water vapor. EBCs currently in service consist of a silicon bond coat and a rare earth silicate topcoat. The melting point of the silicon bond coat (~1410°C) limits the upper use temperature of these coating systems. To protect SiC-based CMCs at temperatures beyond that achievable by the current state-of-the-art, a mullite-based bond coat capable of withstanding temperatures of up to 1482°C has been developed at NASA Glenn Research Center. The mullite-based bond coat can be deposited by either plasma spray physical vapor deposition (PS-PVD) or slurry processing, and various EBC architectures with this bond coat have been developed and tested. In this work, the performance of these EBCs under oxidizing environments including steam and temperature cycling are reviewed, with the effect of coating microstructure, namely porosity, on oxidation being highlighted.

3:20pm **MA1-2-MoA-6 Statistical Correlation between Microstructural Features and Process Forces in Conventional and Ultrasonic-Assisted Milling of Plasma Claddings***, Kai Treutler,* TU Clausthal, Germany*; **Dirk Schröpfer [dirk.schroepfer@bam.de]**,* Bundesanstalt für Materialforschung und -prüfung, Germany*; Maraike Willeke,* TU Clausthal, Germany*; Thomas Kannengießer,* Bundesanstalt für Materialforschung und -prüfung, Germany*; Volker Wesling,* TU Clausthal, Germany

The development of highly efficient and economical steel components in plant and process engineering is crucial for reducing CO2 emissions. To withstand the high combined corrosive, tribological, thermal, and mechanical stresses, wear-resistant coatings tailored to the application and steel grade are employed. The increasing demand to substitute conventional cobalt alloys with nickel alloys, coupled with the need for defined or functional surfaces of high integrity, necessitates the development of novel wear-resistant coatings.

The use of wear-resistant coatings is essential for highly efficient and economical steel components in equipment, process, and power plant engineering. Co-alloys are commonly used as wear-resistant coatings for steel components, tailored to the specific application. The substitutability of Co alloys with Ni-based wear protection systems, in addition to price and supply uncertainties, is facilitated by the combination of innovative welding and machining processes such as ultrasonic-assisted milling.

This study investigates the influence of the microstructure and precipitation morphology adjusted by means of alloy modification on the machinability of wear-resistant plasma cladded coatings. The wear protection alloy NiCrMoSiFeB (trade name: Colmonoy 56 PTA), typically used for screw machines, is employed as a model system. Metallurgical investigations and in-situ measurements of occurring process forces and temperatures at the tool cutting edge during milling, as well as subsequent investigations of tool wear and surface integrity, allow for a detailed analysis and correlation between microstructural properties and machinability.

The primary objective of this study is the statistical correlation between specific microstructural features, like precipitation size, shape and amount with the characteristic process forces of conventional and ultrasonic assisted milling of the claddings.

The addition of Al, Ti, or Nb to the cast samples results in a clear change in the microstructure, hardness and machinability. Al and Ti cause long-needled or star-shaped precipitations and hardness increases, which lead to higher cutting forces and increased tool wear. In the case of the modified alloys, the inclusion of the alloying element Nb results in the formation of a more refined hard phase and reduces the machining force required for C56.

In most cases, the wear resistance potential has been maintained. The statistical model allows to adjust the chemical composition to a better machinability of the hard facings.

4:00pm **MA1-2-MoA-8 Oxidation Resistance of Binary and Ternary Nitrides Obtained by Magnetron Sputtering***, **Ludovic Mereaux [ludovic.mereaux@unilim.fr]**,* IRCER, France*; Edern Menou, Thomas Vaubois,* Safran, France*; Cédric Jaoul,* IRCER, France*; Marjorie Cavarroc,* Safran, France

Increasing aircraft engine temperature is one method, amongst others, to decarbonize aviation. But at high temperature, metallic materials performances are drastically decreased due to the effect of hot corrosion. To limit this impact, metallic materials need to be protected with dedicated coatings with adequate properties, which “entropy-augmented” ceramics could feature.

However, the composition space of complex ceramics is very wide, and comparatively very few bibliographical data are available as these specific ceramics have not been widely studied to date. While the use of data-driven approaches to identify relevant compositions appears necessary, it is not sufficient as (1) it requires data to be trained on, and (2) final properties should be experimentally assessed.

Nitride coatings obtained by PVD methods have been used in the machine tool and aerospace industries for many years. Binary nitride systems exhibit mechanical properties such as high hardness (20-25 GPa [1]). The addition of transition metals, such as Al or Si, improves physical and chemical properties like wear resistance, thermal stability and oxidation resistance [2].

Two main challenges have to be overcome: achieving a single solid solution film to guarantee both material and property homogeneity throughout the coatings, and assessing the long-term mechanical and environmental stability of the materials.

It was decided to creates our own database, starting from simple binary coating with the progressive addition of elements. In this talk, we will present results on the oxidation of binary and ternary nitride coatings. These coatings are obtained by magnetron sputtering in a reactive atmosphere and they are annealed in air up to 900°C, to propose oxidation mechanisms.

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4:20pm **MA1-2-MoA-9 Adaptive Opto-Neuromorphic Device Based on Monolayer MoS_2 for Extreme-Temperature Cognitive Operations***, Pukhraj Prajapat [pukhraj.npl@gmail.com], Govind Gupta,* National Physical Laboratory, India

High-temperature neuromorphic devices are becoming increasingly essential as technology advances to support space exploration and withstand extreme conditions, such as those found in factories. To overcome this need, the researchers are devising technologies that imitate the human brain structure and operation. In this work, we present a scalable neuromorphic device based on a monolayer of MoS_2 that demonstrates operation at 100°C. The device portrays excellent electrical performances, mostly due to the great thermal stability of monolayer MoS_2 and its mechanical flexibility. Among these performances are low power consumption, fast switching, high resistance ratio, low switching voltage, and long stable endurance (~10^3 cycles). Besides, the device mimics neuromorphic behaviour by embedding the synaptic plasticity that is the major functional property of biological neural networks, thus allowing advanced cognitive computing in extreme environments. This is the first step toward a combination of materials science and neuromorphic computing, and it clears the way for smart resilient electronics that could survive in a variety of harsh conditions. This research aimsto achieve a significant breakthrough in the field of high-temperature electronics, paving the way for the development of future high-performance electronics that can meet the demands of modern technology.Keywords: 2D, TMDCs, Neuromorphic, Brain inspired, MoS2

4:40pm **MA1-2-MoA-10 Reactive Sputtering of CrMoNbWxTiCy Carbide Films by High Power Impulse Magnetron Sputtering System: Effect of W and Carbon Contents***, ChunHao Cheng [itsjonardgx@gmail.com], Yung-Chin Yang,* National Taipei University of Technology, Taiwan*; Jyh-Wei Lee,* Ming Chi University of Technology, Taiwan*; Bih-Show Lou,* Chang Gung University, Taiwan*; Chia-Lin Li,* Ming Chi University of Technology, Taiwan

High power impulse magnetron sputtering (HiPIMS) has attracted significant attention for its ability to generate high-density plasma and achieve highly ionized metal species. Compared with conventional DC sputtering, this technique enhances ion bombardment energy, leading to improved film densification and adhesion. In this study, CrMoNbTiWx and CrMoNbWxTiCy high entropy alloy (HEA) coatings were deposited using HiPIMS to investigate the effects of tungsten and carbon incorporation on the microstructure and multifunctional properties of HEA carbide films. By varying the W target contents and controlling the reactive acetylene gas flow rates, the influence of target poisoning on film growth behavior was systematically analyzed. The film morphology and phase structure will be examined using field-emission scanning electron microscopy, X-ray diffraction, transmission electron microscopy, and atomic force microscopy. Mechanical properties, including hardness, adhesion, and wear resistance, will be characterized by nanoindentation, scratch, and pin-on-disk wear tests. Corrosion and oxidation resistance will be evaluated through a potentiodynamic polarization test in 3.5 wt.% NaCl solution and thermogravimetric analysis, while electrical performance will be assessed using a four-point probe to measure their electrical resistivities. This research aims to elucidate the roles of tungsten and carbon contents, as well as target poisoning behavior, in optimizing the structural, mechanical, and electrochemical performance of CrMoNbTiWxCy HEA carbide coatings, demonstrating the advantages of HiPIMS for developing dense and durable multifunctional protective films.

5:00pm **MA1-2-MoA-11 Materials for Aerospace Extreme Environments***, Samir M. Aouadi [samir.aouadi@unt.edu],* University of North Texas, USA **INVITED**

Protective and High-temperature Coatings
Room Town & Country C - Session MA4-1-MoA

Boron-containing Coatings I

Moderator: Martin Dahlqvist, Linköping University, Sweden

2:40pm **MA4-1-MoA-4 Charge Trapping Behavior in BN Films Fabricated by a Reactive Plasma-Assisted Coating Technique and Their Design Strategies***, Koji Eriguchi [eriguchi.koji.8e@kyoto-u.ac.jp],* Kyoto University, Japan **INVITED**

Boron nitride (BN) possesses highly desirable properties for a wide variety of industrial applications [1]. Its properties strongly depend on its microscopic structure: sp^2-bonded hexagonal (h-BN) and sp^3-bonded cubic (c-BN). For example, h-BN films are expected to be superior dielectric materials for electronic devices owing to their high dielectric breakdown field [2], whereas c-BN films have attracted considerable attention because of their high hardness [3]. Historically, using plasma-based technologies, these microscopic structures have been controlled predominantly by the energy of incident ions and the fluxes of B and other species [4]. However, crucial issues remain to be solved—namely, the degradation of dielectric breakdown lifetime for h-BN films and delamination due to residual stress in c-BN films. A fundamental understanding of the various degradation mechanisms in BN films is therefore required.

In this study, we formed BN films and their stacked structures with various bonding phases on Si substrates using a reactive plasma-assisted coating (RePAC) method [5]. After confirming their bonding networks by Fourier-transform infrared spectroscopy and optical properties by spectroscopic ellipsometry [6], we investigated the dielectric degradation of h-BN and the delamination behavior of c-BN in terms of charge trapping dynamics using Al/BN/Si devices. Characteristic charge trapping behaviors during time-dependent dielectric breakdown measurements were enhanced by the bombardment of higher-energy ions and the incorporation of impurities during h-BN film formation [7]. The presence of trapped charges was identified at the c-BN/Si interface and even within stacked BN films (h-/c-BN or c-/h-BN) [8]. In addition, film delamination was found to occur preferentially at the stacked c-/h-BN interface. Moreover, we found that time-dependent film delamination was closely correlated with the trapped charge density. These findings indicate that controlling charge trapping behaviors is key to improving the properties of BN films for various industrial applications.

This work was supported by JSPS KAKENHI (23H01728) and O.S.G. Foundation.

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3:20pm **MA4-1-MoA-6 Development of TiB_2:h-BN:a-C Based Nanocomposite Coatings with Enhanced Wear and Corrosion Resistance for Turbojet and Gas Turbine Components***, Gokhan Gulten [gokhangulten@atauni.edu.tr], Banu Yaylali, Mustafa Yesilyurt, Ali Emre, Yasar Totik,* Atatürk University, Turkey*; Justyna Kulczyk-Malecka, Peter Kelly,* Manchester Metropolitan University, UK*; Ihsan Efeoglu,* Atatürk University, Turkey

Turbojet and gas turbine engines operate under severe thermo-mechanical and chemically aggressive conditions where simultaneous control of friction, wear, and corrosion is essential. This study reports the design and synthesis of a solid-lubricating nanocomposite architecture based on TiB_2:h-BN:a-C deposited by closed-field unbalanced magnetron sputtering (CFUBMS) driven by a hybrid HiPIMS + pulsed-DC power setup. The coating concept employs the synergistic combination of hard TiB_2 domains (load-bearing), hexagonal BN (lamellar solid lubricant, thermal stability), and amorphous carbon (low shear, transfer-film formation). To promote enhanced substrate adhesion and gradient stress accommodation on aerospace alloys (Inconel 718 and Ti-6Al-4V), a thin Cr adhesion layer and a CrN transition layer are incorporated. A Taguchi L9 experimental design is employed to map the influence of TiB_2 target voltage, N_2 flow, duty cycle, and working pressure on structure–property relationships. Comprehensive characterization includes XRD, Raman and XPS, SEM cross-sections, nanoindentation, scratch testing, and pin-on-disk tribometry at room and elevated temperatures. Electrochemical performance is assessed by potentiodynamic polarization and EIS to quantify corrosion resistance. The hybrid power delivery enhances ionization and adatom mobility, producing dense microstructures and superior adhesion. Process–structure–property correlations reveal reduced friction, improved wear resistance, and enhanced corrosion protection, establishing TiB_2:h-BN:a-C coatings as promising candidates for extending component life and reducing maintenance in advanced propulsion systems.

4:00pm **MA4-1-MoA-8 Energy Efficiency in Pulsed-DC Powder-Pack Boriding: A Sustainable Approach to Surface Hardening of Metallic Materials***, Ivan E Campos Silva [icampos@ipn.mx],* Instituto Politecnico Nacional, Mexico **INVITED**

Boriding has emerged as an efficient thermochemical treatment to enhance the wear and corrosion resistance of metallic materials. The resulting boride layer, characterized by its exceptional hardness and outstanding thermal and chemical stability, outperforms nitrided, carburized, and PVD-coated surfaces. However, conventional powder-pack boriding still faces critical challenges (mainly the need for long treatment durations and high temperatures ((≥850 °C)) to achieve protective boride layers (50–75 µm thick). These conditions result in high energy consumption and increased production costs, limiting its industrial sustainability.

The pulsed-DC powder-pack boriding offers a sustainable alternative to conventional method by drastically reducing energy usage and processing time. This technique employs an electric field generated by a power source and a polarity-switching device connected to electrodes immersed in a powder mixture together with the metallic specimen. Remarkably, successful treatments have been performed at lower temperatures (600–750 °C) and shorter durations (up to 1.5 h), producing boride layers with excellent wear and friction performance—an unprecedented advancement in the field of solid boriding media and aligned with the principles of sustainable manufacturing.

4:40pm **MA4-1-MoA-10 Investigation of Technologically Driven Compositional and Structural Changes, Mechanical Properties, and Alloying of Transition Metal Diboride Thin Films***, Viktor Sroba [viktor.sroba@liu.se],* Linkoping University, Sweden, Slovakia **INVITED**

This presentation focuses on the investigation of technologically driven compositional and structural changes, mechanical properties, and on alloying of transition metal diboride (TMB_2) thin films. The films were synthesized using state-of-the-art technological approaches, and modern analytical methods, including scanning transmission electron microscopy (STEM) and computational approaches based on density functional theory (DFT), were used for a complex characterization.

TMB_2 thin films grown by direct current magnetron sputtering (DCMS) are an exciting group of nanocomposite materials with excellent mechanical properties, making them a potential candidate for hard coatings in the cutting tools industry. But there are various structural drawbacks that limit their high-temperature application potential, brittle character, and low oxidation resistance. This work provides several pathways to mitigate these drawbacks.

The main topic is understanding the influence of deposition parameters of high power impulse magnetron sputtering (HiPIMS) on the growth of TMB_2 films. One of the benefits of HiPIMS is a high degree of ionization of the sputtered species, however accompanied by a lower deposition rate. These ions can then be attracted towards the growing film using synchronized bias. This high-energy bombardment results in compositional and structural changes in the film. Advanced hybrid HiPIMS/DCMS co-deposition combines a high degree of ionization provided by HiPIMS and a high deposition rate of DCMS.

In the first part, a study of cross-ionization in hybrid HiPIMS/DCMS co-deposition configuration was performed. It was demonstrated that the cross-ionization of the DCMS flux by HiPIMS is influenced by a relative ratio of two crucial parameters - ionization potentials and masses of the sputtered elements. In the second experimental part of the work, high ionization of the sputtered species during HiPIMS was used to suppress the formation of the amorphous boron-rich tissue phase of understoichiometric ZrB_x films while improving mechanical properties and oxidation resistance in the process. The next part of the research focused on the bombardment by the HiPIMS-generated W-ions showed significant densification of the TiB_2 films' structure and improved their mechanical properties, eliminating the need for external heating of the substrates during deposition. Lastly, on the basis of DFT predictions,alloying of TaB_2 and ZrB_2 films by aluminum and niobium, respectively, using conventional DCMS or hybrid DCMS/HiPIMS co-deposition, showed possible pathways to maintain or even improve mechanical properties at elevated temperatures and improvement in ductility.

Functional Thin Films and Surfaces
Room Palm 5-6 - Session MB2-1-MoA

Thin Films for Emerging Electronic and Quantum Photonic Devices I

Moderators: Shirly Espinoza, ELI Beamlines, ELI ERIC, Czechia, **Jaroslav Vlcek**, University of West Bohemia, Czechia

1:40pm **MB2-1-MoA-1 AlScN Thin Films and Heterostructures for High Temperature Non-volatile Memory***, Nicholas Glavin [nicholas.glavin.1@us.af.mil],* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA **INVITED**

In recent years, strong demand for digital electronics operating in extreme conditions has driven a surge of research and development in new materials and processes. Of particular importance is the development of nonvolatile memory (NVM) capable of operating at temperatures in excess of 500°C. In this talk, scandium-doped aluminum nitride (AlScN) ferroelectric diodes (FEDs) are discussed as a promising solution for NVM operating at high temperatures because of their fast switching speed, high coercive field, high remnant polarization, and temperature resilience. With optimized scandium concentration (30%–40%) and fabrication processes (reactive magnetron sputtering), AlScN FEDs have been demonstrated with on–off ratios as high as 50000, remnant polarizations of >100µC/cm2, and reliable operation at 1000°C with over a million read cycles and 60hours of retention. Additionally, integration of high-k dielectric oxide thin films have shown to improve endurance cycling and performance for future device integration in extreme environments.

2:00pm **MB2-1-MoA-2 Optical and Electrical Properties of Nitrogen-doped p-type Cu_2O Thin Films Prepared by Reactive HiPIMS***, Jan Koloros [koloros@ntis.cz], Jiří Rezek, Pavel Baroch,* University of West Bohemia in Pilsen, Czechia

One of today's challenging scientific topics is finding a suitable p-type TCO that would at least approach the optoelectronic properties of the n-type counterpart [1]. Finding such p-type material is a necessary condition for further sustainable technological development of society. The realization of p-n junctions using transparent conductive materials will enable the development of a new generation of invisible electronics, contribute to reducing the energy requirements of various optoelectronic devices or lead to the production of more efficient solar cells. Transparent conductive materials based on Cu_2O appear to be among the most promising. This is mainly due to the abundance of elements used, their non-toxicity and interesting optoelectronic properties. One of the limiting factors in Cu_2O layers is the low mobility of holes. In our previous work [2], we demonstrated that post-deposition laser annealing can effectively enhance hole mobility.

In our work, we systematically investigated the role of nitrogen incorporated into Cu_2O thin films, with a primary focus on their optical and electrical properties, including the optical band gap and electrical resistivity. The Cu_2O:N films were prepared by reactive HiPIMS of Cu circular target (100 mm in diameter) in Ar+O_2+N_2 atmosphere. The pulse-averaged target power density (S_{da}) was varied from ≈ 100-1300 Wcm^{-2}, and the fraction of N_2 in (Ar+N_2) mass flow was 0–90 %. A decreasing trend in resistivity has been observed with increasing nitrogen content. The prepared p-type Cu_2O:N films with the highest value of a nitrogen fraction of 90% exhibited a very low resistivity about 5×10^{-2} Ωcm exceeding the current state of the art [3].

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2:20pm **MB2-1-MoA-3 Fabrication and Manipulation of Weakly-Interacting Interfaces for Optoelectronic Applications**, ***Kostas Sarakinos* [kostas.sarakinos@helsinki.fi]**, University of Helsinki, Finland **INVITED**

A key challenge in the materials science community is to understand the correlation among nanoscale atomic arrangement, structure-forming mechanisms, and mesoscale morphology during material synthesis. Addressing this challenge will herald a new epoch in which tailor-made materials and devices with unprecedented macroscopic behavior will be created by controlling mesoscale structure via nanoscale manipulation. The present talk demonstrates the implementation of the above-outlined concept of multiscale materials design during the vapor-based synthesis of thin noble-metal films (and nanostructures) on weakly-interacting substrates, including oxides and van der Waals crystals. Such film/substrate systems exhibit a pronounced and uncontrolled three-dimensional (3D) morphology, which is a major obstacle toward fabricating high-quality multifunctional metal contacts in a wide array of devices. Using growth of sliver (Ag) on silicon dioxide (SiO2) as a model system—along with a combination of in situ film growth monitoring, ex situ microstructure and chemical characterization, and modelling—it is shown that the tendency for 3D growth morphology can be effectively reversed, without compromising key physical properties of the film and the substrate, when miniscule amounts of minority gaseous [1,2,3] and metal species [4,5] (surfactants) are deployed with high temporal precision at the film growth front, such that atomic-scale processes that govern key film-formation stages are selectively targeted and affected. The talk concludes with a discussion with regards to the implications and possibilities that this strategy opens for tuning macroscopic performance of devices in the areas of energy saving and generation.

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3:00pm **MB2-1-MoA-5 Investigation of High-temperature Morphology and Electrical Performance of YZr-alloyed Amorphous Al_2O_3 Thin Films**, ***Norma Salvadores Farran* [norma.salvadores@tuwien.ac.at]**, *Florentine Scholz, Tomasz Wojcik,* TU Wien, Austria*; Astrid Gies, Jürgen Ramm, Klaus Böbel,* Oerlikon Balzers, Liechtenstein*; Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials, Austria*; Tobias Huber, Jürgen Fleig, Helmut Riedl,* TU Wien, Austria

Aluminium oxide (Al_2O_3) is a widely used insulating material, particularly in thin-film applications. In addition to its various polymorphs, Al_2O_3 can also exist in an amorphous phase, which is characterized by excellent oxidation resistance and high thermal conductivity. A key advantage of the amorphous form is its uniform structure, free from pinholes. Owing to these properties, amorphous Al_2O_3 being investigated as a dielectric material in electronic and semiconductor devices, as well as in energy storage technologies. Therefore, identifying cost-effective and sustainable deposition methods for the fabrication of high-quality Al_2O_3 insulating thin films is of great importance.

Amorphous Al_2O_3 films were synthesized using a reactive Modulated Pulse Power (MPP) sputtering process. All depositions were carried out in an in-house developed sputtering system equipped with a 3-inch aluminium target and operated in a mixed Ar/O_2 atmosphere. The primary aim of this study was to examine the influence of yttrium–zirconium (YZr) alloying on the thermal stability of the amorphous Al_2O_3 phase, with the goal of preventing phase transitions into crystalline states up to 1200 °C. To achieve this, varying amounts of YZr were incorporated into the aluminium targets. The effects of these YZr additions and their concentrations on process stability, as well as on the resulting film properties – including morphology, structure, and electrical resistivity – were analysed using advanced high-resolution characterization techniques.

Phase formation and evolution were investigated using X-ray diffraction (XRD) over a temperature range from room temperature up to 1200 °C. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were employed to assess the deposition rate and surface morphology of the coatings. The chemical composition of the films was analysed using X-ray photoelectron spectroscopy (XPS), which was also utilized to examine the bonding states of the constituent elements. Additionally, in-situ impedance spectroscopy was used to study variations in the electrical properties as a function of temperature. For electrical characterization, Ti/Pt electrode pads were fabricated via photolithography.

4:00pm **MB2-1-MoA-8 Ion-Beam Assisted Deposition of P-Type Oxide Semiconductor Thin Films in Room Temperature**, ***Tsung-Yu Huang* [huang.tsungyu@mail.mcut.edu.tw]**, Ming Chi University of Technology, Taiwan **INVITED**

Transparent semiconductor oxides are an important class of materials in materials science, including SnO_2, In_2O_3, ZnO, and dozens of doped transparent semiconductor oxides. These materials have been widely used in various electronic and optoelectronic devices. Tin monoxide (SnO), due to the overlap between its 5s orbital and the oxygen 2p orbital, exhibits unique characteristics that enable hole transport. This makes it one of the most promising candidates for p-type oxide semiconductors. In this study, our p-type SnO thin film achieved a mobility of 4.52 $cm^2 V^{-1} s^{-1}$.

4:40pm **MB2-1-MoA-10 Influence of Bonding Temperature on Electromigration Suppression in Cu-Doped Ag Bumps**, ***Chien-Cheng Chiang* [johnson10678@gmail.com]**, *Peng-Hsiang Hsu, Fan-Yi Ouyang,* National Tsing Hua University, Taiwan

The continuous advancement of technology has driven the demand for higher-performance electronic devices, leading to progressive miniaturization of device dimensions. However, further device scaling is fundamentally constrained by physical limits. To overcome these challenges, three-dimensional integrated circuits (3D ICs) have emerged as a promising alternative for enhancing device performance. Compared with conventional flip-chip solder joints, direct metal bonding (DMB) provides higher interconnect density, lower electrical resistance, and improved reliability, making it an attractive technique for advanced packaging. Nevertheless, as interconnect dimensions decrease, reliability issues become increasingly critical, with electromigration (EM) being one of the primary failure mechanisms.

In this study, Ag alloyed with 3.2 at.% Cu was employed as the interconnect material, and a nanotwinned structure was introduced to enhance EM resistance. Thermal compression bonding was performed at various temperatures to investigate the influence of bonding temperature on electromigration behavior and microstructural evolution.Compared with pure silver, Ag doped with 3.2 at.% Cu exhibits not only a better bonding interface at higher bonding temperatures but also retains a larger amount of twin structures, thereby achieving superior electromigration resistance. The results provide valuable insights into the relationship between bonding parameters and EM performance, offering practical strategies to improve the reliability of next-generation advanced packaging technologies.

5:00pm **MB2-1-MoA-11 Piezoelectric MEMS – from Advanced Material Systems to Novel Device Architectures**, ***Ulrich Schmid* [ulrich.e366.schmid@tuwien.ac.at]**, *Daniel Platz, Michael Schneider,* TU Wien, Austria **INVITED**

In a compact introduction, I will motivate the benefits of piezoelectric thin films for MEMS and will give a short overview to state of art device applications.

Next, I will highlight latest results on the electrical, mechanical and piezoelectrical characterization of sputter-deposited aluminium nitride (AlN) including the impact of *e.g.,* substrate pre-conditioning. I will present test structures for determining piezoelectric coefficients (d_{33}, d_{31}) down to an accuracy of about 0.1 pm/V on wafer level. The impact of AlN doping with yttrium which leads to an increase of the moderate piezoelectric coefficient of pure AlN, as known with scandium, will complete the material-related part of my talk.

Next, these films are integrated into fabrication processes of silicon MEMS devices. In combination with a tailored electrode design, cantilever-type resonators are realized featuring Q-factors up to about 350 in water (@1-2 MHz). This enables the precise determination of the viscosity and density of fluids up to dynamic viscosity values of about 300 mPas. Besides this application, such high Q-factors are most essential when targeting mass-sensitive sensors, thus paving the way to *e.g.,* nanosized particle detection even in such highly viscous media like oil. In addition, the characterization of bitumen with dynamic viscosities up to the 10.000 mPas range is demonstrated with these piezoelectric MEMS resonators.

Besides sensing, the field of MEMS actuators is covered. I will present some selected results on buckled, bistable plate-type MEMS devices that allow continuous switching between the two stable states by integrated piezoelectric thin film actuators for realizing *e.g.,* compact ultrasound emitters. Specific features of this device architecture will be discussed**.**

Plasma and Vapor Deposition Processes
Room Town & Country A - Session PP1-2-MoA

PVD Coatings and Technologies II

Moderators: Yen-Yu Chen, National Pingtung University of Science and Technology, Taiwan , **Christian Kalscheuer**, IOT, RWTH Aachen, Germany

1:40pm **PP1-2-MoA-1 Spot Stabilization and Thin Film Synthesis Using an Industrial-Sized DC Vacuum Arc Source with Magnetic Steering and Zr-Cu/Zr-Ni Cathodes***, **Igor Zhirkov [igor.zhirkov@liu.se]**, Andrejs Petruhins,* Linkoping University, Sweden*; Philipp Immich,* IHI Hauzer Techno Coating B.V., Netherlands*; Szilard Kolozsvari, Peter Polcik,* PLANSEE Composite Materials GmbH, Germany*; Johanna Rosen,* Linkoping University, Sweden

Zirconium-based alloys, due to their wide spectrum of properties, are broadly used in various applications, ranging from nuclear reactors to biomedical devices. These alloys are characterized by a favorable combination of high glass-forming ability, high thermal stability, and excellent mechanical properties. Additionally, they exhibit excellent anticorrosion behavior, making them attractive for applications in machinery, microelectronics, and aerospace. Furthermore, the cost of synthesizing Zr-based alloys is relatively low compared to that of other materials, making them economically feasible for large-scale applications. However, reports on the deposition of Zr–Cu and Zr–Ni coatings using DC vacuum arc are very limited, even though this process is commonly used in industry. In this work, we present an analysis of the stability of the arcing process based on the corresponding phase diagrams and the presence of Zr, Cu (or Ni) material grains within the cathode. We show that arcing can be stabilized by utilizing a magnetic arc steering system. The study was performed using an industrial-scale arc plasma source, the Hauzer CARC+, which utilizes planar cathodes 100 mm in diameter. The $Zr_{1-x}Cu_x$ and $Zr_{1-x}Ni_x$ (x = 0.05, 0.10 at.%) cathodes were provided by PLANSEE Composite Materials GmbH. The magnetic arc steering system, based on variation of the electrical current in a solenoid placed behind the cathode, allows tuning of the magnetic field strength at the center of the cathode surface. In this work, using a Hiden EQP mass-energy analyzer, SEM, and XRD, we demonstrate the plasma and resulting film properties over a relatively wide range of operational pressures (from a base pressure of $1x10^{-5}$ Torr to 5×10^{-2} Torr) in the reactive atmosphere of N_2 used here. At base pressure, plasma analysis shows ion energies consistent with the velocity rule: approximately ~70 eV and ~50 eV for Zr and Cu, respectively, and ~65 eV and ~40 eV for Zr and Ni, respectively. In turn, the plasma ion compositions approximately match the compositions of the corresponding cathodes. The plasma properties were correlated with those of the deposited thin films, including their composition and structure across the full range of studied N_2 pressures. In addition, some evaluations of the resulting films were performed using CIELAB color measurements. The results show that DC vacuum arc deposition can be used for Zr–Cu and Zr–Ni layer depositions.

2:00pm **PP1-2-MoA-2 Relationship Between Substrate Bias and Hydrogen Barrier Behavior of Pulsed DC ZrN Thin Films on Zircaloy-4 Deposited by RF Magnetron Sputtering***, **Cheng-Han Wu [Jordan91618@gmail.com]**, Kuan-Che Lan,* National Tsing Hua University, Taiwan

The mechanical integrity of Zircaloy-4 claddings used in light-water reactors is closely related to hydrogen-induced degradation during service. To suppress hydrogen ingress, zirconium nitride (ZrN) thin films were deposited on Zircaloy-4 substrates using an RF magnetron sputtering system operated in pulsed DC mode. This study investigates the relationship between substrate bias and the hydrogen barrier behavior of ZrN coatings by systematically varying the substrate bias during deposition.

Surface morphology and hydride layer formation were examined using scanning electron microscopy (SEM) and focused ion beam (FIB) techniques. Phase constitution, crystallographic texture, grain size, and residual stress were characterized by X-ray diffraction (XRD) and grazing-incidence XRD (GIXRD). Compositional characteristics, including the nitrogen-plus-oxygen-to-zirconium ratio and elemental depth distribution, were analyzed using electron probe microanalysis (EPMA) and X-ray photoelectron spectroscopy (XPS).

The relationship between substrate bias, microstructural features, and hydrogen resistance of the ZrN films is discussed, providing insight into process–structure–property correlations for ZrN coatings deposited by RF magnetron sputtering in pulsed DC mode for zirconium-based nuclear cladding applications.

Keywords: Zirconium nitride ZrN, thin films, Substrate Bias, Hydrogen Permeation Barrier, Magnetron Sputtering

2:20pm **PP1-2-MoA-3 Spherical Tungsten Coating as Inertial Fusion Targets***, **Ali Basaran [ali.basaran@ga.com]**, Priya Raman, Pavel Lapa, Ruben Santana, Hongwei Xu, Wendi Sweet, Fred Elsner, carlos monton,* General Atomics, USA*; Sasikumar Palaniyappan, Eric Loomis,* Los Alamos National Laboratory, USA

High density uniform tungsten coating on microscale spherical shells is of great interest for next generation inertial fusion energy targets since high-z shells are proposed to improve ablator performance and resistance to preheating. In this work, we present deposition of tungsten films on polymeric shells using direct current magnetron sputtering. Spherical shells are agitated on a pan to ensure uniform coverage during deposition. Delamination of high-z metals from the pan during thick coatings and agitation patterns that determine the surface finish of shells are addressed through several strategies. Process parameters such as pressure, power, and target-substrate geometry are optimized to achieve dense coatings with thicknesses up to 50 µm while minimizing residual stress, roughness, and porosity. Metrology of the shells such as thickness, sphericity, and roughness are quantified via x-ray, optical, and electron microscopy techniques. The influence of deposition conditions on coating microstructure and surface morphology will be discussed.

Acknowledgement

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences, under award number DOE/NNSA award 89233124CNA000365.

2:40pm **PP1-2-MoA-4 Structural Transformation and Electrical Transport in Magnetron-Sputtered Pr-Ni-CoThin Films***, **Bisheswor Acharya [bish5197@vandals.uidaho.edu]**, You Qiang, Xavier Naranjo,* University of Idaho, USA*; Wenjuan Bian, Haixia Li,* Idaho National Laboratory, USA*; Hanping Ding,* The University of Oklahoma, USA*; Thomas Williams,* University of Idaho, USA

Understanding and controlling the physics of alloy thin films with designed microstructure and tunable electronic response is essential for enabling emerging nanoscale devices. However, simultaneously achieving structural continuity and efficient charge transport remains difficult. In this work, we deposit Pr-Ni-Co (PNC) alloy thin films via DC magnetron sputtering and reveal how deposition time directs their growth trajectory. At early growth stages, the films consist of isolated metallic domains; with longer deposition, these features rapidly merge into a continuous, well-ordered layer. This change is accompanied by a sharp decrease in electrical resistance, indicating the formation of a fully connected conduction network. These results show that deposition duration is a key lever linking microstructural evolution to electronic transport in rare-earth–transition-metal alloys, highlighting PNC thin films as a versatile platform for next-generation electronic, magnetic, and catalytic applications.

3:00pm **PP1-2-MoA-5 From Anode-Assisted Magnetron Sputtering to Newer Developments Such as Inverted Fireball-Assisted Magnetron Sputtering**, ***Martin Fenker [fenker@fem-online.de]***, fem Research Institute, Germany **INVITED**

Auxiliary anodes have already become an integral part of sputtering technology for some equipment manufacturers: by providing an additional electron sink at positive potential, they reshape current paths, reduce wall losses, and help to "fill" the coating volume with plasma. In multi-cathode arrangements, a positively biased central anode can strongly increase the substrate current and thus enable a permanent, low-energy ion bombardment even on three-dimensional parts and shadowed surfaces during film growth. In related advanced sputter concepts, remote/common anodes biased positive to the chamber wall are used to tune gas/metal ion densities in the coating volume and support stable deposition conditions.

Starting from this classical anode-assisted magnetron sputtering concept, this presentation moves to "active" anodes that do more than stabilize the discharge. A transparent, biased grid anode can act as a plasma-forming element and create an inverted fireball (IFB): a dense plasma confined within the grid with a highly homogeneous plasma potential. In an Ar discharge, IFB ignition requires an anode potential above the gas ionization threshold. In a magnetron environment IFB ignition was demonstrated with a minimum anode voltage of about 22–23 V and can be operated at typical sputter pressures.

The final part focuses on IFB-assisted magnetron sputtering results from Ti deposition on high-speed steel. Multipole resonance probe measurements show electron densities around 2×10^{16} m^{-3} and electron temperatures of about 4 eV in the IFB. Optical emission spectroscopy confirms the presence of Ti ions, consistent with enhanced ionization in the combined magnetron–IFB plasma. Relative to conventional dcMS and to a simple +100 V anode plate, IFB assistance yields a markedly denser Ti film morphology and a pronounced hardness increase (e.g., 429→523 HV, +22% without substrate bias). Together, these results position IFB-assisted magnetron sputtering as a low-complexity route to higher ion flux and improved film performance without sacrificing continuous-process deposition rates.

4:00pm **PP1-2-MoA-8 Particle, Momentum and Energy Fluxes in PVD Processes - Probe Diagnostics Are Still in Vogue?"**, ***Holger Kersten [kersten@physik.uni-kiel.de]***, Kiel University, Germany **INVITED**

4:40pm **PP1-2-MoA-10 High Fidelity Discrete Element Modelling of Particles in Motion for PVD Coating Optimization**, ***Faranak Tayefi Ardebili [faranak.tayefiardebili@unamur.be]***, University of Namur, Namur Institute of Structured Matter (NISM), Namur, Belgium, USA; *Jerome Muller, pavel Moskovkin, Cedric Vandenabeele, stephane Lucas,* University of Namur, Namur Institute of Structured Matter (NISM), Namur, Belgium

Achieving efficient thin-film deposition using PVD methods can be particularly challenging, especially when working with complex geometries or multi-component assemblies where shadowing effects may arise. This is evident in applications implying millimetre to micrometer scale particles, such as ball bearing or battery powder, where uniform coverage is critical. But coating uniformity strongly depends on particle motion and is difficult to quantify experimentally.

In this study, we investigate thin films deposited by magnetron sputtering onto small beads placed inside a vibrating container. The aim is to determine whether conformal coatings can be achieved using this approach, and to identify the conditions required to do so. For that, particle dynamics are simulated using the Discrete Element Method (DEM) implemented in the LIGGGHTS open source code with a Hertz Mindlin contact model. Simulated trajectories are post processed to extract velocity fields, circulation regimes, height distributions, and mixing indices. Predictions are compared with high speed video recordings, showing circulation pattern, and mixing time across a range of excitation amplitudes. From these trajectories we construct spatial maps of collision frequency and particle residence time in a plasma active zone as proxies for coating exposure.

To go further, the PVD process itself can be modelled using the Virtual Coater platform, which combines Monte Carlo model and ray-tracing techniques to compute flux distribution across particle surfaces and predict film properties. This framework identifies motion settings that improve exposure uniformity and reduce dead zones, providing a practical tool for process screening and optimization.

5:00pm **PP1-2-MoA-11 Investigation on Surface Properties Evolution during PVD Duplex Coating Production Steps for H13 Hot Work Steel**, *João Vitor Piovesan Dalla Nora,* Federal University of Rio Grande do Sul, Brazil; *Felipe Canal,* Universidade Federal do Rio Grande do Sul, Brazil; ***Leandro Bettoni Ortega [leandro.bettoni.ortega@gmail.com]***, Oerlikon Balzers, USA; *Steffen Aichholz, Rafael Lopes da Silva,* Oerlikon Balzers, Brazil; *Alexandre Da Silva Rocha,* Universidade Federal do Rio Grande do Sul, Brazil

AISI H13 tool steel is widely used in hot forging applications, where service life is predominantly limited by surface-related failures such as abrasive wear and plastic deformation. While duplex treatments combining plasma nitriding and Physical Vapor Deposition (PVD) coatings have demonstrated significant improvements in surface hardness, wear resistance, and load-bearing capacity, a systematic understanding of how surface integrity changes throughout the entire multi-stage manufacturing sequence - from heat-treated substrate to finished product - remains lacking. This study addresses this gap by characterizing the evolution of surface properties across sequential processing modifications. Adhesion assessment indicated satisfactory coating-substrate bonding, attributed to the synergistic effects of the nitrided load-supporting layer and microblasting-enhanced mechanical interlocking. Wettability measurements showed a hydrophobic final surface. Following hot forging cycles, quenched and tempered dies exhibited more aggressive wear and geometry loss than duplex-treated dies. Failures and cracks on the latter were attributed to substrate hardness loss. The findings provide a holistic framework for optimizing duplex treatment parameters, particularly the integration of microblasting as both intermediate and final steps, to enhance surface quality, coating adhesion, and potential service performance of AISI H13 dies. stages applied to quenched and tempered AISI H13: high-speed milling, mechanical polishing, low-pressure gas nitriding, intermediate microblasting, plasma nitriding, and PVD coating (CrAlTi-based), and final microblasting. At each stage, surface integrity was assessed through roughness, three-dimensional topography parameters, surface and cross-sectional morphology, coating adhesion, and wettability. The performance of the duplex-treated dies was further evaluated against the quenched and tempered baseline through laboratory-scale hot forging cycles under critical conditions. Results reveal that each treatment step imparts distinct modifications to the surface. Gas nitriding produced a compound-layer free diffusion zone, increasing subsurface hardness. Intermediate microblasting significantly altered surface morphology, increasing roughness and promoting mechanical anchoring sites for subsequent coating deposition. The PVD process applied via cathodic arc introduced characteristic droplets and porosity, increasing surface roughness. Final microblasting at reduced pressure attenuated these defects, reducing the presence of droplets and peak heights, as inferred from topography.

Topical Symposium on Sustainable Surface Engineering
Room Town & Country B - Session TS1-2-MoA

Coatings for Batteries and Hydrogen Applications II

Moderators: Chen-Hao Wang, National Taiwan University of Science and Technology, Taiwan , **Martin Welters**, KCS Europe GmbH, Germany, **Fan-Bean Wu**, National United University, Taiwan

2:20pm **TS1-2-MoA-3 Hydrogen-Induced Failure of High-Strength Austenitic Steel Under Wet Friction Conditions**, ***Damian Batory [damian.batory@p.lodz.pl]***, Lodz University of Technology, Poland; *Pedro Avila, Etienne Bousser, Thomas Chagnon, Ludvik Martinu, Jolanta Klemberg-Sapieha,* Polytechnique Montréal, Canada

This work lies in the combined examination of hydrogen-induced damage and tribological loading, an area where current scientific literature remains largely silent. While the deleterious effects of hydrogen on mechanical properties are well documented, and the fundamentals of friction and wear are extensively studied, the intersection of these two domains has not been systematically explored. By evaluating material responses under simultaneous hydrogen charging and friction-induced stresses, this study provides new insights into the synergistic mechanisms that may govern crack initiation, surface damage evolution, and subsurface microstructural transformations. XM19 austenitic steel samples were subjected to electrochemical hydrogen charging processes before and during tribological testing. After the friction tests a geometry of the obtained wear tracks was analyzed and specific wear rates were calculated. Structure and morphology of the wear tracks were analyzed by SEM and TEM techniques. For the comparison dry and wet friction tests in hydrogen charging solution without electical potential were also conducted. As the result of the investigation it was noticed that among all charging procedures, the most effective in deterioration of the surface quality after tribological testing was the one with initial precharging and subsequent tribological testing while charging. The post-mortem wear track analysis of these samples revealed the appearance of blisters exhibiting a network of brittle cracks on the surface with elongated island-shaped precipitations of nickel. The size and intensity of blister appearance, as well as the amount of nickel precipitations on the surface of blisters grew with increasing load applied to the friction contact. The cross-section analysis of the blister revealed noticeable changes in the microstructure. Both SEM and TEM analysis of the area directly beneath the blister cavity exhibited signs of severe plastic deformation with markedly fine-grained microstructure and signs of amorphization. The cracks forming the cavity propagate parallel to the surface, however places resembling small voids or cavities connected by the network of cracks oriented one on each other were also registered. A detailed discussion of hydrogen induced failure and nickel precipitation mechanisms is also presented.

2:40pm **TS1-2-MoA-4 Advances in *Operando* and *In Situ* Cross-sectional Characterization of Thin Films for Battery and Hydrogen Applications***,* ***Juraj Todt [juraj.todt@unileoben.ac.at]****,* Montanuniversität Leoben, Austria*; Francois Lienard, Manfred Burghammer,* ESRF, Grenoble, France*; Tobias Huber,* Huber Scientific, Austria*; Henrik Bratlie, Daniel Rettenwander,* Norwegian University of Science and Technology (NTNU), Norway*; Rostislav Daniel, Markus Alfreider, Michael Tkadletz, Jozef Keckes,* Montanuniversität Leoben, Austria **INVITED**

As we are facing the worldwide need to reduce the carbon footprint of modern technologies, materials relevant to the fields of sustainable energy storage and transport have received widespread attention. A great deal of research effort has been devoted to their study and optimization, where current techniques often measure either bulk or aggregate properties such as specific capacities or power densities. However, to fully understand all the intricate and often localized mechanisms at play, a more detailed look is necessary. Methods such as impedance spectroscopy are able to capture the crucial role of interfaces with the help of some modeling, but direct observations for cross-sectional behavior are usually lacking.

This is where cross-sectional X-ray nano-diffraction (CSnanoXRD) could provide a very effective tool, as it offers the capability of comprehensive insights encompassing phase composition, preferred crystallite sizes and orientations, accumulated lattice defects and crucially also information on internal strains and stresses. This contribution aims to present our recent methodological advances in applying the CSnanoXRD concept to battery and hydrogen applications, showcasing the dedicated experimental set-ups that are necessary to make this possible.

For the study of zero-excess solid state batteries, a test platform capable to apply stacking pressures in the range of several 100 MPa on X-ray-transparent cross-sectional lamellae has been developed within the Horizon Europe project *OPERA*. First results on the role of anode interlayers in Li and Na deposition at the interface between solid electrolytes and current collectors will be shown. A focus will lie on the many technological challenges that had to be overcome until a fully working tool has been achieved, which is now available to the scientific community.

A further novel test platform will be presented, aimed at the study of hydrogen interaction with surface layers. It is based on the application of femtosecond laser ablation for sample patterning and two-photon lithography to create the appropriate microfluidic structures necessary for electrolytic H-charging of thin films at a CSnanoXRD experimental station. The behavior of various metallic layers including Ni and V, as well as Pd/Nb and Ti-V will be examined in detail, showing the formation of hydride phases and decoupling lattice expansion due to H uptake from the formation of residual stress due to mechanical constraints from the substrate and underlying material. Future possibilities for this approach will comprise the study of the role of interfaces and multilayered H-barrier structures.

3:20pm **TS1-2-MoA-6 Atomic Layer Deposition for Enhancing Durability of Fuel Cell Catalysts***,* *Shao-Chuan Chang,* ***Chih-Liang Wang [wangcl@mx.nthu.edu.tw]****,* Department of Materials Science and Engineering, National Tsing Hua University, Taiwan

Fuel cells are promising clean energy devices for hydrogen conversion, yet their commercialization is hindered by the high cost and limited durability of catalysts. To address these challenges, developing low-cost alternatives with enhanced stability is essential. Surface coating has emerged as an effective strategy to improve catalyst durability by suppressing metal particle agglomeration, dissolution, and carbon corrosion. In this study, Ag/C catalysts were prepared via a microwave-assisted method and subsequently coated with zinc oxide (ZnO) using atomic layer deposition (ALD) to evaluate their stability for anion exchange membrane fuel cell (AEMFC) applications. Ag/C catalysts obtained by conventional impregnation were also investigated for comparison. Structural (XRD, FTIR, TEM) and electrochemical (CV, ECSA) analyses demonstrated that the ALD ZnO-coated Ag/C prepared via the microwave-assisted route possessed markedly enhanced durability relative to the impregnated counterpart. Single-cell performance tests further confirmed the superior activity of the microwave-assisted ZnO-coated Ag/C catalyst, which achieved a higher peak power density than the impregnated sample. These results confirm that an optimally engineered ALD ZnO coating effectively mitigates Ag particle aggregation and dissolution, thereby stabilizing the catalyst structure and enhancing overall AEMFC performance.

4:00pm **TS1-2-MoA-8 Electrocatalytic Performance Analysis of FeNixMoWCu High Entropy Alloy Thin Films: Effects of Ni Content***,* ***Yen-Chin Lai [lai.juju0120@gmail.com]****, Po-Chun Chen,* National Taipei University of Technology, Taiwan*; Bih-Show Lou,* Chang Gung University, Taiwan*; Jyh-Wei Lee,* Ming Chi University of Technology, Taiwan

Hydrogen energy has attracted significant attention due to its cleanliness, non-polluting and carbon-free characteristics [1]. Among various hydrogen production methods, water splitting is considered one of the most promising. However, both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) require catalysts to reduce energy losses caused by overpotential. Currently, the most widely used electrocatalysts are based on expensive noble metals, such as platinum and palladium [2], which limits their large-scale application. Therefore, this study aims to develop low-cost, stable, and highly efficient FeNixMoWCu high entropy alloy (HEA) thin films as potential electrocatalyst materials for water-splitting applications [3].

In this research, equimolar FeNiMoWCu targets and pure Ni targets were employed to deposit FeNixMoWCu high entropy alloy (HEA) thin films with different nickel contents onto 304 stainless steel, silicon wafers, and nickel foam (NF) substrates using a co-sputtering system. Grazing-incidence X-ray diffraction (XRD) analysis revealed that all films exhibited a typical amorphous structure. The nickel content has no influence on the crystal structure of thin films. The cross-sectional morphologies indicated that all films possessed dense microstructures without noticeable defects. Mechanical property measurements demonstrated stable hardness values, while scratch testing confirmed excellent adhesion, with all films showing a critical load (L_{C3}) exceeding 100 N.

Lower overpotential results than untreated NF for the evolution reaction (HER) were obtained for the FeNixMoWCu thin films deposited on NF after the electrochemical test in 1 M KOH aqueous solution. The effect of Ni content on the electrocatalysis performance of HEA thin films was explored. We can conclude that the HEA film prepared at a Ni target power of 75 W exhibited the best HER performance, with an overpotential of 121 mV and a Tafel slope of 177.7 mV/dec at a current density of 10 mA/cm^2, indicating excellent electrocatalytic activity for hydrogen evolution. This research develops the novel FeNixMoWCu electrocatalyst thin film materials for water-splitting hydrogen production. The results will provide insights into the potential of FeNixMoWCu HEA films for green energy applications with enhanced electrocatalytic performance.

Keywords: High entropy alloy thin films, Hydrogen evolution reaction, $FeNi_xMoWCu$, electrocatalytic property

4:20pm **TS1-2-MoA-9 Development of FeNiMoWCuN and FeNiMoWCuC High Entropy Alloy Thin Film as Efficient Electrocatalysts for Water-splitting Applications***,* ***TAI Kao Cheng [dylan37859631@gmail.com]****, Lee Jyh-Wei,* Ming Chi University of Technology, Taiwan*; Lou Bih-Show,* Chang Gung University, Taoyuan, Taiwan*; Li Chia-Lin,* Ming Chi University of Technology, Taiwan

This study investigates the microstructure and electrocatalytic properties of FeNiMoWCuN and FeNiMoWCuC high entropy alloy (HEA) thin films deposited by high power impulse magnetron sputtering (HiPIMS) anddirect current (DC) magnetron sputtering techniques, respectively. The HEA films were fabricated at various argon-to-nitrogen and argon-to-acetylene gas flow ratios to assess the impact of nitrogen and carbon contents, respectively, on the phase, microstructure, and electrocatalytic properties of the thin films. A proper nitrogen content was found to promote the formation of the metal nitride phase, thereby enhancing the electrocatalytic activity of the films. Notably, improved performance was observed for the HEA films with different N contents in the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), characterized by lower overpotentials and smaller Tafel slopes. Similarly, a proper carbon content was achieved for FeNiMoWCuC, resulting in improved electrocatalytic performance. Overall, FeNiMoWCuN and FeNiMoWCuC thin films deposited using HiPIMS and DC with optimized nitrogen content exhibited superior electrocatalytic properties, highlighting their potential for applications in water splitting.

4:40pm **TS1-2-MoA-10 High-Entropy Oxide Thin Films for Sustainable Battery Applications***, **Pavel Soucek [soucek@physics.muni.cz]**, Tatiana Pitonakova, Tomas Rada,* Masaryk University, Czechia*; Tomas Kazda, Antonin Simek,* Brno University of Technology, Czechia*; Petr Vasina,* Masaryk University, Czechia **INVITED**

High-entropy materials represent a rapidly growing frontier in materials science, offering new routes toward multifunctional and resource-efficient technologies. While high-entropy alloys (HEAs) have gained considerable attention, the concept has now been successfully extended to ceramics, including oxides, nitrides, borides, and carbides. These materials derive their unique properties from four synergistic effects: high configurational entropy, severe lattice distortion, sluggish diffusion, and the cocktail effect. The resulting structural stability, chemical resilience, and tunable electronic properties make high-entropy oxides (HEOs) highly promising candidates for advanced electrochemical applications such as lithium-ion and sodium-ion batteries.

In this contribution, we present a study of the Mg-Co-Ni-Cu-Zn-O system, crystallizing in a rock salt-type (MgCoNiCuZn)O structure, and Cr–Mn–Fe–Ni–Cu–O system, crystallizing in a spinel-type $(CrMnFeNiCu)_3O_4$ structure. While the first system represents a “conservative” choice close to current materials used in batteries, the second is entirely free of critical raw materials while offering the potential for improved electrochemical performance and long-term stability, aligning with the vision of sustainable and circular energy storage technologies. The thin films are deposited by reactive DC and High Power Impulse Magnetron Sputtering (HiPIMS), allowing precise control of elemental composition and plasma energy input. The influence of deposition temperature, stoichiometry, and process parameters on the morphology and crystalline structure of the as-deposited coatings is systematically investigated.

Special emphasis is placed on the fabrication of porous thin films, achieved by adjusting the deposition pressure, target-to-substrate distance, and substrate tilt angle—from normal to glancing-angle configurations. The resulting morphological variations strongly affect ion transport and electrochemical activity. Finally, the electrochemical behavior of selected coatings against lithium and sodium is evaluated and correlated with their structural and compositional features. The findings open new pathways for designing high-entropy oxide electrodes that combine sustainability, structural tunability, and superior performance for next-generation battery systems.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

10:00am **CM1-1-TuM-7 High Spatial Resolution Electrical Characterization of Crystal Defects in Metals and Alloys*, Hanna Bishara [hbishara@tauex.tau.ac.il]*,** Tel Aviv University, Israel

Microstructural defects such as Grain boundaries (GBs) and dislocations significantly affect the electrical properties of metallic materials. Generally, the GB interfacial resistivity or dislocation specific resistivity are captured as an accumulative property of all the defects within the material. However, for example, it is evident that different boundary types exhibit distinct structural and chemical characteristics. Therefore, the GB electrical properties are expected to span over a spectrum of values. Yet, the relationship between the boundary's characteristics and their electron transport properties is not well-understood. This research employs SEM in-situ local electrical measurements to study on the impact of GB (and dislocations) structure, chemistry and precipitates on its resistivity.

The talk initially introduces an experimental procedure to measure the local electrical resistivity of GB segments with high sensitivity and spatial resolution *in-situ* scanning electron microscopy (SEM). The local electrical properties are correlated with microstructural characters resolved 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. Multiple materials system will be addressed, namely, pure Cu, dilute Cu alloys, aluminum alloys, and Half Huesler alloys. In addition the disolcation-dislocation interaction on resistivity will be demonstrated for Full-Heusler alloy.

The talk provides insights to the high-resolution methodology of assessing local electrical resistivity of well-defined complexions. The directly-measured interfacial resistivity are discussed in means of thermodynamic excess properties, segregation, and material type.The novel results contribute to a better understanding of the defects' resistivity, and opens new horizons in in knowledge-based defect engineering of smart materials. The present research is promising to be applied on phase boundaries and internal interfaces.

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

Stainless steels exposed to high temperatures undergo sensitization, a process that significantly reduces corrosion resistance due to chromium carbide precipitation along grain boundaries [1]. This precipitation depletes chromium in the surrounding matrix below the threshold required for passivity, creating galvanically active regions prone to intergranular corrosion [2].

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

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

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Protective and High-temperature Coatings
Room Palm 3-4 - Session MA3-1-TuM

High Entropy and Other Multi-principal-element Materials I

Moderators: Frederic Sanchette, Université de Technologie de Troyes, France, **Frédéric Schuster**, CEA, France

8:00am **MA3-1-TuM-1 A Combinatorial Approach to Develop Sputter-Deposited Lanthanide-Containing High Entropy Alloys for ICF Applications***, **Daniel Goodelman [goodelman1@llnl.gov]***, Lawrence Livermore National Laboratory, USA*; Minsuk Seo,* Lawrence Livermore National Laboratory, Republic of Korea*; Gregory Taylor, Alison Engwall-Holmes, Swanee Shin, David Strozzi, Brandon Bocklund, John Chesser, Jimmy Aut, Sergei Kucheyev, Leonardus Bimo Bayu Aji,* Lawrence Livermore National Laboratory, USA

In indirect-drive inertial confinement fusion (ICF) experiments at the National Ignition Facility (NIF), the hohlraum plays a critical role in achieving increased implosion yield, as it drives the fuel capsule's compression. Our simulations with the radiation hydrodynamics code LASNEX suggest that the fusion yield can be improved by using hohlraums made of high entropy alloys (HEAs) containing rare-earth (RE) elements. Here, we present results from a systematic study using combinatorial radio-frequency magnetron co-sputtering to develop a family of Gd-Ta-W-Au-Bi coatings with properties favorable for ICF applications, including high electrical resistivity for consideration in magnetically-assisted ICF schemes. These results provide a framework for the future development of RE-HEA hohlraum materials.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 26-ERD-011.

8:20am **MA3-1-TuM-2 Lanthanide- and Actinide-Containing High-Entropy-Alloy Coatings for Inertial Confinement Fusion Hohlraums***, **Leonardus Bimo Bayu Aji [bayuaji1@llnl.gov]***, Lawrence Livermore National Laboratory, USA

A hohlraum, centimeter-scale sphero-cylindrical heavy-metal cans with wall thicknesses of 10–100 µm, is a key component of indirect-drive inertial confinement fusion (ICF) targets, as they determine the x-ray drive that implodes the fuel capsule. Our simulations predict that hohlraums made from rare-earth-containing high-entropy alloys (RE-HEAs) or depleted-uranium-containing high-entropy alloys (DU-HEAs) can achieve significantly higher x-ray coupling efficiencies than the best-performing single-element hohlraums made from Au or DU. Here, we present our progress in developing sputter-deposited RE- and DU-HEAs with material properties compatible with ICF target fabrication processes.

This work was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and LDRD project 26-ERD-011.

8:40am **MA3-1-TuM-3 Machine Learning Assisted Design of Complex and High Entropy Alloys by Hybrid Hipims/Pulsed Dc Pvd Process for Low Carbon Energy Applications in Extreme Environments***, **Paul Foulquier [paul.foulquier@cea.fr]***, CEA-INSTN, France*; Frédéric Schuster, Ryma Haddad, Fanny Balbaud-Célérier,* CEA, France*; Jean-Philippe Poli,* CEA List, France*; Eric Monsifrot,* AZ Concept, France **INVITED**

Materials and Data sciences convergence is the new paradigm governing the discovery acceleration of new materials, always more complex and integrating, in a virtuous approach, new durability and sovereignty requirements. Every great transitions are concerned: towards a sustainable future and energies, towards frugal digital applications, towards a medicine of the future always more personalised. This dynamic is organised at the national level by the PEPR DIADEM, a program gathering universities and research institutes to shape and promote this trend.

To achieve these ambitious goals of discovery acceleration, the role of acceleration platforms and self-driving laboratories is more and more significant. If numerical simulation tools are always more coupled to artificial intelligence approaches and allow the realisation of custom-made materials, in reality things are often much more complex. Indeed, no material can be made without elaboration processes and any materials keeps the memory of its elaboration process.

In this race to the discovery acceleration of materials, artificial intelligence may play a significant role in always more complex synthesis and shaping processes proficiency. Any types of Materials are concerned by these new approaches: metals, polymers, ceramics, composites including the industrials sectors in which they are involved : mobility, energy, microelectronics, construction, health. Among these high impact generic processes for many industrial sectors, thin film deposition technologies play a key role, in particular driven towards excellence by constraints and specifications imposed by the requirements always more specific of microelectronics applications.

We will present developments for applications in extreme environments using a hybrid pulsed direct current/HiPIMS system with multiple cathodes. In particular, these developments are related to applications in nuclear reactors.

In particular, a new approach to discovering new HEA-type coatings for corrosion in molten salts for small modular reactors will be presented. We will explore the feasibility of Ni-Al-Cr-Mo alloys.

Combinatorial approaches made possible by instrumented multi-target PVD technologies, coupled to artificial intelligence allowing the extraction of inter-parametric relations between processes parameters, are at the heart of this study dedicated to the development of a hybrid pulsed-DC/HiPIMS PVD process digital twin for the deployment of complex coatings for extreme media.

9:20am **MA3-1-TuM-5 EELS Study of Fe–Co–Ni Phosphides electrocatalysts for Hydrogen Evolution Reaction***, Chun-Te Chiang* ***[tony25477210@gmail.com]****,* Southern Taiwan University of Science and Technology, Taiwan*; Yu-Min Shen,* National Dong Hwa University (NDHU), Taiwan*; Yu-Tsung Lin, Jow-Lay Huang,* National Cheng Kung University (NCKU), Taiwan*; Sheng-Chang Wang,* Southern Taiwan University of Science and Technology, Taiwan

Abstract

Hydrogen is widely recognized as a promising clean energy carrier, with the hydrogen evolution reaction (HER) serving as a crucial step in sustainable hydrogen production. Transition-metal phosphides have attracted considerable attention owing to their excellent electrical conductivity and catalytic activity. In this study, Fe–Co–Ni phosphides were synthesized via a solution-based precursor route followed by phosphorization, forming nanostructured multimetallic phases with uniform morphology. Transmission electron microscopy (TEM) revealed nanoscale features, while energy-dispersive X-ray spectroscopy (EDS) confirmed the homogeneous distribution of Fe, Co, and Ni.

Electron energy loss spectroscopy (EELS) played a central role in elucidating the electronic structure evolution of the catalysts. The spectra revealed distinct edges corresponding to O (538.5 eV), Fe (712.0 eV), Co (783.0 eV), and Ni (857.0 eV), clearly reflecting the hybridization between metal 3d and P 2p orbitals and providing direct evidence of charge redistribution among the transition-metal sites. These findings demonstrate the strong correlation between the local electronic configuration and catalytic performance.

Electrochemical analysis further confirmed that Fe–Co–Ni phosphides exhibit remarkable HER activity, requiring only -0.176 V overpotential to reach −10 mA cm^{-2}. The polarization (I–V) curves showed rapid current response and low activation energy, while a Tafel slope of 109 mV dec^{-1} indicated a favorable Volmer–Heyrovsky mechanism. Long-term chronoamperometric measurements verified excellent durability, and subsequent durability and accelerated cycling tests lasting up to 100 hours will be conducted to comprehensively evaluate structural and electrochemical stability under realistic conditions.

This work not only demonstrates the successful synthesis of multimetallic phosphides but also highlights EELS as a powerful tool for probing the structure–property relationship, offering valuable insights for the rational design of efficient and durable hydrogen electrocatalysts.

Keywords: NiCoFeP ; EELS; electrocatalyst

9:40am **MA3-1-TuM-6 Solid-State Synthesis and In-Situ XRD Analysis of Titanium-Based Composite Oxides for Lithium-Ion Battery Anodes and Application***, Guan-Hong Lin* ***[m56144031@gs.ncku.edu.tw]****,* *Hsing-I Hsiang,* National Cheng Kung University (NCKU), Taiwan*; Yu-Min Shen,* National Dong Hwa University (NDHU), Taiwan

The rational design of multi-component oxide systems provides an effective pathway to balance high capacity and structural robustness in lithium-ion battery anodes. In this study, TiO_2–SnO_2 composite solid solutions were synthesized via a controlled solid-state reaction to explore the interplay between structural evolution and electrochemical performance. Structural analyses (XRD and TEM) confirmed the partial incorporation of Sn^{4+} into the rutile TiO_2 lattice, accompanied by limited phase segregation into SnO_2-rich domains at higher Sn contents. The coexistence of solid-solution and segregated regions generated a nanoscale heterostructure that enhanced Li^+ diffusion and mitigated volume fluctuation during cycling. Among the synthesized samples, ST1450 initially delivered the highest capacity of 635.5 mAh g^{-1} at 0.2 C, but gradually declined to 231.9 mAh g^{-1} after 100 cycles, corresponding to the lowest degree of phase segregation. Electrochemical impedance spectroscopy (EIS) and distribution of relaxation time (DRT) analyses revealed that coherent TiO_2/SnO_2 interfaces effectively facilitated charge-transfer kinetics while preserving mechanical integrity. The optimized ST1450 sample exhibited an extremely low charge-transfer resistance of 3.85 Ω, reflecting improved electronic transport pathways. Furthermore, in-situ XRD measurements directly captured phase transitions during lithiation and delithiation, providing crucial insight into the dynamic reaction mechanism. The observed spinodal decomposition within the TiO_2–SnO_2 system forms a self-organized nanoscale microstructure that reinforces both ionic transport and structural stability. These results elucidate the lithiation pathway of TiO_2–SnO_2 composite oxides and highlight spinodal decomposition as a promising strategy for developing structurally adaptive, high-performance oxide anodes for next-generation lithium-ion batteries.

Keywords: **Composit**e **oxides**, **Anode materials**, **Fast-charging materials**, **In-situ XRD**, **Solid-state reaction**

Protective and High-temperature Coatings
Room Town & Country D - Session MA4-2-TuM

Boron-containing Coatings II

Moderators: Martin Dahlqvist, Linköping University, Sweden, **Anna Hirle**, TU Wien, Austria

8:00am **MA4-2-TuM-1 Tuning Structure and Mechanical Properties of TaB_x Films using HiPIMS***, Kateryna Smyrnova* ***[kateryna.v.smyrnova@gmail.com]****,* *Tomáš Roch, Martin Truchlý,* CENAM FMPI, Comenius University in Bratislava, Slovakia*; Peter Švec,* Institute of Physics, SAS, Slovakia*; Rainer Hahn, Helmut Riedl,* TU Wien, Austria*; Leonid Satrapinskyy,* CENAM FMPI, Comenius University in Bratislava, Slovakia*; Viktor Šroba,* Linkoeping University, Sweden*; Marián Mikula,* CENAM FMPI, Comenius University in Bratislava, Slovakia

Both experimental and theoretical studies have reported TaB_x to be promising for high-temperature and wear-resistant applications due to its exceptional hardness and oxidation resistance. However, achieving dense, nanocrystalline TaB_x with controlled stoichiometry remains a challenging task. To date, TaB_x films have been deposited only by conventional magnetron sputtering and high target utilization sputtering. This study demonstrates the pressure-controlled structure transformation of TaB_x films deposited by HiPIMS.

TaB_x coatings were deposited from a TaB_2 target in an Ar atmosphere at 340 °C using HiPIMS. Three groups of films were grown under three pressures (0.3 – 0.9 Pa) and two substrate bias conditions. The target current density was maintained at 1 A/cm^2 by adjusting the pulse frequency. The microstructure was analyzed using XRD and TEM. TaB_x films exhibited an amorphous structure at low pressure, a nanocomposite nature at moderate pressure, and a dense nanocrystalline structure at high pressure. This work presents the first systematic investigation into how energy flux controlled by pressure influences phase evolution in TaB_x deposited by HiPIMS. Cross-sectional SEM confirmed uniform thicknesses and sufficient adhesion. The chemical composition, as determined by WDS, showed that the B/Ta ratios rose from 1.05 to 1.4. This might be attributed to the reduced resputtering of B by thermalized reflected Ar neutrals at higher pressure. The nanoindentation method yielded a nanohardness of 26.2 GPa and Young's modulus of 344.6 GPa for amorphous films, improving to 42.4 GPa and 469.8 GPa for nanocrystalline ones. Fracture toughness (K_{IC}) was also determined by cantilever fracture testing in SEM.

These results establish working pressure in HiPIMS as a powerful parameter for controlling the crystallinity, stoichiometry, and mechanical properties of refractory borides. This study clarifies how changes in microstructure affect the densification and hardening of boron-rich films. The demonstrated ability to obtain dense, hard, and tough TaB_x films by HIPIMS highlights its potential for preparing next-generation materials for extreme environments. This work was funded by the Slovak Research and Development (No. APVV-24-0038) and the European Union under grant agreement No. 101158464 (COLOSSE).

8:20am **MA4-2-TuM-2 Solid Self-Lubrication Mechanism of B_2O_3 in Boride Based Thin Film Materials Under Various Atmospheres**, ***Daniel Pölzlberger [daniel.poelzlberger@tuwien.ac.at]***, Institute of Materials Science and Technology, TU Wien, Austria; *Norma Salvadores Farran, Tomasz Wojcik, Philip Kutrowatz, Rainer Hahn,* Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria; *Eleni Ntemou, Daniel Primetzhofer,* Department of Physics and Astronomy, Uppsala University, Sweden; *Carsten Gachot,* Institute of Engineering Design and Product Development, Research Unit Tribology, TU Wien, Austria; *Helmut Riedl,* Institute of Materials Science and Technology, TU Wien, Austria

Transition metal borides (TMBs) represent a highly promising family of materials for functional coatings due to their abundance, cost-effectiveness, and exceptional mechanical properties. These include a high melting point, hardness of up to 60 GPa, excellent chemical and thermal conductivity, and outstanding resistance to wear. Their distinct self-lubricating behavior arises from the formation of boron oxide, which reduces friction, although the fundamental mechanisms behind this tribo-reaction remain not fully understood, particularly for TMB-based thin films. Temperature and atmosphere play a significant role in boron oxide formation, making it essential to understand the oxidation behavior of physical vapor-deposited boride based films to interpret their friction and wear performance at elevated temperatures. Tribological tests reveal that sputter-deposited super-stoichiometric $TiB_{2.9}$ exhibits a significantly lower friction coefficient (~0.3) than sub-stoichiometric $TiB_{1.5}$ (~0.4) at 500°C, attributed to the higher oxidation rate of $TiB_{2.9}$ and the presence of B-rich tissue phases at column boundaries. Similarly, α-$WB_{2\pm z}$ coatings display self-lubrication via boron oxide formation, although growth related sub-stoichiometry limits boron availability during oxidation. The surrounding atmosphere further influences friction behavior: in oxygen-depleted conditions, oxidation and lubrication are minimal, whereas under humid conditions, water vapor reacts with boron oxide to form boric acid with layered, lubricious properties. To investigate these processes, we conducted ex-situ and in-situ oxidation studies of the TMB based thin films using elastic backscattering spectrometry (EBS) over a temperature range from room temperature to 940°C. The oxidation data, correlated with tribological, X-ray photoelectron spectroscopy, X-ray diffraction, and transmission electron microscopy analyses, provide new insights into the temperature-dependent lubrication mechanisms of boron oxide in TMB thin films.

8:40am **MA4-2-TuM-3 Super-Ordered MAB Phases: Theoretical Design of Novel Boron-Containing Materials with Simultaneous in-Plane and Out-of-Plane Chemical Ordering**, ***Martin Dahlqvist [martin.dahlqvist@liu.se]***, *Johanna Rosen,* Materials Design Division, Linköping University, Sweden

Chemical ordering in layered materials, such as MAX and MAB phases, enables precise tailoring of functional properties through structural motifs like in-plane (*i*-MAB, *i*-MAX) and out-of-plane (*o*-MAB, *o*-MAX) configurations. This study introduces super-ordered MAB phases (*s*-MAB), a novel structural material combining simultaneous in-plane and out-of-plane chemical ordering, previously unreported in synthesized MAB phases. Using first-principles density functional theory, we systematically investigated the thermodynamic stability of hypothetical quinary s-MAB phases with 314 ($M1_4M2_2M3_3Al_3B_{12}$) and 416 ($M1_4M2_2M3_6Al_3B_{18}$) compositions (M1, M3 = transition metals; M2 = Sc, Y) against a comprehensive set of competing phases, including ternary and quaternary MABs, disordered configurations, and binary/ternary borides at 2000 K. Our calculations predict 27 thermodynamically stable *s*-MAB compositions, predominantly featuring M1 = Cr, Mo, W, Mn, Fe and M3 = V, Nb, Ta, with M2 = Sc or Y promoting the combined in-plane and out-of-plane order. Notably, 416 structures exhibit conditions favoring partial or complete disorder, highlighting the nuanced stability landscape. These *s*-MAB phases offer a theoretical roadmap for synthesizing novel boron-containing compounds with precisely controlled atomic arrangements, potentially yielding unique mechanical, thermal, and electronic properties. Additionally, stable *s*-MABs can serve as precursors for 2D boridene (MBene) synthesis, expanding compositional flexibility for property tuning compared to existing boridenes. This work establishes a framework for designing advanced boride-based materials, with implications for high-temperature coatings, structural components, and electronic devices. Future experimental efforts should prioritize optimizing synthesis conditions to validate predicted chemical ordering and explore application-driven property enhancements.

Functional Thin Films and Surfaces
Room Palm 5-6 - Session MB2-2-TuM

Thin Films for Emerging Electronic and Quantum Photonic Devices II

Moderators: Ufuk Kilic, University of Nebraska - Lincoln, USA, **Ulrich Schmid**, TU Wien, Austria

8:00am **MB2-2-TuM-1 Polyoxometalate Thin Film Heterostructures and Blends with Neuromorphic Computing Capabilities**, ***Dimitra Georgiadou [D.Georgiadou@soton.ac.uk]***, University of Southampton, UK **INVITED**

Neuromorphic computing holds promise for lowering power consumption and increasing the computation speed of Artificial Intelligence (AI) applications, as it is emulating the parallel manner of memorising and processing information in the brain. Although machine learning algorithms inspired by the spiking neural networks in the brain have recently made gigantic leaps into the field of neuromorphic computing, scalability and power efficiency remain a challenge. There is, therefore, a clear need for redesigning the neuromorphic hardware systems using radically novel materials and architectures that can better emulate the chemical processes in the mammalian brain and lead to efficient computation with added functionalities.

Polyoxometalates (POMs), a class of redox active molecular metal oxides, have emerged as promising candidates for next generation neuromorphic devices. Their discrete molecular structure, tunable electronic properties, and compatibility with silicon-based platforms have made them attractive materials for advanced memory applications with tunable long- and short-term memory characteristics. POMs can accept multiple electrons without compromising their structural integrity, notably acting as “electron reservoirs” or “electron sponges”, while the highly tunable surface chemistry of these metal oxide clusters offers many routes for electronic device optimisation.

In this talk, I will present a two-terminal redox-based resistive switching memory using the Keggin phosphomolybdate POM $H_3PMo_{12}O_{40}$. By combining this Mo-POM with nanogap coplanar metal electrodes, we create nanoelectronic devices that offer significant advantages, such as low power consumption and fast switching times. Emphasis will be placed on the diverse strategies used to integrate POMs with different metal substrates and functional layers, such as dielectric and conjugated polymers. I will also discuss the influence of counterions and encapsulating layers in resistive switching mechanisms.

This combination of redox active nanomaterials and nanogap architecture holds great potential for advancing electronic technologies, while being also fully compatible with large area manufacturing and flexible substrates. Overall, this work introduces POM-based systems as a viable alternative to the limitations of conventional CMOS memory, offering a blueprint for future developments in molecular electronics.

8:40am **MB2-2-TuM-3 Yttrium-Doped Aluminum Nitride Memristors to Enhance the Pattern Recognition Accuracy of Unsupervised Spiking Neural Network**, ***Jer-Chyi Wang [jcwang@mail.cgu.edu.tw]***, Chang Gung University, Taiwan **INVITED**

Recently, an increasing requirement for pattern recognition and decision-making in computing systems has led to the development of artificial neural network (ANN). Although ANN is inspired by the working principle of the biological nervous system, the learning rule and computing architecture are still inconsistent with nervous behaviors, making it difficult to realize the functionalities of the human brain. To overcome these issues, spiking neural network (SNN) with high biological plausibility has been proposed for next-generation neuromorphic computing systems. SNN performed with the spike-timing-dependent plasticity (STDP) learning rule can mimic the learning behaviors of living beings. Hence, the design of electronic devices with STDP behavior, such as synaptic transistors, memristors, and ferroelectric memories, has become a crucial task. Among them, memristors have been considered as the most promising candidates because of their synapse-like morphology, high scaling ability, and low power consumption. Nitride-based memristors, such as AlN, Si_3N_4, WN, and CuN memristors, have been reported to exhibit superior memory characteristics; however, most of the devices require specific operation methodologies to mimic the synaptic properties. Thus far, no studies have focused on the process-related influences on the STDP behavior of memristors and further implementation of the devices in the SNN system.

In this study, yttrium (Y)-doped AlN memristors are proposed to investigate the dependence between the Y-doping concentration and SNN performance. With an increase in the Y-doping concentration, both the memory characteristics and synaptic behaviors of the AlN memristors significantly improved. In addition, the STDP parameters of the memristors were extracted and fed into the SNN to simulate the pattern recognition capability. The optimized pattern recognition accuracies of 75.89 and 60.21% for the MNIST and ETH-80 datasets, respectively, were achieved for the AlN memristors with a Y-doping concentration of 3.4%, which is promising for implementation in future neuromorphic computing system and artificial intelligence.

9:20am **MB2-2-TuM-5 Impact of Interlayers on the Electrical and Microstructural Stability of Cu Films Deposited on SiC Substrates***, **Jui-Wei Hsu [michaelhsu33@gmail.com],*** College of Semiconductor Research, National Tsing Hua University, Hsinchu, Taiwan*; Fan-Yi Ouyang,* Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan

Silicon carbide (SiC) has become a key substrate material for high-voltage and high-temperature power devices due to its wide bandgap, high breakdown field, and excellent thermal conductivity. However, its distinct surface chemistry and higher thermal budget pose challenges for metallization. In conventional Si-based systems, interlayers such as TiN, Ta, and TaN are widely used as Cu diffusion barriers and adhesion layers. Yet, their effectiveness on SiC substrates remains insufficiently understood. Establishing a stable, low-resistance Cu film stack on SiC is therefore critical for ensuring both electrical performance and reliability under high-temperature operation.

In this study, TiN, Ta, and TaN interlayers were deposited on SiC substrates using a sputtering system, followed by a 5000 Å Cu overlayer. This configuration enables direct comparison of how each interlayer affects Cu texture, interfacial stability, and diffusion behavior during subsequent thermal processing. The as-deposited Cu/TiN structure exhibited the lowest sheet resistance, followed by Cu/TaN and Cu/Ta. After annealing at 200–300 °C, the Cu/Ta stack demonstrated the best stability, while Cu/TaN maintained a slightly higher but stable value around 2.0 Ω/sq. TiN showed more pronounced resistance variation with temperature. The temperature-dependent evolution of resistivity and interfacial structure, along with the underlying diffusion mechanisms, will be discussed in detail. These findings contribute to a deeper understanding of Cu/interlayer/SiC interfaces, providing design guidance for reliable metallization schemes in next-generation power electronics.

Keywords: SiC, TiN/Ta/TaN interlayer, diffusion barrier, Cu metallization, thermal stability

9:40am **MB2-2-TuM-6 Ternary-Blending Energetics and 3d Packing in Thin Films Enable Ultralow-Noise Nir Opds and Thermally Durable All-Polymer Opvs***, **Chih-Ping Chen [cpchen@mail.mcut.edu.tw],*** Ming Chi University of Technology, Taiwan **INVITED**

We report complementary molecular- and ternary blend-control thin-film strategies that concurrently suppress non-radiative loss and dark current in near-infrared (NIR) organic photodetectors (OPDs) and deliver record-level thermal durability in all-polymer organic photovoltaics (OPVs). (i) In OPDs, introducing PTQ10 into PM6:PY-IT forms a ternary film that suppresses unfavorable molecular packing and tunes interfacial energetics, thereby mitigating thermally activated carrier generation/leakage. A ternary OPD incorporating PTQ10 into PM6:PY-IT suppresses unfavorable packing and optimizes energy-level alignment, thereby mitigating thermally activated carrier generation and leakage. The devices achieve $J_d < 1.0 \times 10^{-9}$ A cm^{-2} at −2 V and shot-noise-limited detectivity D*_shot ≈ 5.0×10^{13} Jones (830 nm, −2 V) without sacrificing responsivity. In the case of donor D18 paired with Y-series acceptors of varied surface energies and frontier orbitals identifies D18:Y18 blends with optimized 3D packing (GIWAXS), reduced trap density, and minimized non-radiative recombination, yielding D*_shot = 4.2×10^{13} Jones at −2 V, with superior linear dynamic range, cutoff frequency, and response time. For OPVs, blending the polymer donor PBQx-TF with high-crystallinity D18 followed by sequential deposition of PY-IT tunes morphology and balances carrier mobilities while minimizing energy losses. The ternary all-polymer OPV attains PCE = 16.07%, surpassing the corresponding binaries (15.26% for PBQx-TF:PY-IT; 14.39% for D18:PY-IT), and exhibits outstanding durability, retaining 80% of its initial PCE after 1500 h at 120 °C, with intact layer structure. Together, these results establish clear design rules—ternary-blend energetics and controlled 3D packing—for achieving ultralow dark current in NIR OPDs and unprecedented thermal stability in all-polymer OPVs.

Tribology and Mechanics of Coatings and Surfaces
Room Town & Country C - Session MC3-1-TuM

Tribology of Coatings and Surfaces for Industrial Applications I

Moderator: Osman Eryilmaz, Argonne National Laboratory, USA

8:00am **MC3-1-TuM-1 Bridging Research and Industrial Application: Advanced Coatings and Surface Treatments for Tribological Challenges***, **Andras Korenyi-Both [andy.korenyi-both@woodward.com],*** Woodward Inc., USA **INVITED**

Surface engineering and advanced coatings are critical for addressing complex tribological challenges across diverse industrial applications, from aerospace to manufacturing. This talk provides an overview of key advancements in coating technologies, spanning decades of research and development, with a focus on linking fundamental insights to real-world applications.Highlights include the investigation of faults and failures in sprayed MoS_2 coatings on the Galileo spacecraft, which informed the development of improved PVD MoS_2 coatings through doping and layering for enhanced performance transitioning to rocket engine turbo pump gears. The transition from PVD coatings to tribomechanical deposition applications is explored, leveraging techniques such as laser surface texturing and WAM testing to bridge laboratory results with production-scale implementation.Emerging technologies, such as autocatalytic in situ diamond-like carbon formation from hydrocarbons, are also discussed, showcasing their potential to enable self-lubricating surfaces in extreme industrial environments. The application of duplex and triplex treatments is highlighted as a powerful approach to solving complex tribological problems, combining multiple surface engineering techniques to optimize performance across diverse conditions.Additional contributions include the development of high-performance coatings for forging and die-casting applications, high-temperature plasma electrolytic oxidation combined with solid film lubricants and the use of nanoparticles in liquids to enhance lubrication. Case studies like the MISSE-to-production pipeline highlight the challenges of translating terrestrial -proven coatings to flight applications, addressing the "flight history conundrum."This work demonstrates the importance of combining advanced surface engineering strategies—ranging from thin-film deposition to hybrid treatment approaches—to tackle emerging challenges in multi-fuel and dry gas environments. Collectively, these efforts underscore the value of a multidisciplinary approach to the development, characterization, and deployment of coatings and surface treatments for solutions in transportation, manufacturing, and beyond. Closing remarks include the role of solid film lubricants towards environmental stewardship.

8:40am **MC3-1-TuM-3 DLC-Based Coatings with Enhanced Cavitation Resistance for Automotive Applications***, Kenny Bislin,* Oerlikon Surface Solutions AG, Liechtenstein*; Martin Bohley,* Oerlikon Balzers Coating Germany GmbH, Germany*; Christian Fleischmann, **Astrid Gies [astrid.gies@oerlikon.com]**, Theresa Huben, Kaushik Hebbar Kannur, Felix Oelschlegel, Stefan Moser,* Oerlikon Surface Solution AG, Liechtenstein*; Timea Stelzig,* Oerlikon AM Europe GmbH, Germany

Since several years, automotive manufacturers focus on enhancing the engine performance while reducing the fuel consumption and therefore emissions of gasoline internal combustion engines (ICE). Consequently, the usage of high-pressure direct injection systems, already known from diesel ICEs, is increasing. In these systems, the fuel is accumulated in a central high-pressure rail and injected via injectors into the cylinder. The injection pressure has increased over time; current state-of-the-art systems operate between 200bar and 500bar. By increasing the injection pressure from 200bar to 500bar, the particle emission of the engine can be reduced by 95%. In most of the high-pressure injection systems, the injector valves consist of a ball opening and closing against a seat. Any leakage between the ball and the seat must be avoided to guarantee the lifetime of the system. In most of the current systems, the components like for example the balls are often coated with diamond-like-carbon (DLC) based coatings in order to prevent any premature wear in the systems.

However, the constantly rising injection pressures, but also the use of different fuel blends with incorporation of certain amounts of ethanol and methanol for reduced CO_2 emissions lead to drastically increased loads on the different components, especially due to severe cavitation occurring inside the injectors, exceeding sometimes the mechanical strength of common DLC coatings. The resulting wear of the injectors causes fuel leakage into the combustion chamber and significantly reduces the lifetime of such systems.

In this study we compare the tribological performance as well as the cavitation resistance of a standard DLC coating optimized for tribological applications with a DLC coating with enhanced cavitation resistance. The tribological performance of the coatings is investigated using a translatory oscillating friction and wear test (SRV® from Optimol Instruments). To study the cavitation resistance of the coatings, a cavitation test bench (sonotrode tester) was employed using test procedures according to ASTM 32.

While the tribological performance of both coatings is similar, the standard DLC coating shows first indication of cavitation erosion after 90 minutes testing time, whereas the DLC coating with enhanced cavitation resistance shows first indications of cavitation resistance by a factor of 3 later and at a lower intensity. Therefore, this coating is more suitable for the application in high-pressure direct injection systems and enables the use of more environmentally friendly gasoline blends with higher ethanol or methanol share due to the drastically increased cavitation resistance.

9:00am **MC3-1-TuM-4 Surface Technologies for Geothermal Energy Applications***, **Oyelayo Ajayi [ajayi@anl.gov]**, Levent Eryilmaz, Aaron Greco,* Argonne National Laboratory, USA **INVITED**

Geothermal power systems rely on equipment that must perform in exceptionally harsh environments—high temperatures, high flow rates, chemically aggressive brines containing chlorides, CO_2 and H_2S, and suspended solids. These conditions make many components susceptible to surface-initiated or surface-related failure modes. Vulnerable systems include drilling tools, casing strings, valves and piping, and rotating equipment such as pumps, motors and turbines. Under these extremes, abrasive wear, particle erosion, corrosion and mineral deposit formation can rapidly degrade performance, shorten component life. Mitigating surface-related failures is therefore essential to reliable, cost-effective construction and operation of geothermal plants.Surface engineering offers a practical, cost-effective pathway to extend service life without wholesale changes to base materials. Incumbent surface technologies used in geothermal applications include hardfacing overlays with metal-matrix composite claddings (e.g., carbide-reinforced Ni/Co systems); thermochemical conversion treatments such as boriding/boronizing that create hard, wear-resistant diffusion layers; and thermal spray coatings—HVOF, plasma and arc spray deposition to apply corrosion- and erosion-resistant alloys, cermets and ceramics.This presentation will review where and how these technologies are applied, their benefits and limitations, and the practical technical considerations that determine success. Key property and performance attributes most relevant to geothermal service—hardness, fracture toughness, coating adhesion, erosion and slurry wear rates, corrosion resistance, scaling propensity, thermal stability will be discussed.Emerging advances in surface technologies, such as functionally graded coatings, nanostructured and amorphous metal overlays, high-entropy alloy and cermet systems, will be highlighted. Gaps where further development is needed: standardized test protocols representative of geothermal conditions, long-duration field data and models that bridge laboratory results to plant performance, coatings that resist silica-rich scaling while maintaining mechanical integrity will be discussed. Together, these insights aim to highlight opportunities for surface-engineered solutions across geothermal power systems.

9:40am **MC3-1-TuM-6 Tailoring Ice Adhesion Behavior of Erosion Resistant Coatings: Tuning Surface Chemistry and Physical Properties***, **Olayinka Abegunde [Olayinka.Abegunde@sdsmt.edu]**, Nathan Madden, Grant Crawford, Forest Thompson,* South Dakota School of Mines and Technology, USA*; Emily Asenath-Smith,* US Army Engineer Research and Development Center (ERDC) Cold Regions Research and Engineering Laboratory (CRREL), Hanover, NH 03755, USA

The mitigation of ice accretion on critical infrastructure, including aircraft components and energy installations remains a significant challenge in cold and arctic regions. Conventional de-icing methods based on thermal and chemical approaches are widely used and have been explored extensively but are inherently energy-intensive and environmentally unsustainable. Thus, passive approaches which rely on the surface properties of a material to reduce ice adhesion strength, delay ice nucleation, or repel ice accretion have gained significant attention.

This study explores the design, deposition, and characterization of durable, erosion resistant coatings engineered to minimize interfacial adhesion strength with ice in cold environments by tuning their surface chemistry, physical properties, and surface microstructure. A series of nitride-based coatings were deposited using magnetron sputtering process. Deposition parameters were optimized to tailor key surface characteristics, including roughness, topography, surface energy, crystallographic texture, and Young's modulus.

The surface morphology and topography were examined using scanning electron microscopy (SEM) and atomic force microscopy (AFM), while grazing-incidence X-ray diffraction (GIXRD) was employed to identify crystalline phases. X-ray photoelectron spectroscopy (XPS) provided insights into the surface chemical states and contact angle goniometry was utilized to evaluate surface wettability. The sub-zero coefficient of friction and wear rate were assessed using a low-temperature tribometer. Ice adhesion strength was quantified through a shear-testing procedure which enabled controlled growth of ice on the durable coatings.

This work provides new insights into the structure–property–performance relationship governing ice adhesion and demonstrates a pathway for scalable fabrication of durable, low-adhesion coatings suitable for extreme service conditions in the aerospace and energy sectors.oi

10:00am **MC3-1-TuM-7 2D MXene Coatings – Combining Macro-Scalesuperlubricity and Durability***, **Andreas Rosenkranz [arosenkranz@ing.uchile.cl]**,* University of Chile **INVITED**

MXenes nano-sheets have experienced tremendous attention in the scientific community since their discovery in 2011. In the last 5 years, the tribological research community has started to explore their friction and wear performance when used as lubricant additives, solid lubricant coatings and reinforcement phase in composites. Especially when using MXenes for solid lubrication, promising results have been verified. MXene coatings tend to demonstrate an ultra-high wear resistance being particularly beneficial for the durability and longevity of these coatings. These beneficial properties are traced back to the formation of a thin MXene-rich tribolayer. Little is known about the structural and compositional properties of these tribolayers. The underlying kinetics and driving forces are yet to be explored. More knowledge about the involved mechanisms and kinetics is urgently needed, which is expected to significantly boost this entire research topic.

Therefore, we have designed tribological ball-on-disk experiments to understand the influence of the number of layers (few- versus multi-layers), the coatings thickness and the tribological testing conditions (normal load, sliding velocity and relative humidity) on the tribofilm formation. Combined with advanced materials characterization, these tests allow us to draw some important conclusions about the involved thermomechanical aspects and underlying kinetics of the layer formation.

Based upon the experiments conducted, we verify thermomechanical and kinetic aspects of the involved tribolayer formation, which align well with the respective temporal evolution of the coefficient of friction. When exceeding a critical value of the applied normal load (Hertzian contact pressure), the formation of a stable tribolayer with beneficial friction and wear properties is not possible. More importantly, the same conclusion can be drawn when exceeding a critical sliding velocity, which clearly shows the kinetic aspect of the involved layer formation. We also verify that increasing the respective thickness of the MXene coatings does not necessarily result in more beneficial effects (low friction, low wear, and long-lasting effects). Concerning energy application, the material of choice tends to go towards mono-layer MXenes. Regarding tribological research, no scientific study has systemically addressed whether it is more beneficial to use few- or multi-layer MXenes. This contribution also sheds some light on this open question, thus giving some important guidelines and recommendation for future tribological experiments using MXenes.

10:40am **MC3-1-TuM-9 Friction and wear of composite MXene/MoS_2 coating under low viscosity fuels under reciprocating sliding***, **Ali Zayaan Macknojia [alizayaanmacknojia@my.unt.edu]**, Mohammad Eskandari,* University of North Texas, USA*; Stephan Berkebile,* Army Research Laboratory, USA*; Andrey Voevodin, Samir Aouadi, Diana Berman,* University of North Texas, USA

Friction and wear-related failures remain major challenges in moving mechanical assemblies operating under various conditions. For example, the components of fuel systems made of AISI 52100 steel are susceptible to scuffing-induced wear when operated in fuel environment. This study demonstrates the decreased friction and wear characteristics achieved by spray-coating 52100-grade steel surfaces with solution-processed multilayer $Ti_3C_2T_x$-MoS_2 blends. Study analyzed performance of the coating in different fuels. Raman spectroscopy, scanning electron microscopy, and transmission electron microscopy results revealed the formation of an in-situ robust tribolayer responsible for the outstanding performance observed at high contact pressures and sliding speeds. This study has broad implications for the development of solid lubricants that can operate under extreme conditions and low viscosity fuel environment, inspiring further research and development in this field.

Surface Engineering of Biomaterials, Devices and Regenerative Materials: Health, Food, and Agriculture Applications
Room Town & Country B - Session MD1-2-TuM

Coatings and Surfaces for Medical Devices: Mechanical, Corrosion, Tribocorrosion, and Surface Processing II

Moderators: Po-Chun Chen, National Taipei University of Technology, Taiwan , **Jean Geringer**, Ecole Nationale Superieure des Mines, France

8:00am **MD1-2-TuM-1 Metallic-Capped Nanoslit Structure Integrating with Microfluidic Devices for Biosensing Applications.**, ***Yu-Jui (Ray) Fan [rayfan@nycu.edu.tw]***, National Yang Ming Chiao Tung University (NYCU), Taiwan **INVITED**

A localized surface plasmon Resonance (LSPR) is the result of the confinement of a surface plasmon in a nanoparticle/nanostructure of size comparable to or smaller than the wavelength of light used to excite the plasmon. The plasmon resonant frequency is highly sensitive to the refractive index of the environment; a change in refractive index results in a shift in the resonant frequency. As the resonant frequency is easy to measure, it can be used as an immunosensor. We will introduce the metallic-capped nanostructures as LSPR biosensors integrating with microfluidic devices. In this talk, I will show two examples: (1) an LSPR sensor integrating with microfluidic-based polymerase chain reaction (PCR) for DNA detection, and (2) an LSPR sensor integrating with a microfluidic-based preconcentrator for antigen detection.

8:40am **MD1-2-TuM-3 Plasma-Activated Chitosan-Hydrogel Coating Incorporating Natural Immunomodulatory Protein (GMI) for Enhanced Tissue Regeneration and Oral Cancer Inhibition**, *Yu-Rou Lin, Meng Yun Wu, Sheng-Yen Lin,* ***Ying-Sui Sun [yingsuisun@tmu.edu.tw]***, Taipei Medical University, Taiwan **INVITED**

Dental implant regeneration aims not only to restore alveolar bone integrity but also to re-establish the physiological functions of periodontal tissues and sensory feedback lost in conventional osseointegration. Conventional titanium implants, while mechanically stable, often lack the biological complexity of natural teeth. Therefore, regenerative implant strategies that promote bone formation, soft tissue integration, and nerve recovery are increasingly essential for long-term functional success. Meanwhile, oral cancer remains the sixth most prevalent malignancy globally, particularly in Southeast Asia. Betel nut chewing, smoking, and alcohol consumption are major etiological factors contributing to late-stage diagnosis, high recurrence, and impaired oral functions. Hence, developing biomaterials that simultaneously enhance tissue regeneration and suppress cancer progression represents a critical frontier in oral biomedical materials research. In this study, a plasma-activated chitosan-hydrogel coating incorporating a natural immunomodulatory protein, Ganoderma lucidum microspore immunomodulatory protein (GMI), was developed as a dual-functional platform for tissue regeneration and oral cancer inhibition. Plasma activation was employed to enhance the surface energy and introduce hydrophilic reactive groups (–OH, –COOH, $–NH_2$) on the chitosan hydrogel, improving protein immobilization efficiency and biointerface activity. GMI, known for modulating MAPK-related immune signaling, exhibits anti-inflammatory, antiviral, and anticancer properties while promoting tissue repair. The plasma-activated hydrogel surface was characterized using FESEM and immunofluorescence microscopy, confirming an extracellular matrix (ECM)-like morphology favorable for cell attachment. Biological performance was evaluated using dental pulp stem cells (DPSCs) and oral cancer cell lines. The AlamarBlue assay demonstrated that the plasma-activated GMI–hydrogel coating significantly enhanced DPSC viability and proliferation compared to untreated controls. Wound healing and migration assays revealed accelerated cell migration and coverage on the plasma-treated surfaces. Western blot analysis further confirmed the upregulation of MAPK-associated proteins involved in regenerative signaling. In parallel, the GMI-loaded coatings induced apoptosis in oral cancer cells, inhibiting their adhesion, spreading, and colony formation. These results collectively demonstrate that the synergistic combination of plasma surface engineering and GMI bioactivity enables precise modulation of cellular behavior toward regeneration while suppressing malignant cell functions.

9:20am **MD1-2-TuM-5 Low Temperature Plasma Assisted Strategies to Surface Engineering of Biomaterial**, *Claude Côté, Noureddine Oudini, Alexa Bagdasarian,* PLASMIONIQUE Inc., Canada*; Kambiz Chizari,* PLSMIONIQUE Inc, Canada*; Eduardo Loreto,* PLASMIONIQUE Inc, Canada*; Anita Sarkissian, Ryan Porter,* ***Andranik Sarkissian [sarkissian@plasmionique.com]***, PLASMIONIQUE Inc., Canada **INVITED**

The unique characteristics of materials at the nanoscale make them some of the most promising molecular building blocks in nanotechnology. Nanostructured materials have attracted significant attention across various industrial fields due to their exceptional mechanical, chemical, electrical, and optical properties, which enable a wide range of potential applications. However, each specific application demands precisely engineered structures tailored to its unique requirements. Consequently, the development of specialized strategies for selective processes - such as etching, deposition, functionalization, ion implantation, and synthesis - with excellent control is essential.

Biomaterials present additional challenges, as they must simultaneously satisfy multiple, and often competing, requirements, including biocompatibility, hemocompatibility, cytotoxicity, biodegradability, and mechanical and chemical stability.

Plasma- and vacuum-based technologies offer several distinctive advantages, particularly their ability to enable surface engineering with single-monolayer precision.

In this presentation, we will discuss a range of plasma-assisted surface modification strategies, illustrated with examples of their application to the surface engineering of biomaterials, including biodegradable materials.

10:00am **MD1-2-TuM-7 Superhydrophilic Metallic Coating: PVD Fabrication and Applications**, *Sea-Fue Wang,* National Taipei University of Technology, Taiwan*;* ***Jinn P. Chu [jpchu@mail.ntust.edu.tw]***, National Taiwan University of Science and Technology, Taiwan

Superhydrophilic coatings represent a powerful class of biomimetic technologies that address diverse real-world challenges—from maintaining building cleanliness and optical clarity to enhancing safety in medical settings and efficiency in industrial processes. In this presentation, I will report a novel superhydrophilic coating based on a sputter-deposited 316 stainless steel layer. The coated surface exhibits a water contact angle of approximately 10 degrees. Furthermore, this coating demonstrates notable antifouling and underwater superoleophobic properties, making it highly advantageous for application in separation membranes designed for oil/water emulsions. In addition to its antifouling and separation capabilities, this coating has proven highly effective at enhancing electrochemical responses, making it an excellent functional layer for sensor electrodes. This presentation will provide specific application case studies to demonstrate its practical utility in this domain.

10:20am **MD1-2-TuM-8 Ti-Nb-Mo Alloy Coatings Sputter-Deposited on 316L for Biomedical Applications**, *Katherine Martinez-Orozco, Bruno Aquino,* Federal University of Sao Carlos, Brazil*; Raira Apolinario, Haroldo Pinto,* University of Sao Paulo, Brazil*; Conrado Afonso,* ***Pedro Nascente [nascente@ufscar.br]***, Federal University of Sao Carlos, Brazil **INVITED**

Medical grade AISI 316L stainless steel (SS) has been widely used as prosthetic material due to its adequate biomechanical and biocompatibility properties, however, the cytotoxicity caused by the release of Cr and Ni ions can have toxic effects and cause allergies in human tissues. β phase (body-centered cubic) Ti-based alloys present lower elastic moduli, better biocompatibility, lower density, and better wear and corrosion resistance in biological environments than the 316L SS, however, they are much more costly. An economical option would be to coat a SS implant with a β-Ti alloy thin film with adequate composition to enhance the material biocompatibility. Nb and Mo are non-toxic and non-allergenic biocompatible metals, and their addition to Ti helps to stabilize the β phase. Ti-Nb-Mo alloy ternary alloys present a low elastic modulus that could prevent the stress shielding effect that can cause bone loss. We report on Ti-Nb-Mo alloy coatings deposited on 316L substrates by direct current magnetron sputtering. The following atomic compositions were produced: Ti74Nb21Mo5, Ti74Nb19Mo7, Ti72Nb19Mo9, and Ti67Nb22Mo11; a Ti80Nb20 coating was used as reference. Only the β phase was identified by grazing incidence X-ray diffraction. Scanning electron microscopy images revealed the presence of agglomerates and porous; the grain sizes decreased with the increasing in Mo content. The residual stresses presented a combination of compressive and tensile stresses. An inverse Hall-Petch effect was observed with the hardness reduction with the decreasing in grain size. X-ray photoelectron spectroscopy (XPS) analysis revealed that the Ti-Nb-Mo coatings presented oxidized surface layers, which can be beneficial for biomedical applications.

Exhibitors Keynote Lecture
Room Town & Country A - Session EX-TuM

Exhibitors Keynote Lecture
Moderator: Peter Kelly, Manchester Metropolitan University, UK

11:00am **EX-TuM-1 Thin Film Tribological Coatings to Enhance the Durability of Engineered Bearings and Industrial Motion Components**, ***Ryan Evans [ryan.evans@timken.com]***, The Timken Company, USA **INVITED**

Thin film tribological coatings can substantially improve the wear resistance of bearings and industrial motion components. This talk reviews proven thin-film solutions, including chemical conversion treatments such as black oxide, electrodeposited Ni–W coatings, and reactively sputtered diamond-like carbon (including WC/a–C:H), and examines their real-world performance on bearings and gears. Case studies cover wind-turbine bearing wear reduction, cost-effective Ni–W implementations, and ball-coating options. The presentation addresses coating-lubricant interactions, coating selection criteria, and implementation challenges required to translate laboratory results into field reliability gains. Attendees will gain actionable guidance and insights for specifying coatings that deliver measurable durability and maintenance benefits in industrial motion applications.

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

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

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

2:00pm **CM1-2-TuA-2 Advancements in XPS Depth Profiling using Femtosecond Laser Ablation (fs-LA) for Thin Film and Metal Oxide Surfaces***, **James Lallo [james.lallo@thermofisher.com]**,* Thermo Fisher Scientific, USA*; Tim Nunney, Robin Simposn,* Thermo Fisher Scientific, UK*; Mark Baker, Charlie Chandler,* University of Surrey, UK

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

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

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

3:00pm **CM1-2-TuA-5 Automated XPS/XAS Multiplet Fitting for Reproducible Orbital Covalency Extraction in Transition-Metal Systems***, **Mariela Bravo-Sanchez [mariela.bravo@academicos.udg.mx]**, Mario U. Delgado-Jaime, Tania E. Gonzalez-Robles,* Universidad de Guadalajara, Mexico **INVITED**

X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) are widely used to study the local electronic structure of transition-metal systems. However, extracting physically meaningful descriptors from these spectra is still challenging. In charge-transfer multiplet (CTM) analysis, which is required to reproduce the experimental data in highly covalent materials such as those based on molecular systems. However, the large number of parameters involved make it difficult to find a suitable solution and historically has taken several months to find a single fit under this approach.

In this work, we present an automated fitting framework for the joint analysis of XPS and XAS spectra to derive details of their electronic structure and to extract covalency. The approach treats spectral fitting as a constrained inverse problem and combines systematic parametric exploration with convergent search grids to identify stable regions of physically equivalent solutions. In this way, it becomes possible to obtain a more robust estimation of electronic parameters related to charge transfer and hybridisation.

The methodology is evaluated using thin films based on transition-metal phthalocyanines (Fe, Co, Mn, and Ni) as model systems. These materials are of great interest in the field of science materials, as they exhibit intriguing magnetic properties, but their origin has remained elusive. However, our approach has been effective in reproducing their XPS/XAS multiplet features, which are highly sensitive to metal–ligand covalency. Beyond achieving spectral agreement, the framework focuses on parameter stability, internal consistency between XPS and XAS, and the symmetry-based decomposition of orbital covalency as a relevant electronic descriptor.

This contribution is especially relevant for advanced characterisation workflows because it integrates spectroscopy, physics-based modelling, and automated data analysis into a reproducible pipeline. The proposed strategy can be extended to other transition-metal-containing materials, including engineered surfaces, where a reliable interpretation of XPS/XAS data is essential to understand structure–property relationships.

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

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

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

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

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

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

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

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

Protective and High-temperature Coatings
Room Town & Country A - Session MA2-1-TuA

Hard and Nanostructured Coatings I

Moderators: Stanislav Haviar, University of West Bohemia, Czechia, **Kuan-Che Lan**, National Tsing Hua University, Taiwan , **Norma Salvadores Farran**, TU Wien, Austria

1:40pm **MA2-1-TuA-1 The Fabrication, Microstructure, and Characterization of Functional Electroless Ni-P Composite Surface Coatings on Dried Luffa as Bio-Plate**, *Tzu-Hsiu Hung [andybenny2012@gmail.com], Kai-Tse Tsai, Fan-Bean Wu,* National United University, Taiwan

This study employed luffa sponge as a natural substrate for the electroless deposition of nickel-phosphorus, Ni-P, alloy to enhance its structural performance. The phosphorus contented the Ni-P coating was controlled by adding sulfuric acid to adjusting the pH value of the plating bath, allowing analysis of compositional and property variations. The luffa sponge was first sensitized and activated using $SnCl_2$ and $PdCl_2$, followed by deposition in a solution containing $NiSO_4$, NaH_2PO_2, and $Na_2C_4H_4O_4$, with sulfuric acid used to adjust pH. Sodium hypophosphite acted as the reducing agent, promoting the co-deposition of Ni and P. Since the electroless plating rate was approximately 0.1–0.3 μm/min, electroplating was subsequently applied to increase film thickness and investigate its microstructure and mechanical behavior. This technique demonstrates a promising route for the functional surface modification of natural porous materials, enabling the fabrication of lightweight, high-strength composites with potential applications in electronic, structural, and environmental fields.

2:00pm **MA2-1-TuA-2 Erosion-Corrosion Analysis of Cr2N/Ni3N Multi-Layer Coating System Deposited on Nickel Aluminium Bronze (Nab) Using the Dc Magnetron Sputtering**, *Aakanksha Jain [aakanksha_j@me.iitr.ac.in], Ramesh Chandra, Rahul S Mulik,* Indian Institute of Technology Roorkee, India

Nickel–aluminium bronze (NAB) alloys are extensively used in marine environments owing to their strength and corrosion resistance, yet they remain highly susceptible to erosion–corrosion during long-term service. In this work, multilayer Cr_2N/Ni_3N coatings were deposited on NAB substrates using DC magnetron sputtering to address these limitations. The multilayer design combines the chemical stability of Cr_2N with the mechanical robustness of Ni_3N, thereby enhancing hardness, corrosion protection, and erosion resistance, while also modifying surface wettability. Microstructural and chemical characterisation was performed using FE-SEM, EDX, XRD, XPS, AFM, and TEM. Mechanical and functional properties were evaluated through nanoindentation, contact angle measurements, electrochemical corrosion tests, and solid particle erosion studies. The multilayer coating exhibited a hardness of 26.29 GPa and a hydrophobic contact angle of ~134.7°. Electrochemical testing confirmed a drastic reduction in corrosion rate, from 0.184 mm/y for bare NAB to 0.117×10^{-3} mm/y for the coated sample. Erosion resistance was also significantly improved, with material loss reduced to 4.59 mm^3/kg. These results demonstrate the synergistic benefits of Cr_2N/Ni_3N multilayers in enhancing the durability of NAB alloys, highlighting their potential application in marine turbine blades and related components.

2:20pm **MA2-1-TuA-3 Characteristics of TiBCN-based Thin Film with Different Mo Content by Direct Current Plasma Chemical Vapor Deposition**, *Takeyasu Saito [t21165j@omu.ac.jp], Rizu Kurogi, Noki Okamoto,* Osaka Metropolitan University, Japan

Recently, the concept of high-entropy alloys (HEAs) has been extended from metallic systems to ceramic compounds such as nitrides, carbides, and borides, offering a promising strategy to develop next-generation protective thin films with superior hardness, thermal stability, and oxidation resistance. Ti-based thin film such as TiN, TiC, and TiCN was widely used as conventional protective thin films. Further improvements in hardness and oxidation resistance were carried out by incorporating elements such as B, to from TiBCN thin films composed of Ti(C,N) nanocrystals in an amorphous TiBCN matrix. Incorporating refractory metals such as Mo into Ti-based systems is also expected to enhance solid-solution strengthening and oxidation resistance due to their high melting points and in oxide formation resistance. However, the effects of Mo addition in multi-component hard thin films remain unclear. Most previous studies employed physical vapor deposition (PVD) methods such as magnetron sputtering or arc evaporation, while plasma enhanced chemical vapor deposition (CVD) provides potential advantage on higher conformality, stronger interfacial adhesion strength and low temperature fabrication for complex-shaped tools and components fabrication. The objective of this study is to investigate the role of Mo addition in TiBCN thin film containing Ti(C,N) nanocrystals and amorphous TiBCN, as well as the role of Mo addition on solid-solution hardening and oxidation resistance.

TiBCN thin films with different Mo contents were deposited on Si and cemented carbide (WC–Co) substrates using direct current (DC) plasma CVD at around 600℃ where WC–Co substrates were pretreated with aqua regia to improve interfacial adhesion. The precursor gases were $TiCl_4$, CH_4, N_2, BBr_3, and $MoCl_5$. It was confirmed that, B content in TiBCN films increased with increasing BBr_3 flow rate. The effects of Mo incorporation on phase formation, microstructure, and mechanical properties were systematically evaluated using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and nanoindentation. The results from the TiBCN film with Mo will be discussed in order to demonstrate the HEA design concept thin film by DC plasma CVD, which provides a promising method for low temperature next generation hard thin film procedures to enhance mechanical and chemical durability.

2:40pm **MA2-1-TuA-4 CrAlN-based Protective Nanostructured Coatings: Process–Structure–Property Correlations and Performance in Energy-Related Applications**, *Juan Carlos Sanchez-Lopez [jcslopez@icmse.csic.es], Teresa Cristina Rojas,* Institute of Materials Science of Seville (ICMS), Spanish National Research Council (CSIC), Spain; *Ramón Escobar-Galindo,* Universidad de Sevilla (US), Spain; *Santiago Dominguez-Meister, Marta Brizuela,* TECNALIA, Basque Research and Technology Alliance (BRTA), Spain; *Sonia Mato, Francisco Javier Pérez,* Universidad Complutense de Madrid (UCM), Spain **INVITED**

Chromium aluminum nitride (CrAlN)-based coatings represent a model system for understanding and engineering protective nanostructured materials operating under extreme environments. Over the past decade, our research has focused on correlating deposition parameters, microstructure, and functional performance of magnetron-sputtered CrAlN coatings. Particular attention has been paid to the influence of multiple factors, such as film architecture (single- or multilayered), aluminum and dopant concentrations and distributions (Y, Zr, Si, and O), the nature of the substrate, and the type of surrounding atmosphere (air or steam), on oxidation mechanisms, thermal stability, and functional behavior at high temperatures. These studies reveal how nanoscale architecture and compositional design govern mechanical integrity and resistance to degradation at high temperature. Complementary investigations have addressed tribological behavior and oxidation resistance in steam atmospheres, representative of demanding industrial and energy-generation conditions.

Building on this knowledge, recent developments have extended CrAlN-based coatings toward advanced energy technologies, including concentrated solar power systems, where coatings must combine optical functionality with long-term durability above 550 °C. This invited talk will review the evolution of CrAlN-based protective coatings from model hard systems to multifunctional materials for energy-related applications, emphasizing the process–structure–property relationships and degradation mechanisms that underpin their outstanding performance in harsh and sustainable operating environments.

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4:00pm **MA2-1-TuA-8 Enhancement of Thermal Stability of Sputtered Nanotwinned Ag Thin Films by Cu Doping for Reliable Electronic Applications**, ***Jun-Hui Qiu [junhui-qiu@gapp.nthu.edu.tw]***, Department of Engineering and System Science, National Tsing Hua University, Taiwan; *Yu-Lin Liao,* College of Semiconductor Research, National Tsing Hua University, Taiwan; *Fan-Yi Ouyang,* Department of Engineering and System Science, National Tsing Hua University, Taiwan

The rapid expansion of artificial intelligence, data centers, and electric vehicles has intensified the demand for reliable interconnect materials capable of withstanding high-temperature and high-current operating conditions. Silver (Ag) is a promising candidate for electronic applications due to its exceptional electrical conductivity; however, its poor thermal stability often leads to reliability concerns. To address this issue, this study investigates the effect of copper (Cu) doping on the thermal stability of sputtered nanotwinned Ag thin films.

Nanotwinned Ag and co-sputtered 6 at% Cu-doped Ag thin films were fabricated via magnetron sputtering and subsequently annealed at 200 °C, 300 °C, 400 °C, and 500 °C under a vacuum of 5.5 mTorr. In pure Ag films, the nanotwinned structure remained stable up to 400 °C for 1 hour but progressively transformed into large grains with increasing annealing time. After 48 hours at 400 °C, nanotwins disappeared completely due to abnormal grain growth, resulting in a (200)-oriented microstructure. In contrast, the 6 at% Cu-doped Ag films exhibited significantly slower grain coarsening and superior structural stability even after prolonged annealing. At 400 °C, nanotwins were still observed after both 1 hour and 24 hours of annealing. Cu doping also suppressed the orientation transition from (111) to (200), indicating enhanced thermal stability. Furthermore, Cu addition increased hardness from 1.29 GPa to 3.33 GPa through solid-solution strengthening, while causing only a slight rise in electrical resistivity from 2.03 μΩ·cm to 2.90 μΩ·cm. These findings demonstrate that Cu doping effectively improves the thermal and mechanical stability of nanotwinned Ag thin films, providing a promising pathway toward reliable metallic interconnects for next-generation electronic devices.

4:20pm **MA2-1-TuA-9 Backscattered Argon Neutrals: Hidden Architects of Hf–Al–N Nanostructure Evolution**, ***Naureen Ghafoor [naureen.ghafoor@liu.se]***, *Marcus Lorentzon,* Linköping Univ., IFM, Thin Film Physics Div., Sweden; *Rainer Hahn,* TU Wien, Austria; *Diederik Depla,* Ghent University, Belgium; *Justinas Palisaitis, Jens Birch,* Linköping Univ., IFM, Thin Film Physics Div., Sweden

Transition metal aluminum nitrides (TM–Al–N) are multifunctional ceramics whose nanostructure can be tailored for extreme mechanical performance. However, the Hf–Al–N system remains largely unexplored. Here, we demonstrate that energetic backscattered argon neutrals, inherently produced during magnetron sputtering of heavy targets, dominate the structure formation in $Hf_{1-x}Al_xN_Y$ thin films—surpassing the influence of both ion assistance and substrate temperature.

Single-crystal cubic (c) $Hf_{1-x}Al_xN_Y$ films with x < 0.30 deposited on MgO(001) exhibit a unique three-dimensional checkerboard superstructure composed of HfN- and AlN-rich nanodomains aligned along the <001> directions. This periodic modulation, detected via XRD satellites and high-resolution STEM, originates from sub-surface spinodal decomposition triggered by backscattered Ar neutrals with energies exceeding the displacement threshold (~40–50 eV). SDTrimSP and SIMTRA simulations reveal that ~40 % of the neutrals impinging on the film surface possess sufficient energy to induce bulk atomic displacements, leading to compositional modulations even at low growth temperatures (300 °C). In contrast, varying ion flux (up to 15 ions per atom at 20 eV) or substrate temperature (300–900 °C) produced negligible structural changes, underscoring the primary role of energetic neutrals.

The superstructure period increases linearly with Al content (9–13 Å), correlating with hardness enhancements from 26 GPa for HfN_Y to ~38 GPa for c-$Hf_{1-x}Al_xN_Y$ due to dislocation pinning by strain fields. For Al-rich compositions (x > 0.41), a nanocrystalline wurtzite phase with 0001 texture forms, yielding ~22 GPa hardness. Micropillar compression of c-$Hf_{0.93}Al_{0.07}N_{1.15}$ confirmed brittle fracture along {110}<011> slip systems, reflecting superstructure-induced dislocation confinement.

These findings reveal a previously unrecognized mechanism of film nanostructuring in heavy-element sputtering: backscattered neutral atoms act as energetic sculptors, promoting coherent superstructure formation and enhanced mechanical performance. This insight extends beyond Hf–Al–N, providing a general framework for controlling nanostructure evolution in metastable nitrides through energetic neutral engineering.

4:40pm **MA2-1-TuA-10 From Grain Refinement to Precipitation Hardening: Si-Driven Microstructural Control in (Al,Mo,Ta,V,W)C Coatings**, *M.A. Altaf, Balint Hajas,* TU Wien, Austria; *Szilard Kolozsvári,* Plansee Composite Materials GmbH, Germany; *Tomasz Wojcik, Alexander Kirnbauer,* ***Paul Mayrhofer [paul.mayrhofer@tuwien.ac.at]***, TU Wien, Austria

High-entropy carbides (HECs) are emerging as promising candidates for extreme-environment applications due to their exceptional hardness and thermal resistance. This work investigates the influence of Si incorporation (0, 1, and 7 at%) on the microstructure, mechanical properties, and thermal stability of reactively sputtered (Al,Mo,Ta,V,W)C_y coatings. X-ray diffraction and transmission electron microscopy (TEM) confirm single-phase face-centered cubic structures for all compositions. Increasing Si content strongly refines the columnar grain morphology—from ~500 nm in the Si-free coating to ~20 nm in the 7 at% Si variant—and induces a pronounced (200) texture.

Upon annealing at elevated temperature, Si segregates to column boundaries and forms coherent nanoscale SiC precipitates, as evidenced by HAADF-STEM and EDS mapping. These precipitates act as effective barriers to boundary motion and dislocation activity, stabilizing the microstructure against coarsening. Mechanical testing shows very high as-deposited hardness values of 41 GPa (Si-free), 39 GPa (1 at% Si), and 41 GPa (7 at% Si). After annealing, all coatings retain excellent mechanical performance, with the Si-rich variants exhibiting minimal hardness reduction.

These results demonstrate that controlled Si addition enables precipitation-driven microstructural stabilization in HECs through strong carbide-forming enthalpies and multi-element chemical/size mismatch—rather than configurational-entropy effects. This mechanism provides a robust pathway for designing thermally stable, ultrahard ceramic coatings for demanding applications such as aerospace, energy, and high-temperature manufacturing environments.

5:00pm **MA2-1-TuA-11 Influence of Interlayers on Thermal Stability and Abnormal Grain Growth in Co-Sputtered Nanotwinned Cu–Ag Alloy Thin Films**, ***Ding-Peng Lin [teddy910106@gmail.com]***, *Yu-Lin Liao, Fan-yi Ouyang,* National Tsing Hua University, Taiwan

As electronic and power devices operate under increasingly high temperatures and voltages, bonding and interconnect materials must exhibit superior thermal stability and reliability. Silver-based nano-twinned films provide excellent electrical and thermal conductivity but are prone to abnormal grain growth during annealing, which degrades performance. This study investigates the effect of titanium (Ti) and tantalum (Ta) interlayers on the thermal stability and grain growth behavior of co-sputtered nano-twinned Cu–Ag alloy thin films during annealing. All films were deposited by magnetron co-sputtering and annealed at 200 °C, 300 °C, 400 °C, 500 °C, and 600 °C for 1, 24, and 48 hours under a vacuum of 5.5 mTorr. In the Ti-interlayer samples, the nano-twinned structure remained stable up to 400 °C for 1 hour but disappeared after prolonged annealing due to abnormal grain growth and texture transition. In contrast, the Ta-interlayer samples preserved a stable nano-twinned (111) structure even after annealing at 400 °C for 48 hours and 500 °C for 1 hour. The Cu–Ag alloy films with Ta interlayers also retained higher hardness and lower resistivity after annealing, indicating reduced interdiffusion and structural degradation. These results demonstrate that Ta effectively enhances the thermal and microstructural stability of nano-twinned Cu–Ag alloy thin films, establishing it as a superior diffusion barrier for high-temperature interconnect applications in next-generation power and electronic devices.

Protective and High-temperature Coatings
Room Palm 3-4 - Session MA3-2-TuA

High Entropy and Other Multi-principal-element Materials II

Moderators: Alexander Kirnbauer, TU Wien, Austria, **Pavel Soucek**, Masaryk University, Czechia

1:40pm **MA3-2-TuA-1 On the Structure and Properties of Refractory-Metal-Based High-Entropy Metal-Sublattice Ceramics***, **Alexander Kirnbauer [alexander.kirnbauer@tuwien.ac.at]**,* TU Wien, Thin Film Materials Science Division, Austria **INVITED**

The development of materials that can withstand high thermal and mechanical loads is in focus of many materials' science activities. In recent years high-entropy materials gained attraction of many researchers due to their vast compositional possibilities and therefore tuneable properties for many applications.

Here we show the beneficial effect of the high-entropy concept applied to several thin film material systems including borides, carbides, nitrides, and oxides. All the investigated coatings are based on refractory metals, including Cr, Hf, Nb, Ta, Ti, V, W, and Zr. The study focuses on the preparation by physical vapor deposition, their thermal stability and mechanical properties. All coatings investigated are comparably insensitive to the change of deposition parameters, such as reactive gas flow and bias potential. Additionally, they exhibit outstanding thermal stability and significantly retarded decomposition and softening processes, outperforming their commonly used binary or ternary constituents. Furthermore, we recently investigated the influence of He-ion irradiation on the mechanical properties of borides, carbides, and nitrides having the same metal sublattice. The results show that these coatings, if optimized regarding their structure, are possible materials to protect bulk materials from degradation due to the implantation of He.

2:20pm **MA3-2-TuA-3 Influence of Nitrogen Contents on the Microstructure, Mechanical, and Electrochemical Behaviors of AlCrNbSiTiMoNx high entropy alloy films deposited by HiPIMS***, **CHANG-YI JIANG [a910225y@gmail.com]**,* Department of Materials Engineering Ming Chi University of Technology, Taiwan*; Chia-Lin Li,* Center for Plasma and Thin Film Technologies, Taiwan*; Bih-Show Lou,* Chemistry Division, Center for General Education, Chang Gung University, Taiwan*; Jyh-Wei Lee,* Department of Materials Engineering Ming Chi University of Technology, Taiwan

High entropy alloy (HEA) films have attracted significant attention for applications in harsh environments due to their outstanding mechanical strength and excellent corrosion protection. In our earlier research, the increasing amount of Mo in the AlCrNbSiTiMo thin films can increase the hardness and significantly improve the corrosion resistance of thin films in harsh corrosive environments. Previous studies have demonstrated that nitrogen addition can significantly enhance the mechanical performance of HEA films effectively. In this study, AlCrNbSiTiMoNx HEA films with different nitrogen concentrations were deposited on silicon wafers, AISI 420, and 304 stainless steel substrates using a high power impulse magnetron sputtering (HiPIMS) system. The AlCrNbSiTiMoNx HEA films without nitrogen content exhibited a body-centered cubic (BCC) phase structure, while those with nitrogen contents between 15 and 26.3 at.% showed an amorphous structure. As the nitrogen content increased to 33.0 and 36.3 at.%, the films transformed into a face-centered cubic (FCC) nitride phase. Mechanical characterization revealed that the 36.3 at.% contained thin film achieved the highest hardness of 27.5 GPa. Potentiodynamic polarization tests demonstrated that the thin film with 33.0 at.% nitrogen exhibited a superior corrosion resistance, which is 319.3 times greater than that of 304 stainless steel. These findings indicate that AlCrNbSiTiMoNx HEA films possess excellent mechanical strength and corrosion resistance, underscoring their potential applications in harsh corrosive environments. The research provides valuable insights into the relationship between nitrogen content and the structural, mechanical, and electrochemical properties of AlCrNbSiTiMoNx HEA films.

KEYWORDS: (AlCrNbSiTiMo)Nx high entropy alloy thin films, high power impulse magnetron sputtering, mechanical properties, corrosion resistance

2:40pm **MA3-2-TuA-4 Development of CrMoNbWTi and CrMoNbTiWC high entropy alloy films by HiPIMS: effect of Ti and C contents***, Han-Chieh Chen, Chia-Lin Li, Bih-Show Lou,* ***Jyh-Wei Lee [jefflee@mail.mcut.edu.tw]**,* Ming Chi University of Technology, Taiwan

High entropy alloys (HEAs) and multicomponent alloys (MCAs) were first proposed independently by Professor Jien-Wei Yeh and Professor Brian Cantor in 2004. Since then, the research on HEAs and MCAs has been widely explored because of their unique properties, such as good mechanical strength and excellent corrosion resistance. Among the fabrication of HEAs, the HEA thin films have been studied extensively. In this work, we fabricated two series of HEA thin films. In the first series, CrMoNbW and Ti targets were co-sputtered using high power impulse magnetron sputtering (HiPIMS) technique to fabricate CrMoNbWTi films with different Ti contents ranging from 0 to 15.69 at.%. All CrMoNbWTi films exhibited a BCC structure. The 15.69 at.% Ti contained CrMoNbWTi film deposited at a Ti target power of 400 W showed excellent wear resistance, achieving a low wear rate of 1.3×10^{-6} $mm^3/N\cdot m$.

In the second series, CrMoNbTiWC thin films were fabricated using the same Ti target power of 400 W and with varying carbon contents via a plasma emission monitoring (PEM) feedback control by a HiPIMS deposition system. With increasing carbon content, the CrMoNbTiWC thin film structure transitioned from BCC to FCC and then to amorphous. Wear tests revealed that the T80 film, containing 83.1 at.% carbon, exhibited the lowest friction coefficient (COF = 0.16) and a lower wear rate of 2.1×10^{-7} $mm^3/N\cdot m$, demonstrating excellent wear resistance. Corrosion tests showed that the T20 film with 36.5 at.% carbon had superior corrosion resistance in 0.5 M H_2SO_4 (~1,500 times higher than 304SS), and in 3.5 wt.% NaCl (~33 times higher than 304SS). The detailed microstructure, mechanical, and corrosion properties of CrMoNbWTi and CrMoNbTiWC films with different Ti contents and varying carbon contents are comprehensively investigated in this study.

3:00pm **MA3-2-TuA-5 Synthesis and Characterization of Amorphous CrCuTaTiV High-Entropy Thin Films: The Role of Sputter Yield in Custom Target Design***, Uriel Cárdenas-Rojas,* ***Sandra E. Rodil [srodil@unam.mx]**, Carlos Ramos-Vilchis,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México

High-Entropy Alloys (HEAs) are a class of materials with exceptional properties driven by their high-entropy stabilized atomic structures. Since their introduction in 2004, HEAs have gained widespread attention because of their compositional versatility, which allows for designing materials with tailored properties for various applications. Thin film synthesis, especially through magnetron sputtering, is a powerful method for exploring new HEA compositions and coatings.

This work presents the synthesis and characterization of a new quinary HEA system, CrCuTaTiV, deposited as thin films using a single, custom-designed sputtering target. The target was created by combining five pure-element sectors, with each sector's area calculated based on its reported sputter yield to account for differences and achieve an equiatomic composition in the resulting film. Films were deposited at room temperature via DC magnetron sputtering with varying deposition times and powers (100, 200, and 300 W) to systematically examine how these parameters and sputter yields influence the final film composition and structure.

Comprehensive analysis confirms that all CrCuTaTiV coatings produced were amorphous. Compositional data showed that, despite the custom target design, the films had non-uniform compositions. Early in deposition, the composition was mainly affected by the element with the largest target area. Over longer deposition times, the composition became more uniform, settling at around 17-18 at% for Cr, Ti, and V, while Cu and Ta ranged from 20-30 at% (with some uncertainty due to Cu-Ta signal overlap). X-ray Photoelectron Spectroscopy (XPS) revealed the films had low oxygen content and retained a metallic nature, though surface analysis indicated a lower Cu presence and Ta enrichment at the very surface. These results provide important insights into the complex relationship between target design, deposition process, and compositional control in multi-element thin films.

4:00pm **MA3-2-TuA-8 Combinatorial Approach for the Synthesis of High-Entropy-Like Protective Nitride Coatings for Highly Aggressive Tribo-Corrosion Applications***, **Etienne Bousser [etienne.bousser@polymtl.ca]**, Olayinka Abegunde, Fellipy S. Rocha, Pedro Avila, Ludvik Martinu, Jolanta Ewa Klemberg-Sapieha,* Polytechnique Montréal, Canada

High-entropy alloys (HEAs) and high-entropy nitrides (HENs) have attracted increasing attention as protective coatings for demanding tribological and corrosive environments due to their high entropy, lattice distortion, and sluggish distortion effect. Compared to conventional transition-metal nitrides, HEN coatings can exhibit superior hardness–toughness, reduced wear, low friction coefficients, and enhanced corrosion resistance.

In this study, CrZrSiTiN coatings were deposited using a combinatorial magnetron sputtering process, generating a controlled compositional gradient across nine Ti6Al4V substrate samples deposited simultaneously. The depositions were carried out under a constant substrate bias, and a chromium sublayer was pre-sputtered to improve coating adhesion. The nitrogen flow rate was optimized to achieve a near-stoichiometric metal–nitrogen ratio (~1:1) characteristic of NaCl-type crystal structure nitride films.

Nanoindentation showed hardness values ranging from ~17 to 31 GPa and reduced moduli between ~138 and 282 GPa, depending on film composition. Tribo-corrosion testing in 1 M H_2SO_4 at open circuit potential (OCP) demonstrated that the most wear-resistant samples also exhibited the lowest coefficients of friction (~0.2), while sustaining the highest positive open circuit potentials (> 0.2 V) during sliding. Chromium-rich coatings with intermediate to low Si content, and reduced Ti and Zr concentrations outperformed the other compositions in terms of both wear and corrosion resistance. Wear volume analysis using optical profilometry revealed that all coatings significantly reduced wear compared to bare Ti6Al4V (by up to 260 times better), with the lowest wear rate of 1.3 x 10^{-6} $mm^3/N \cdot m$.

XRD revealed peak broadening, peak shifts, and texture variations, indicating lattice distortion, small grain size, and partial amorphization. Amorphized TiCrSiZrN coatings exhibited the best wear resistance and the highest recorded OCP values during and after wear. Samples with a dominant FCC (220) texture showed the second-best tribo-corrosion performance, whereas those with a dominant FCC (200) texture exhibited comparatively lower performance, but still significantly better than the bare substrate.

In conclusion, elemental composition plays a significant role in determining the preferred crystallographic texture of multi-element nitride coatings, which in turn governs tribo-corrosion performance. Lower concentrations of strong nitride-forming elements (e.g., Ti and Zr), combined with higher Cr content and adequate Si content, promote an amorphized microstructure with excellent wear and tribo-corrosion resistance.

Tribology and Mechanics of Coatings and Surfaces
Room Palm 5-6 - Session MC2-1-TuA

Mechanical Properties and Adhesion

Moderators: **Chia-Lin Li**, Ming Chi University of Technology, Taiwan , **Michael Meindlhumer**, Montanuniversität Leoben, Austria, **Balila Nagamani Jaya**, Indian Institute of Technology, India

1:40pm **MC2-1-TuA-1 Mechanical and Interfacial Behavior of Liquid-Like Polymer Surfaces at Extremes***, **Megan J. Cordill [megan.cordill@oeaw.ac.at]**,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria **INVITED**

Ice buildup presents significant obstacles for both power generation and air transportation in cold regions requiring effective ice protection strategies. Passive anti-icing methods, such as icephobic coatings have garnered increasing interest due to their cost-effectiveness and eco-friendliness. Effective passive ice removal requires very low ice adhesion strength values of less than 20 kPa so that the ice can be easily removed with natural forces such as wind and gravity. Recent studies have shown that liquid-like surfaces (LLS) with ice-shedding properties can be generated through the covalent attachment of linear polymer chains onto smooth substrates bearing sufficiently high hydroxyl group densities. The durable coating retains its slippery properties after exposure to laboratory conditions of icing/deicing and heating cycles, organic solvents, and acid treatment. However, little is known about mechanical stability and longevity of the LLS at relevant temperatures and wind speeds. Nanoindentation, both traditional and AFM-indentation, was used to measure the mechanical properties at various temperatures to establish a ductile to brittle transition of the coating. Additionally, scratch and wear testing were utilized to mimic scratch induced debris and removal of the LLS. As a final check, bulge testing was used to evaluate the adhesion of the ice-phobic coating to the aluminum substrate. These experiments were then compared to the same coatings subjected to various ice and wind tunnel experiments performed on a NACA 0012 aerofoil that would simulate actual conditions during take-off and landing. The combination of assessments demonstrates that the developed LLS coating is robust for wind turbine applications as well as to replace anti-icing fluids currently used for airplanes.

2:20pm **MC2-1-TuA-3 In Situ Observation of Multicracking in Thin Films and Nanostructures***, **Damien Faurie [faurie@univ-paris13.fr]**,* Université Sorbonne Paris Nord, France **INVITED**

Multicracking in brittle thin films on compliant substrates is a critical reliability issue in flexible electronics, optical coatings, and protective thin-film technologies. While characteristic fracture patterns have been reported for decades, the fundamental mechanisms governing crack initiation, spacing, and multiplication still remain unclear. Classical models link average crack spacing to film thickness, yet they do not account for the local stress heterogeneity and accumulation of damage that precede fracture.In this invited talk, we present an *in situ* experimental methodology that combines synchrotron X-ray diffraction with real-time optical imaging during controlled uniaxial and biaxial mechanical loading of brittle thin films (10–500 nm) supported on polymer substrates. This approach enables the simultaneous monitoring of stress evolution, diffraction peak broadening (FWHM), and crack nucleation. We show that variations in FWHM provide a quantitative diffraction signature of local stress concentration and correlate directly with the onset and multiplication of cracks. This establishes a direct link between microscopic stress heterogeneity and the formation of multicracking networks.Looking forward, we extend this methodology to lithographically patterned thin films, where periodic architectures (e.g., parallel wires, modulated-width structures, multilayered or architectured interconnects) offer new degrees of freedom to tailor stress distribution and confinement effects during deformation. We will discuss how such artificial architectures can promote or suppress crack formation, enable stress redistribution, and ultimately improve thin-film reliability.Overall, this work provides a new framework to understand and engineer multicracking in thin films and opens pathways toward mechanically robust architectured coatings and interconnects for next-generation flexible technologies.

3:00pm **MC2-1-TuA-5 Numerical and Experimental Evaluation of Cyclic Contact Loads on Titanium Borides***, Hugo Alberto Pérez Terán, GERMAN ANIBAL RODRIGUEZ CASTRO, ALFONSO MENESES AMADOR, **Felipe Nava Leana [felnaval@gmail.com]**,* Instituto Politécnico Nacional, Mexico*; Daybelis Fernández Valdés,* Tecnológico Nacional de México*; VICTOR MANUEL ARAUJO MONSALVO,* Instituto Nacional de Rehabilitación Luis Guillermo Ibarra Ibarra, Mexico

In this work a Ti6Al4V alloy hardened by the boriding process was evaluated by cyclic contact loads. Powder-pack boriding process was used to modify the alloy surface where two phases TiB and TiB_2 were obtained on the sample due to the boron diffusion into the substrate material. The thermochemical treatment was carried out at a temperature of 1100°C for 10, 15 and 20 h of exposure time. Titanium borides (TiB and TiB_2) formed on the surface of the Ti6Al4V alloy was confirmed by means of the XRD analysis.Berkovich nanoindentation test was conducted to determine both hardness and Young's modulus of the borided samples. Cyclic contact loads were applied on the borided sample using a MTS Acumen equipment to evaluate the quality of the titanium borides based on the damage caused on the sample surface. Finite element method was used to obtain the stress field due to cyclic contact loads. Results showed that the sample with thicker thickness because of longer treatment time showed the best mechanical behavior under cyclic contact loads.

4:00pm **MC2-1-TuA-8 Grain Boundaries and "Complexions" in Metallic Thin Films: New Insights on the Interplay of Atomic Structure, Chemistry and Material Properties***, **Gerhard Dehm [dehm@mpi-susmat.de]**,* Max Planck Institute for Sustainable Materials, Germany **INVITED**

Similar to surface reconstructions, grain boundaries in polycrystalline materials can undergo phase transformations (sometimes referred to as "complexion" in the literature), which alter the resulting properties. Temperature, stress, and chemical composition are the main driving forces for such transformations. Understanding and controlling such transformations allows additional control over the relationships between structure, processing, properties, and performance, especially in materials with a high content of grain boundaries.

The first part of the presentation shows examples of grain boundary phases and transitions in pure and alloyed metallic thin films. Surprisingly, grain boundary phase transitions are observed even in pure metals. The second part of the presentation focuses on electrical and mechanical properties. A workflow is presented that allows to investigate the contribution of individual grain boundary structures to electrical resistivity. The results show that the excess volume of a grain boundary is the main contributor to electron scattering in a pure fcc metal such as copper. However, impurities segregated at the grain boundary can significantly alter electron transport. This can be exploited positively, but can also be detrimental, as exemplified with two examples.

Also mechanical properties are strongly influenced by grain boundaries and their phases. While this has long been known for cases of grain boundary embrittlement, such as Bi in Cu or Ga in Al, the influence on strength and shear-coupled grain boundary motion has only recently been studied in detail and will be presented in the lecture. Finally, strategies to make use of grain boundary “complexions” for property design are discussed.

Acknowledgment: This work gas been partially supported by the ERC advanced grant GB-Correlate (Correlating the State and Properties of Grain Boundaries [https://www.mpie.de/3893203/GB-correlate]) and the German Science Foundation DFG within the SFB 1394 Structural and chemical atomic complexity – from defect phase diagrams to material properties. Fruitful interactions with many colleagues, especially T. Brink, C. Liebscher, L. Langenohl, K. Bhat, A. Kanjilal, J. Duarte, and H. Bishara are gratefully acknowledged.

4:40pm **MC2-1-TuA-10 Many-to-one Mapping Between Stress-Strain Curves and Spherical Indentation Load-Displacement Curves***, **Santosh Thapa [sth230@g.uky.edu]**, Yang-Tse Cheng, Madhav Baral,* University of Kentucky, USA

The stress-strain relationship is key to understanding material behavior, yet conventional tensile testing provides only bulk-averaged properties and fails to capture local heterogeneities. Instrumented indentation testing (IIT), particularly with spherical indenter, is often assumed capable of uniquely determining stress-strain relationships from a single load-displacement curve. However, our results challenge this assumption showing that different combinations of elastic modulus, yield stress, and work-hardening exponent can produce indistinguishable indentation responses, highlighting the non-uniqueness of the inverse problem of obtaining stress-strain relation from spherical indentation load-displacement curves. Thus, the quest for obtaining local mechanical properties from spherical indentation measurements continues.

5:00pm **MC2-1-TuA-11 Tribological Performance and Mechanistic Insights of Aluminium-Sic Composites Fabricated by Computerized Bottom-Pouring Stir Casting***, Vishal Mehta,* Automobile Engineering Department, Parul Institute of Technology, India*; **Anand Joshi [anandyjoshi@gmail.com]**,* Micro Nano Research and Development Center, Parul University, India*; Unnati Joshi,* 3Mechanical Engineering Department, Parul Institute of Engineering & Technology, India

The growing demand of lightweight structural material with enhanced wear resistance has accelerated the study of aluminium based metal matrix composites that are reinforced using ceramic particulates. The composites in the present research were Aluminium-Silicon Carbide (Al-SiC) produced by computerized bottom pouring type stir casting, which has a high level of control on the process parameters giving accurate dispersion of reinforcement and fewer defects in the casting. This work is devoted to the evaluation of the friction and wear properties of the developed composites in the dry sliding mode and to determine the prevalent wear mechanisms by means of the surface and compositional analyses.

In the present investigation, pure aluminium (Al) was considered as a matrix material due to easy availability. Pure Al was reinforced with 5 wt.% SiC having size of 40-50 microns. Rockwell hardness of the developed AMCs were measured and 13% higher values were observed as compared to unreinforced matrix. The pin-on-disc tribometer was used for a tribological test in wet conditions. The Al-SiC AMCs were found to have a significant decrease in the coefficient of friction and wear rate with those of the unreinforced aluminium matrix. The ability of the SiC particles to prevent direct contact between metal and metal contributed to the increased performance and was attributed to the bearing role of the particles. The smoother worn surfaces and reduced scars of adhesive wear were observed post-test SEM analysis, whereas the EDX spectra proved the absence of intermetallic Al_4C_3 in the developed composite with C/Al mass ratio value of ~0.176 referring to theoretical stoichiometric value for Al_4C_3 (~0.334). The EDS result confirms the defect free AMC development for the further applications. The wear mechanisms observed in SEM characterization indicates transition from adhesive wear in the base alloy to mild abrasive and oxidative wear in the reinforced composites.

These findings suggest that computerized bottom-pouring stir casting provides both an effective and quality production pathway to high-integrity Al-SiC AMCs with improved friction and wear properties and therefore promising in surface engineering, tribological finishes and other lightweight component applications.

Keywords

Aluminium matrix composites, Friction and wear, SEM, EDX, Stir casting, Tribology

Surface Engineering of Biomaterials, Devices and Regenerative Materials: Health, Food, and Agriculture Applications
Room Town & Country B - Session MD2-1-TuA

Coatings and Sensors for Health, Food and Agriculture: Antibacterial, Bioactive, and Flexible Interfaces I

Moderators: Diego Mantovani, Université Laval, Canada, **Phaedra Silva-Bermudez**, Instituto Nacional de Rehabilitación Luis Guillermo Ibarra Ibarra, Mexico

1:40pm **MD2-1-TuA-1 Deposition and Surface Characterization of Low-Pressure Plasma Ultra-Thin Coatings Designed for Biomedical Applications***, **Laurent Houssiau [laurent.houssiau@unamur.be]**,* University of Namur, Belgium **INVITED**

Our research group combines expertise in surface characterization techniques, namely X-ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), with low-pressure plasma deposition of thin films and nanoparticles. This approach enables projects across diverse fields, including biomaterials, biosensing, tissue imaging, hybrid materials, adhesion, and cultural heritage. In this presentation, we will focus on the deposition and characterization of ultra-thin (<100 nm) films that impart new functionalities to substrate materials.

We will first present our work on gradient coatings for dental implants, designed to promote osseointegration while providing antibacterial properties. These coatings are deposited on Ti-6Al-4V (Ti64) alloys using Plasma-Enhanced Chemical Vapor Deposition (PECVD) from a titanium-containing organometallic precursor (titanium isopropoxide) injected in gas phase with argon and oxygen. By gradually decreasing the oxygen flow during the deposition, a compositional gradient is created, from an inorganic TiO_2-like layer at the implant interface to a more organic TiO_xC_y layer near the bone interface, ensuring a smooth transition between the metallic implant and bone tissue. A final magnetron sputtering step, within the same plasma chamber, introduces ZnO nanoparticles into the top TiO_xC_y layer, enhancing antibacterial activity. Depth profiling by XPS and ToF-SIMS confirms the compositional gradient and nanoparticle deposition.

We will then highlight our collaboration with Prof. Mantovani’s group at Université Laval on plasma-deposited diamond-like carbon (DLC) and fluorocarbon coatings. Here, XPS and ToF-SIMS have been instrumental in elucidating coating quality, composition, and behavior under various conditions.

Finally, we will present recent research on graphene-based biosensors—an application that also integrates plasma modification and surface analysis for biomedical use. As a proof of concept, the biotin–streptavidin interaction was employed. Graphene layers were amine-functionalized by plasma polymerization, followed by biotin grafting, with XPS monitoring each surface modification step. Electrical I–V measurements revealed a Dirac point shift correlated with streptavidin concentration, demonstrating detection capabilities down to 0.1 nM.

2:20pm **MD2-1-TuA-3 Silver-Copper Nanocoating (Sakcu®) Deposited on Stainless Steel Brackets to Reduce Biofilm Formation of *Streptococcus Mutans* and Potentially Prevent Early Dental Caries***, **Alejandra Cervantes-Ramírez [aleebathory1@gmail.com]**, Lorena Reyes-Carmona, David Eduardo Martínez-Lara, Andrea Quiroz-Cervantes, Gina Prado-Prone, Sandra E. Rodil, Argelia Almaguer-Flores,* UNAM, Mexico

Introduction: Dental brackets facilitate the accumulation of bacteria during orthodontic treatments, favoring the biofilm formation of bacteria that produce organic acids, such as *Streptococcus mutans* (*S. mutans*). This bacterium can lead to enamel demineralization and cavity development. Therefore, creating antibiofilm devices can significantly contribute to preventing early-stage cavities during orthodontic treatments.

Objective: To deposit the Ag-Cu nanocoating (SakCu®) on conventional metallic brackets and evaluate its capacity to reduce the biofilm formation of the cariogenic strain *S. mutans.*

Methods: The deposition of the Ag-Cu nanocoating on stainless steel brackets (American Orthodontics®) was carried out using the magnetron sputtering technique. The micro-morphology and chemical composition of the coated and uncoated bracket surfaces were evaluated using scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS), respectively. The *in vitro* antibiofilm effect of surfaces was assessed by Alamar blue kit and the counting of colony-forming units (CFU) assay using *S. mutans* (ATCC 25175). The evaluation was conducted after 1, 3, and 7 days of incubation under anaerobic conditions. Qualitative observation of bacterial adhesion on the surfaces was performed using SEM.

Results: The stainless-steel surface of the orthodontic brackets was coated with a uniform nanolayer of silver and copper without significantly changing their surface morphology. The microbiological results showed that the Ag-Cu nanocoating reduced the biofilm formation of *S. mutans*, especially at the initial incubation times (55% on day 1 and 85% on day 3), compared to the biofilm formed on the surface of brackets without the nanocoating.

Conclusion: The SakCu® nanocoating on orthodontic brackets reduced biofilm formation of the cariogenic *S. mutans* strain, especially during early contact periods. This suggests that the Ag-Cu nanocoating can potentially prevent biofilm formation on orthodontic devices and the development of initial caries, thereby improving treatment and rehabilitation in the mid-term.

Acknowledgments: Financial support of UNAM-PAPIIT # IT207824, # TA10424and SECTEI #159, projects.

2:40pm **MD2-1-TuA-4 ZnO Nanowires: A Platform for Biosensing Applications**, *Rafael Salinas, Shirlley Martínez, Guillermo Santana Rodriguez, Carlos Ramos,* ***Ateet Dutt [adutt@iim.unam.mx]***, UNAM, Mexico **INVITED**

Our research focuses on the design and characterization of advanced nanomaterials, particularly hybrid gold–zinc oxide (Au–ZnO) nanowires, for chemical and biosensing applications. We investigate how variations in size, morphology, and composition influence their structural and functional performance. The synergistic combination of Au and ZnO imparts these nanowires with distinctive physicochemical properties, enabling the creation of highly sensitive and efficient sensing platforms.

In one study, we developed one-dimensional ZnO nanowire-based systems for the rapid detection of cancer biomarkers, demonstrating precise photoluminescent signal generation through the integration of nanoscale receptors. Furthermore, we achieved tunable photoluminescence responses across analyte concentrations ranging from 1×10^2 to 1×10^8 CFU mL^{-1}, allowing direct visualization of targeted bacterial cells on ZnO nanowire surfaces.

This contact-based nano-biosensing approach enables real-time detection while substantially reducing both processing and response times—an essential advantage for rapid pathogen identification in critical scenarios. By deepening our understanding and control of these hybrid nanostructures, we aim to advance their practical implementation in clinical diagnostics and broader biomedical technologies.

4:00pm **MD2-1-TuA-8 Photoresponsive Bilayer Coating Integrating Zinc and a Chitosan-Antibiotic Drug Delivery Film for on-Demand Antimicrobial Photodynamic Therapy in Biomedical Implants**, ***Samuel Santana Malheiros [samuelsmalheiros@gmail.com]***[1], *Maria Helena Rossy Borges,* University of Campinas (UNICAMP), Brazil; *João Gabriel Silva Souza,* UnG, Brazil; *Elidiane Cipriano Rangel,* UNESP, Brazil; *Carlos Fortulan,* University of São Paulo, Brazil; *Nilson Cristino da Cruz,* UNESP, Brazil; *Eduardo Buozi Moffa,* University of Saskatchewan, Canada; *Bruna Egumi Nagay, Valentim Adelino Ricardo Barão,* University of Campinas (UNICAMP), Brazil

Despite significant advances in surface treatments, failures of biomedical implants due to bacterial colonization, wear and insufficient bioactivity remain persistent clinical challenges. Here, we engineered a light-responsive antimicrobial bilayer coating for titanium implants consisting of: (i) an inner porous oxide layer doped with bioactive elements Ca, P, and Zn produced by plasma electrolytic oxidation (PEO) and covered by (ii) an outer biodegradable chitosan (CS) thin film for controlled delivery of the photosensitive antibiotic demeclocycline (DMC), enabling antimicrobial photodynamic therapy, a light-activated process where a photosensitizer produces reactive oxygen species (ROS) to eliminate microorganisms. After preparation, samples underwent morphological, physical, chemical, optical, crystallinity, and tribological characterization. Coating's photo-responsiveness was indirectly assessed via methylene-blue degradation under illuminated and dark conditions. Antimicrobial performance was tested under illuminated and dark conditions using a 96-hour polymicrobial biofilm model (human saliva as inoculum). Bioactivity was assessed by hydroxyapatite formation, proteomic analysis of the adsorbed proteins from human blood, and cytocompatibility with pre-osteoblastic cells. Regarding results, PEO generated a moderately rough, porous oxide layer (Ra ≈ 1 µm) composed of calcium, phosphorus, and zinc oxide, partially covered by the CS film, which reduced roughness to Ra ≈ 0.6 µm while maintaining hydrophilic behavior (contact angle < 40°). CS and DMC incorporation was confirmed by EDS, FTIR, and XPS analyses and UV–Vis spectroscopy attested DMC's photoactive absorption within the visible light wavelength spectra (Soret band ~450 nm). XRD confirmed high crystallinity of the PEO inner oxide layer which imparted mechanical robustness under tribological loading, while the outer polymeric film provided a cushion effect evidenced by the lowest friction coefficient, minimal mass loss, and preservation of the inner layer morphology. Upon light irradiation, photoexcited DMC generated ROS, leading to > 3-$\log_{10}$ reductions in biofilm viability and > 50% decreases in metabolic activity, dry mass, and protein content, along with favorable shifts in microbial community composition. Beneficial protein adsorption profiles, enhanced hydroxyapatite formation, and cytocompatibility confirmed the coating's bioactive potential. Overall, the developed smart light-responsive coating unites ROS-mediated antimicrobial action on-demand, wear protection, and bioactivity in an industry-scalable platform, with potential to enhance biomedical implants longevity and reliability.

4:20pm **MD2-1-TuA-9 Electrospun Nanocomposite Membranes for the Development of Osteoinductive Microambients**, ***Phaedra Silva-Bermudez [pssilva@inr.gob.mx]***, *Julieta García-López,* Unidad de Ingeniería de Tejidos, Terapia Celular y Medicina Regenerativa; Instituto Nacional de Rehabilitación Luis Guillermo Ibarra Ibarra, Mexico; *Gina Prado-Prone,* Laboratorio de Biointerfases, DEPeI, Facultad de Odontología, Universidad Nacional Autónoma de México; *Monserrat Ramirez-Arellano, Gustavo E. Martínez-Murillo,* Unidad de Ingeniería de Tejidos, Terapia Celular y Medicina Regenerativa; Instituto Nacional de Rehabilitación Luis Guillermo Ibarra Ibarra, Mexico; *Lucia S. Flores-Hidalgo,* Posgrado en Ciencia e Ingeniería de Materiales, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México; *Sandra E. Rodil,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México

Displaced, particularly open fractures, represent a significant clinical challenge due to their complexity, variability andhigh complication rate, predominantly due to infections and delayed bone healing rates. In Mexico, approximately 50,000 cases occur annually, with infection rates reaching up to 10%, which is notably higher than those reported in developed countries. Given this concern, there is a growing interest for developing biomedical materials capable of promoting bone regeneration while minimizing infection risk.

Electrospinning is a versatile technique that enables the fabrication of polymeric nanofibrous membranes with high porosity, conformability, and suitable for controlled drug release and degradation. Recently, nanomaterials have attracted significant interest to develop composite materials with specific biofunctionalities. In particular, magnesium oxide nanoparticles (MgONPs) have demonstrated osteogenic properties by promoting cellular proliferation and differentiation towards the osteoblastic phenotype.

Thus, the aim of the present project is to develop composite (polycaprolactone, type B gelatin and MgONPs) membranes capable of thriving an appropriate microambient at the site of the bone fracture, aiming to contribute to increase osteogenesis and decrease bacterial infection. Membranes were fabricated via electrospinning based on polycaprolactone (PCL) and gelatin (Gel), and incorporated with MgO NPs at different concentrations (2, 5, and 7 wt%). Their micro-morphology, chemical composition, wettability, and mechanical properties were examined using SEM, EDS, FTIR, WCA, TGA, DSC and tension tests. The biocompatibility and osteoinductive capability of the membranes was assessed using human bone marrow-derived mesenchymal stem cells (BM-MSCs). Cell viability was assessed after 24 h exposure to membrane lixiviates (MTT assay), and after 24 and 72 h of cells directly cultured on the membranes surfaces (calcein/ethidium homodimer assay). The osteoinductive potential of the membranes was evaluated by assessing the osteogenic differentiation of BM-MSC in contact with membranes lixiviates, by using Alizarin Red staining and immunofluorescence assays against collagen Type I, Osteocalcin and Osteopontin.

[1] **Graduate Student Award Finalist**

The nanocomposite membranes exhibited a microfibrillar-porous structure, and appropriate wettability and mechanical properties for clinical use. The cytocompatibility and osteoinductive effects were dependent on the MgO NPs concentration, with higher NPs concentration increasing cell differentiation towards the osteoblastic phenotype.

Topical Symposium on Sustainable Surface Engineering
Room Town & Country C - Session TS3-TuA

Circular Strategies for Surface Engineering

Moderators: Marcus Hans, RWTH Aachen University, Germany, **Arnaud Le Febvrier**, Uppsala University, Sweden

1:40pm **TS3-TuA-1 Rethinking Resources: Circular Strategies in Target Material Production*, Lukas Zauner [l.za@rhp.at]*,** *Marie Friedl, Laszlo Sajti, Mariangela Fedel, Emanuel Feuerstein, Michael Kitzmantel, Erich Neubauer,* RHP Technology, Austria **INVITED**

The continuing expansion of thin-film technologies across diverse industries is intensifying the demand for reliable supply chains of high-quality target materials. At the same time, targets are frequently manufactured from scarce, geopolitically restricted, precious or energy-intensive materials, rendering conventional extract–produce–dispose supply models increasingly unsustainable. In addition, technological limitations such as an inefficient utilization of sputter targets – often at levels of only 20-40% – necessitate process innovations and direct recycling strategies to retain valuable material of spent targets in a closed loop.

This presentation explores how innovative approaches contribute to enhancing circularity across the life-cycle of target materials, reduce environmental impacts and support stable supply. We evaluate powder-technological processes with respect to repurposing industrial waste into valuable target materials or the feasibility to directly recycle and re-use spent targets in the production process. Furthermore, efficiency improvements of geometry-driven target optimization through detailed magnetic field and erosion simulations are highlighted. Finally, we present conversion technologies such as laser-ablation-based nanoparticle formation as alternative processing routes for high-value scrap material.

Selected case studies from industry and research demonstrate both the technical and ecological potential of integrating circular strategies into target production, while maintaining stringent performance requirements for advanced thin-film applications. Together, these approaches underline that improving circularity is not only feasible and impactful for target materials, but also an important aspect to future-proof thin-film manufacturing against volatility in raw material supply and environmental constraints.

2:20pm **TS3-TuA-3 Opportunities of Combinatorial Thin Film Materials Design for the Sustainable Development of Magnesium-Based Alloys*, Marcus Hans [hans@mch.rwth-aachen.de]*,** RWTH Aachen University, Germany*; Philipp Keuter,* GTT-Technologies, Germany*; Aparna Saksena,* Max Planck Institute for Sustainable Materials, Germany*; Janis Sälker, Markus Momma,* RWTH Aachen University, Germany*; Hauke Springer,* Universität Duisburg-Essen, Germany*; Jakub Nowak, Daniela Zander,* RWTH Aachen University, Germany*; Daniel Primetzhofer,* Uppsala University, Sweden*; Jochen Schneider,* RWTH Aachen University, Germany

Magnesium-based lightweight structural materials exhibit potential for energy savings. However, the state-of-the-art quest for novel compositions with improved properties through conventional bulk metallurgy is time, energy, and material intensive. Here, the opportunities provided by combinatorial thin film materials design for the sustainable development of magnesium alloys are evaluated. To characterize the impurity level of (Mg,Ca) solid solution thin films within grains and grain boundaries, scanning transmission electron microscopy and atom probe tomography are correlatively employed. It is demonstrated that control of the microstructure enables impurity levels similar to bulk-processed alloys. In order to substantially reduce time, energy, and material requirements for the sustainable development of magnesium alloys, we propose a three-stage materials design strategy:

(1) Efficient and systematic investigation of composition-dependent phase formation by combinatorial film growth.

(2) Correlation of microstructural features and mechanical properties for selected composition ranges by rapid alloy prototyping.

(3) Establishment of synthesis–microstructure–property relationships by conventional bulk metallurgy.

2:40pm **TS3-TuA-4 Life Cycle Analysis for Next Generation Sustainable Flexible Food Packaging Materials*, Glen West [G.West@mmu.ac.uk]*,** Manchester Metropolitan University, UK **INVITED**

This work describes an extensive Life Cycle Analysis (LCA) study into the Product Life Cycle (PLC) of sustainable, recyclable, mono-material, flexible food packaging solutions for a circular economy. Comparison is drawn to existing, non-sustainable solutions. The LCA process, and in particular the establishment of life cycle inventory is discussed, drawing on primary source data and trial data from across the industry and comparing to published inventory data. The end of life of the packaging solutions will be evaluated against industry legislations and standards with improvements to be suggested.

A major aim of this work is to provide academia and industry an evaluation and best practice on how to undertake an LCA for packaging to address the overall lack of knowledge in this area.

4:00pm **TS3-TuA-8 Advanced Chemical and Environmental Design of Coatings: From TG-Mass Spectrometry Through Thermodynamic and Life Cycle Analysis Application*, Francisco Javier Perez Trujillo [fjperez@ucm.es]*,** Calle Cantalejo 11, Spain **INVITED**

The design of coatings for steam turbines have been based in the past on the testing different chemical compositions. In the recent years, the application of computational tools to predict most favorable chemical compositions have been applied. In this way the role of the themodynamic calculations to simulate the interaction at high pressure steam with alloy surfaces have been a successful tool to know the liquid, solid and gas phases formed in the equilibrium of the high temperature corrosion conditions. From those results the first approach of the chemical compositions of coatings have been done. Moreover, in order to validate the volatile oxyhidroxydes species formed, TG-Mass spectrometry have been applied in order to validate the computational results and to optimize the coatings compositions. At the end a LCA-Life Cycle Analysis have been perfomed in order to know the CO2-foot print and the environmental impact of the final coatings design. In order to know the combination of computational tools with experimental advanced characterization techniques, the application to uncoated and coated steels by metallic and ceramic coatings will be show.

4:40pm **TS3-TuA-10 Reversible Solid Oxide Cells for Hydrogen Production and Storage Developed by Reactive Magnetron Co-Sputtering*, Justyna Kulczyk-Malecka [j.kulczyk-malecka@mmu.ac.uk]*,** *Kleitos Panagi, David Shaw, Peter Kelly,* Manchester Metropolitan University, UK

Reversible solid oxide cells (RSOC) are promising technology for high-efficiency energy conversion and storage, enabling electrolysis and fuel cell operation within a single device. In this work, ultrathin (~1-3 μm) anode functional layers (AFL) were deposited using oblique angle reactive magnetron co-sputtering, enabling precise control over the cell microstructure at the nanoscale. The AFLs were deposited onto commercial YSZ electrolyte support cell and consisted of V-doped Ni/YSZ composite to reduced Ni content and its agglomeration during the long-term cycling, and therefore, to improve cell durability. The study shows that V-doped cells showed superior electrochemical performance relative to benchmark Ni/YSZ in fuel cell mode, delivering higher power densities under H_2-rich conditions. In electrolysis mode the cells sustained electrolysis current densities approaching 0.5 A cm^{-2} at 850°C under steam-rich conditions, exhibiting good polarisation behaviour without immediate voltage rise. During prolonged operation in high steam content (up to 90%) the cells demonstrated enhanced tolerance to high oxygen chemical potential and improved resistance to redox induced anode degradation.

The post-mortem analysis of RSOCs using FIB-SEM/EDS, TEM and XPS revelated that low vanadium contents promote homogeneous dopant distribution and stabilise the Ni/YSZ microstructure, whereas higher vanadium loadings promote surface enrichment and secondary phase formation associated with accelerated cell degradation. The key findings indicate that optimised microstructure and composition of the AFLs facilitate increased performance and durability presenting a promising pathway towards RSOCs for hydrogen generation, utilisation and storage.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Surface Engineering - Applied Research and Industrial Applications
Room Palm 1-2 - Session IA2-1-WeM
Surface Modification of Components in Automotive, Aerospace and Manufacturing Applications I

Moderators: Satish Dixit, Plasma Technology Inc., USA, **Tanifuji Shinichi**, Kobe Steel Ltd., Japan

8:00am **IA2-1-WeM-1 Micro-Impact Testing to Develop Multilayer Coating Systems with Enhanced Durability Under Cyclic High-Stress Contact***,* ***Ben Beake [ben@micromaterials.co.uk]****,* Micro Materials Ltd, UK*; Tomasz Liskiewicz,* Manchester Metropolitan University, UK*; Sam McMaster,* Anglia Ruskin University, UK*; Daniel Tobola,* Lukasiewicz, Poland*; Luis Isern, John Nicholls,* Cranfield University, UK*; Hannah Zhang, Mark Gee,* National Physical Laboratory, UK **INVITED**

The lifetime of components operating in harsh environments subjected to repetitive contacts in high performance manufacturing operations, gas turbines and automotive engines can be extended by the application of advanced multilayer coating systems. These coating systems need to combine high hardness with resistance to fracture. The cyclic nano- or micro-scale impact test has been shown to be a convenient test method to rank coating resistance to fracture, with coating performance in the test with typically a 1:1 correspondence to the application performance.

In this presentation we will provide an overview of the technique and describe several recent technical developments including (1) higher data acquisition for multi-metric analysis of every impact (2) inclined impact to combine shear and compression forces (3) impact at elevated temperature (4) spatially distributed impact, and show how these are being used in testing (i) thermal barrier coatings (TBCs) in gas turbines (ii) DLC coated steel components in automotive engines (iii) PVD coated steel and coated WC-Co cutting tools.

The multi-metric analysis reveals significantly more about the deformation and wear behaviour in the test than the impact depth alone, showing that in some cases the % dissipated energy in cyclic impact can act as an “early warning signal” for failure as it can be sensitive to the initiation and growth of sub-surface crack networks before crack coalescence and fracture occurs. To simulate applications where cyclic impact events are not perpendicular to the surface inclined impact tests have been performed which have, for example, revealed markedly different effects on the durability of DLC coatings and TBCs. Reasons for these differences will be discussed. To replicate the spatial distribution of multiple impacts that occur when a coated component is subjected to solid particle erosive wear the method has been adapted to produce controlled impacts at different statistically-distributed locations on the sample surface. Tests on the TBCs 7YSZ and gadolinium zirconate clearly showed that the spatially-distributed micro-impact test could replicate differences in erosion resistance and also reproduce the main damage mechanisms and surface morphology that occur.

8:40am **IA2-1-WeM-3 From Lab to Industry: Scaling Atmospheric Plasma Coatings for Metal Protection Against Corrosion***,* ***Daphne Pappas [daphne.pappas@plasmatreat.com]****,* Plasmatreat USA **INVITED**

Magnesium and aluminum alloys are extensively used in the automotive, aerospace and other industries due to their robustness, lightweight, and excellent weight-to-strength ratios. The manufacturing of lightweight structural components for aircraft and various types of vehicles leads to improved fuel efficiency and lower greenhouse gas emissions. However, long term exposure to moisture, pollution, salt and other harsh environments make them susceptible to corrosion. Common mitigation strategies involve surface treatments like ion implantation and protective coatings that can enhance the corrosion resistance of common metals.

In the first part of this talk, an overview of plasma-based coating methods for corrosion protection will be presented. For decades, low pressure plasma systems were employed in the deposition of thin coatings on steel, aluminum and other metals. While the coatings provided significant improvement in corrosion protection, vacuum chambers are often limited in volume, making it difficult to treat large or irregularly shaped parts efficiently.

In recent years, atmospheric pressure plasma systems are preferred for scalable, continuous, and flexible surface treatments. In the second part of this work, the plasma-assisted, large area deposition of dense, organosilicon coatings on Al 6061, AM60 and AZ91D Mg alloys using atmospheric pressure plasma jets will be presented. For the deposition process, clean dry air was used as the plasma generating gas, along with 2 types of siloxane precursors. The process was fully automated, as the plasma jets were moved over the substrates at constant speed with the assistance of a robotic system.

Results from the analysis of coatings with thicknesses ranging from 200nm to 1200nm will be shown. The electrochemical characterization involved immersion of the Mg alloy substrates in a 3.5wt.% NaCl solution, whereas the aluminum substrates were exposed to highly corrosive HCl solutions. Multi-scale image characterization and chemical analysis was performed using scanning electron microscopy (SEM) equipped with energy dispersive X-ray spectrometry (EDS) and scanning transmission electron microscopy system. More information correlating the plasma process parameters to the elemental composition, thickness and corrosion resistance of the coated metals will be presented.

Overall, large area plasma deposition enables uniform, scalable application of anti-corrosion coatings on metal surfaces, making it ideal for industrial components like automotive and aircraft panels. Its atmospheric operation allows integration into continuous production lines, reducing costs while enhancing durability and surface protection.

9:20am **IA2-1-WeM-5 Directed Energy Deposition of Bronze Coatings on Aluminium Substrates: Microstructure, Phase Evolution, and Process Optimization***,* ***Christoph Witte [christoph.witte@fh-kiel.de]****,* *Claus-Henning Solterbeck,* University of Applied Science Kiel, Germany*; Hannes Freiße,* Kugler Bimetal SA, Switzerland*; Johannes Wiesheier, Thomas Rubenbauer,* Schlenk Metallic Pigments GmbH, Germany*; Andreas Ebert, Jürgen Barz,* Schmelzmetall Deutschland GmbH, Germany*; Jana Schloesser,* University of Applied Science Kiel, Germany

With the increasing demand for efficiency and sustainability in aerospace applications, the development of lightweight parts represents a critical challenge. This study presents an integrated approach that covers the entire process chain, from alloy and powder development to the production of functional components, made possible through close collaboration between a research institute and industrial partners. Bronze coatings are applied onto aluminium substrates using a laser powder based Directed Energy Deposition (DED) process, aiming to combine low weight with enhanced wear resistance for the production of sliding bearings.

The metallurgical interaction between aluminium and copper-based alloys is highly complex. In addition to differences in physical properties such as thermal expansion, melting point and diffusion behaviour, brittle intermetallic phases tend to form at the interface. These phases often act as crack initiation sites and can lead to delamination.

In this work, bronze coatings are deposited on aluminium substrates using a powder-based Directed Energy Deposition (DED) process. Prior to the deposition, the aluminium substrates undergo appropriate surface preparation, and post-deposition heat treatments are applied to optimise adhesion and coating properties. The resulting microstructure and phase formation at the interface are investigated. Furthermore, this study identifies critical process parameters that affect coating quality and discusses strategies to mitigate interfacial defects.

This study demonstrates the potential of laser-powder-based DED process for the fabrication of lightweight, wear-resistant sliding bearings, and provides valuable insights into the application of copper-based coatings on aluminium substrates for a variety of applications, particularly in the aerospace sector.

9:40am **IA2-1-WeM-6 Plasma Electrolytic Oxidation Coatings on Mg Alloy AE44 Prepared from Mixed Aluminate-silicate Electrolytes***, Tianyi Zhang* ***[Zhang4x3@uwindsor.ca]****, Ran Cai, Xueyuan Nie, Henry Hu,* Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Canada

Magnesium–aluminum alloys are increasingly utilized in areas requiring lightweight materials, such as the automotive industries and humanoid robotics, due to their advantageous properties. However, their relatively low strength, hardness, and corrosion resistance limit their broader engineering applications. To address these shortcomings, surface modification techniques such as plasma electrolytic oxidation (PEO) are employed to form protective oxide layers that enhance surface performance. In previous studies, sodium phosphate (Na_3PO_4) solutions were commonly used as electrolytes, while other electrolyte systems have been less frequently investigated. In this study, aluminate–silicate mixed electrolytes with varying concentrations were utilized to fabricate PEO coatings. The surface morphologies were examined using scanning electron microscopy (SEM), and elemental contents were quantified through energy-dispersive X-ray spectroscopy (EDS), the phase compositions were identified by X-ray diffraction (XRD). Furthermore, potentiodynamic polarization, hardness, and indentation tests were conducted to assess the coatings' performance. The results revealed that the addition of silicate to the aluminate electrolyte enhanced the coating growth rate. Moreover, coatings produced from electrolytes with different concentrations exhibited distinct surface morphologies, as well as varying corrosion and indentation resistance.

11:00am **IA2-1-WeM-10 Low-Adhesion Carbon Coatings for the Sustainable Utilization of Geothermal Power Plants***, Yuya Nakashima* ***[nakashima-yuuya@fujielectric.com]****,* Fuji Electric Co., Ltd., Japan*; Noritsugu Umehara,* Nagoya University, Japan*; Hiroyuki Kousaka,* Gifu University, Japan*; Takayuki Tokoroyama,* Nagoya University, Japan*; Motoyuki Murashima,* Tohoku University, Japan **INVITED**

Geothermal power generation is one of the renewable power generation systems and they emit only 1 – 3 % CO_2 compared to emissions from coal-fired thermal power plants. Additionally, geothermal power plants provide stable electricity supply in contrast to the other renewable power sources such as solar and wind power which fluctuate power outputs depending on time and weather. However, geothermal steam, which is origins to rotate steam turbine, contains much amount of dissolved silica. It precipitates and accumulates on the turbine components and clogs steam flow throats and eventually causes power output drop and frequent maintenance. In this study, Diamond-like Carbon (DLC) is adopted as coating to suppress the silica accumulation on turbine blades. DLC is carbon based thin coating consist of sp2 and sp3 structures and has high chemical stability which may also has low chemical interaction against silica. Hence, chemical structure of DLC to reduce silica adhesion is revealed. To identify chemical structure of DLC on the outermost surface, X-ray analysis fine structure (XAFS) and Elastic recoil detection analysis (ERDA) is employed since outermost surface is quite important for adhesion and chemical structure of DLC completely differ from its bulk to outermost surface. As a result, DLC has lower sp2 fraction can reduce adhered silica amount to 3% compared with that on steel and if DLC has higher sp2 fraction but it also has higher hydrogen content, adhered silica amount is reduced to same level with DLC with lower sp2 fraction. It indicates lower sp2 fraction and higher hydrogen content can reduce silica adhesion. Then, chemical interaction against silica from DLC is revealed by calculating adsorption energy between sp2 structure and silica through ab initio calculation. sp2 structure itself physically adhere to silica, but if it has atomic defect as dangling-bond, adhesion state is changed from physical to chemical adhesion. If that dangling-bonds are terminated by hydrogen atoms, chemical adhesion is changed back to physical adhesion. Hence, adhesion mechanism between DLC and silica as chemical adhesion sites against silica is reduced by reducing sp2 fraction and adhesion state is changed to physical adhesion by increasing hydrogen content is proposed. Finally, DLC coated turbine blade samples is exposed under geothermal steam for 5 months. Then, almost no silica accumulation occurs on DLC even no-coated blade get certain amount of silica accumulation. As a result of above, we believe that DLC is new solution can solve silica accumulation troubles generally happens in geothermal power generation systems.

11:40am **IA2-1-WeM-12 Application-Driven Research in Surface Engineering for Advanced Cutting Tool and Component Applications - 25 years of cooperation between Plansee and Oerlikon -***, Peter Polcik* ***[peter.polcik@plansee.com]****, Szilard Kolozsvari,* Plansee Composite Materials GmbH, Germany*; Denis Kurapov,* Oerlikon Surface Solutions AG, Liechtenstein*; Helmut Riedl, Paul Heinz Mayrhofer,* Institute of Materials Science and Technology, TU Wien, Austria **INVITED**

The persistent challenges in the field of PVD coatings—both in established and emerging applications—can be effectively addressed through close collaboration along the entire value chain. This paper highlights key milestones achieved through the long-standing partnership between Plansee Composite Materials and Oerlikon Surface Solutions, which has now spanned more than two decades. Substantial support from the Austrian Christian Doppler Research Association has enabled a strong collaboration between industry and a broad network of scientists from leading Austrian research institutions: Montanuniversität Leoben, the University of Innsbruck, and Technische Universität Wien.

Initiated in 2000, this collaboration was guided by clear objectives to advance the development of TiAl- and AlCr-based nitride coatings. Plansee contributed through innovations in target materials design, while Oerlikon provided the industrial platform for PVD coating processes. This paper provides an overview of systematic investigations on how variations in composition influence the properties of PVD-deposited thin films, ultimately leading to the industrial implementation of novel AlCrB- and AlCrSi-based hard coatings. These achievements were realized by establishing fundamental concepts, evaluating new coatings in both laboratory settings and industrial PVD systems, and consistently integrating findings into iterative development cycles.

To address new applications in machining, forming, and high-temperature environments, the research scope expanded beyond nitrides to include borides and carbides, with particular emphasis on enhancing oxidation resistance without compromising hardness.

The outcomes of this collaboration led to the development and successful market introduction of several coating solutions that contribute to a more sustainable and environmentally responsible economy.

International Union for Vacuum Science, Technique, and Applications Special Session
Room Palm 5-6 - Session IUVSTA-WeM

IUVSTA Special Session

Moderator: Ivan G. Petrov, University of Illinois at Urbana-Champaign, USA

8:00am **IUVSTA-WeM-1 The Enabling Power of Vacuum Science, IUVSTA and Field-Deployable Quantum-Based Innovations with the NIST-on-a-Chip Program***, Jay Hendricks* ***[jay.hendricks@nist.gov]****,* NIST, USA **INVITED**

I'll bring context to the talk with a short introduction of IUVSTA, the International Union for Vacuum Science, Technique and Application. As President, a main priority is public outreach to highlight the impact of vacuum technology on everyday life. Our IUVSTA Divisions are making significant contributions to the development of faster, smaller, and more energy-efficient technologies, from computer chips to artificial intelligence systems, self-driving cars, and more energy-efficient systems.

The redefinition of the International System of Units (SI) has opened up new avenues for realizing fundamental units, enabling the development of innovative measurement technologies that are quantum-based. The emergence of these quantum-based metrology systems has the potential to transform various fields, but also raises important questions about their miniaturization, deployment, and impact on the metrology ecosystem. This talk will explore the exciting possibilities and challenges arising from these advancements, with a focus on the role of metrology institutes in the new era of quantum-based measurement.

The vacuum technology technical core of the presentation will delve into recent breakthroughs in quantum-based measurement methods, including the Fixed Length Optical Cavity (FLOC) for pressure measurement and the Cold Atom Vacuum Standard (CAVS) for vacuum metrology. These cutting-edge approaches leverage fundamental physics, quantum mechanics, and photonics to achieve high accuracy and precision. The use of photons for measurement readout enables the exploitation of the rapidly growing field of photonics, paving the way for the development of compact, field-deployable measurement systems.

The NIST on a Chip program will be highlighted as a key initiative driving the miniaturization of measurement technologies. By exploring the intersection of quantum-based metrology, photonics, and miniaturization, this talk aims to spark a discussion on the future of metrology and the role of metrology institutes in this new ecosystem where field-deployable systems are in use.

8:40am **IUVSTA-WeM-3 Chalcogenide Ovonic Threshold Switch (OTS) and Selector-Only Memory (SOM) Devices for Neuromorphic Applications***,* ***Jong-Souk Yeo [jongsoukyeo@yonsei.ac.kr]****, Siwon Park, Young-Min Kim, Sangyeop Kim,* Yonsei University, Republic of Korea **INVITED**

As artificial intelligence and data-intensive applications continue to drive rapid changes in computing paradigms, energy-efficient and highly scalable hardware architectures are increasingly important. Resistive switching devices have emerged as promising building blocks for next-generation memory due to their simple structure, low power consumption, and compatibility with high-density integration.

Ovonic Threshold Switches (OTS) are particularly attractive as selector devices in cross-point memory arrays because of their abrupt threshold switching behavior and high on/off ratios, which effectively suppress sneak currents. However, achieving reliable operation and scalability requires a thorough understanding of the switching mechanisms and systematic optimization at the material level.

In this work, we present a comprehensive optimization strategy for OTS devices by investigating how material composition influences electrical switching characteristics. Switching behavior is shown to depend strongly on compositional tuning and local bonding configurations. By extending to more complex multi-component material systems,we develop a deeper understanding of how specific bonding configurations influence device characteristics, resulting in significantly enhanced on/off ratios and improved stability. These results establish clear composition–structure–property relationships that provide practical guidelines for high-performance OTS design.

Based on the optimized device, we demonstrate a low-power artificial neuron that exhibits leaky-integrate-and-fire behavior. The firing frequency of the neuron can be modulated by external load conditions, confirming its capability to emulate key features of biological neural dynamics.

In addition, polarity-dependent threshold voltage modulation is observed in OTS devices and is attributed to asymmetric local structural configurations, as confirmed by molecular dynamics simulations. This intrinsic asymmetry allows controllable threshold tuning to be used as a memory element, thus enabling a selector-only memory architecture that potentially replaces conventional selector–resistor functionality with a single device.

This enhanced understanding of OTS devices provides valuable insights and design strategies for compact and energy-efficient neuromorphic applications.

This research was supported by Samsung Electronics Co., Ltd. (Project No. IO2102021-08356-01), the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No.2023R1A2C2006811), and the BK21 FOUR (Fostering Outstanding Universities for Research) funded by the Ministry of Education (MOE) and NRF of Korea.

9:20am **IUVSTA-WeM-5 Quantum Effects of Hydrogen in Metal Thin Films***,* ***Katsuyuki Fukutani [fukutani@iis.u-tokyo.ac.jp]****,* University of Tokyo, Japan **INVITED**

Hydrogen absorption in metals is relevant to a variety of energy- and environment-related applications, including hydrogen storage, high-temperature superconductivity, and catalytic reactivity [1]. Because hydrogen is the lightest atom, it is often argued that hydrogen in metals exhibits quantum effects arising from zero-point vibrations and quantum tunneling. To investigate the behavior of hydrogen in metal thin films, our group has developed nuclear reaction analysis (NRA) [2] combined with channeling and electrical resistance measurements. Using this approach, we have studied the structure and diffusion of hydrogen in typical hydrogen-absorbing metals of titanium and palladium, in which quantum effects play a significant role [3-5].

Titanium hydride thin films with a thickness of 90 nm were fabricated on MgO(110) substrates by reactive magnetron sputtering. Two-dimensional NRA mapping revealed axial and planar channeling patterns. By comparison with trajectory simulations, approximately 10% of the hydrogen was found to occupy octahedral sites, while the remaining hydrogen resided at tetrahedral sites. In contrast, deuterium was found to occupy exclusively the tetrahedral sites, a difference attributed to zero-point vibrational effects [3]. A palladium thin film with a thickness of 10 nm was fabricated on a glass substrate and hydrogenated either by hydrogen gas exposure followed by quenching or by low-energy hydrogen ion irradiation. In both cases, hydrogen initially occupied metastable hydride states and was observed to migrate to stable states. By measuring the time evolution of the film resistance, hydrogen diffusion in the films was analyzed, revealing a crossover from a classical thermally activated regime to a quantum regime [4,5].

1. K. Fukutani et al., Chem. Rec. 17, 233 (2017).
2. M. Wilde and K. Fukutani, Surf. Sci. Rep. 69 (2014) 196;
3. T. Ozawa et al., Nat. Commun. 15, 9558 (2024).
4. T. Ozawa et al., J. Phys. Chem. Solids 185, 111741 (2024).
5. T. Ozawa et al., Sci. Adv. 11, eady8495 (2025).

11:00am **IUVSTA-WeM-10 Stable and Metastable High Entropy Alloys***,* ***Sven Ulrich [sven.ulrich@kit.edu]****, Dimitri Litvinov, Jarir Aktaa, Adam Bichler, Michael Stueber,* Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM), Germany **INVITED**

In stable high entropy alloys (HEA) the individual elements must have the same crystal structure. Of the 80 non-radioactive elements in the periodic table, 14 metallic elements (Al, Ca, Ni, Cu, Ag, Au, Pb, Pd, Pt, Rh, Ir, Sr, Ce, Yb) have a face-centered cubic structure at room temperature, 14 elements (Li, Na, K, Rb, Cs, Ba, Eu, V, Cr, Fe (α), Nb, Mo, Ta, W) have a body-centered cubic crystal structure, and 22 elements have a hexagonal close-packed crystal structure (Be, Mg, Sc, Ti, Co, Zn, Zr, Cd, Hf, Y, La, Nd, Gd, Tb, Dy, Ho, Er, Tm, Lu, Ru, Os, Re). They represent the maximum number of elements of the corresponding stable HEA. Adding an element with a foreign crystal structure below the solubility limit also results in a stable HEA. Examples are given for the various cases. However, metastable HEA can form above this solubility limit. As an example, single-phase, body-centered cubic Ni-containing (Cr, Mo, Nb, Ta, V, W) HEA thin film are examined in detail with regard to their global and local elemental composition (EPMA, STEM, EDX), topology using SEM, and microstructure using XRD and HRTEM. The coatings were produced by non-reactive d.c. magnetron sputtering of a Cr-Mo-Nb-Ta-V-W-Ni target in argon plasma at 0.2 Pa.

Protective and High-temperature Coatings
Room Town & Country A - Session MA2-2-WeM

Hard and Nanostructured Coatings II

Moderators: **Stanislav Haviar**, University of West Bohemia, Czechia, **Kuan-Che Lan**, National Tsing Hua University, Taiwan , **Norma Salvadores Farran**, TU Wien, Austria

8:00am **MA2-2-WeM-1 Dual-Phase Crystalline-Amorphous Coatings Based on Thin-Film Metallic Glasses: Synthesis and Properties***,* ***Petr Zeman [zemanp@kfy.zcu.cz]****,* University of West Bohemia, Czechia **INVITED**

Magnetron sputter deposition has been demonstrated to be a suitable technique for synthesizing metallic glasses as thin films (TFMGs). Thanks to the non-equilibrium conditions of low-temperature plasma and extremely high cooling rates at the atomic scale on the substrate, TFMGs can be prepared with a much wider composition variety and solubility than bulk metallic glasses (BMGs). Moreover, TFMGs exhibit properties and characteristics that surpass those of BMGs as well as conventional metallic and ceramic coatings, particularly in achieving an optimized balance between ductility and strength.

The amorphous structure of TFMGs, characterized by short- and medium-range atomic ordering, combined with their exceptional properties, offers opportunities to create dual-phase architectures incorporating both TFMGs and crystalline materials. These architectures have the potential to overcome the limitations inherent to each constituent phase while enhancing existing properties or even enabling novel functionalities through synergistic phase interactions.

Dual-phase crystalline-amorphous coatings based on TFMGs can be relatively easily prepared in multilayer architectures comprising alternating crystalline and TFMG sublayers. We demonstrated this concept with multilayer Zr-Cu-N coatings consisting of hard ceramic ZrN and ductile glassy ZrCu sublayers. The coatings exhibited enhanced damage tolerance due to effective crack deflection at sublayer interfaces, yielding superior fracture stress and toughness values. Incorporating ZrN-Cu nanocomposite surface sublayers further imparted antibacterial functionality, expanding their potential applications.

The formation of dual-phase crystalline-amorphous coatings based on TFMGs in a nanocomposite architecture presents significant challenges. However, we successfully synthesized such coatings in the Zr-Cu-N and Zr-Cu-B systems using a one-step process of reactive and non-reactive magnetron co-sputtering, respectively. The coatings prepared under optimized conditions were nanocomposites comprising nanocrystalline ZrN or ZrB_2 and glassy ZrCu phases, representing a novel class of nanocomposite coatings combining ceramic and TFMG phases.

The talk will detail the compositional design, synthesis, microstructural evolution, and structure-property relationships of these coatings. Results from ab initio simulations that complement the experimental findings will also be presented, and key differences between the two coating systems will be discussed. It will be shown that these coatings offer promising potential for applications requiring a balance of hardness, toughness, and durability.

8:40am **MA2-2-WeM-3 Solubility Limit of Al in Cubic Transition-Metal Nitrides: Case Study of (Al,Cr)N***, **Fedor F. Klimashin [fedor.klimashin@empa.ch]**,* Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; M. Učík,* PLATIT a.s., Czechia*; D. Casari,* Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland*; S. Lellig,* RWTH Aachen, Germany*; T.J.E. Edwards,* NIMS, Japan*; H. Bolvardi, A. Lümkemann,* PLATIT AG, Switzerland*; J.M. Schneider,* RWTH Aachen, Germany*; J. Michler,* Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

The addition of Al to cubic transition-metal nitrides (TMNs) has been a cornerstone in the development of hard, protective coatings for high-performance applications. Increasing the Al content in cubic TMNs typically enhances hardness, oxidation resistance, and thermal stability. However, under thermodynamic equilibrium, AlN and cubic TMNs are immiscible, as AlN favours the wurtzite (w-) structure. The formation of hexagonal w-AlN, in turn, is generally detrimental to mechanical performance and abrasive-wear resistance.

Theoretical and experimental studies have shown that high compressive residual stresses, high deposition rates, and low substrate temperatures can extend the metastable cubic solubility limit (along with Al subplantation or coherency-strain-stabilised multilayer architectures, which, however, are outside the scope of this study). This behaviour is well captured by metastable phase-diagram calculations for magnetron-sputtered (Ti,Al)N and (V,Al)N films [1,2].

High reported Al solubility levels in cubic TMNs are often inferred solely from the absence of w-AlN reflections in X-ray diffractograms. We investigated a series of sputter-deposited (Al,Cr)N films with Al metal fractions up to 0.72, which exhibited only fcc reflections in X-ray diffractograms. However, selected-area electron diffraction revealed the presence of w-AlN, indicating that the true solubility limit is lower. We discuss the influence of residual stress, substrate temperature, and deposition kinetics on the stabilisation of metastable cubic solid solutions, and propose indirect, experimentally accessible indicators for the onset of wurtzite-phase formation. These findings refine the understanding of Al solubility in (Al,Cr)N and, more broadly, in cubic TMNs.

References:

[1] S. Liu et al., *Acta Mater.* 165 (2019) 615–625.

[2] S. Liu et al., *Acta Mater.* 196 (2020) 313–324.

9:00am **MA2-2-WeM-4 Hardness and Fracture Toughness Enhancement in Non-Stoichiometric Diboride Superlattices***, **Marek Vidiš [marek.vidis@fmph.uniba.sk]**,* *Tomáš Fiantok, Martin Truchlý, Vitalii Izai, Leonid Satrapinskyy, Tomáš Roch,* Comenius University Bratislava, Slovakia*; Rainer Hahn, Helmut Riedl,* TU Wien, Austria*; Peter Švec,* Slovak Academy of Sciences, Slovakia*; Viktor Šroba, Marián Mikula,* Comenius University Bratislava, Slovakia

Superlattice architecture presents a promising strategy for the simultaneous enhancement of hardness and fracture toughness in hard ceramic films. We demonstrate the success of this approach in transition metal diboride films and report the structural and mechanical properties of films composed of nanocrystalline $ZrB_{2+x}$and disordered TaB_{2-y} layers. Superlattice films with a wide range of bilayer periods (Λ = 1.8–31.5 nm) were prepared by magnetron sputtering. Deposition was performed at 300 °C with a floating bias to minimize interdiffusion. The formation of sharp interfaces for all Λ values is confirmed by X-ray reflectivity. The films consist of strongly understoichiometric $TaB_{1.4}$ layers, which lack long-range ordering, and overstochiometric $ZrB_{2.6}$ layers with a preferential (001) crystalline orientation. With decreasing Λ, we observe a change in preferential orientation and the formation of a true superlattice structure, evidenced by satellite peaks. This indicates crystallization of the $TaB_{1.4}$ layers, as confirmed by STEM data which shows both layers exhibiting a (001)-oriented hexagonal structure. This is a result of two effects: locally induced stabilization by the underlying ZrB_{2+x}layer and boron diffusion at the interface, enhanced by the boron concentration gradient and the bombardment of Ar neutrals reflected from the targets. This transition is accompanied by a remarkable increase in hardness from 34.1 ± 1.9 to 47.2 ± 2.3 GPa as Λ decreases to 3.4 nm. The observed hardening exceeds estimations based on Koehler's strengthening mechanism for two layers with a shear modulus difference of only 39 GPa. Improved mechanical properties are observed also from DFT calculations for defect-free ZrB_2/TaB_2 cells (Λ = 1.4–8.2 nm), which reveal a stabilizing effect with decreasing Λ and a significant increase in stiffness, peaking at Λ = 2.7 nm. At the same time, the fracture toughness K_{IC}, obtained from notched cantilever bending tests, increases from 3.3 ± 0.2 $MPa \cdot m^{1/2}$ (average of both monolithic films) to 4.6 ± 0.3 $MPa \cdot m^{1/2}$ for the superlattice film with Λ = 1.8 nm. This improvement is attributed to coherent stresses at the interfaces due to lattice mismatch. The suppression of brittle response under mechanical load is also confirmed by cube-corner indents, which show shorter radial cracks with decreasing Λ. This work demonstrates that the superlattice approach is highly effective in transition-metal diborides and highlights the crucial role of stoichiometry. It was supported by the Slovak Research and Development Agency (Grant No. APVV-21-0042 and APVV-24-0038), Scientific Grant Agency (Grant No. VEGA 1/0473/24) and COLOSSE project (No. 101158464).

9:20am **MA2-2-WeM-5 Effects of Nitrogen Flow Rate and Deposition Temperature on the Structure and Properties of VMoN Thin Films Deposited by High Power Impulse Magnetron Sputtering***, **Jia-Hong Huang [jhhuang@ess.nthu.edu.tw]**,* *Pei-Fen Peng,* National Tsing Hua University, Taiwan

In this study, vanadium molybdenum nitride (VMoN) thin films were deposited on Si substrate using high power impulse magnetron sputtering (HiPIMS). The purpose of this research was to investigate the effects of process parameters including nitrogen flow rate (N-series) and deposition temperature (T-series) on the structure and properties of VMoN thin films. The results showed that for the coatings deposited at 400 °C, the lattice parameters linearly increased with increasing N/metal ratio, while those deposited at temperatures ranging from 200 to 350 °C, did not follow the Vegard's law. The texture of the VMoN films also significantly affected by the two process parameters. VMoN thin films deposited at 400 °C exhibited a (200) texture, and the texture coefficient of (200) increased with nitrogen flow rate, which could be explained by the steering effect and competitive growth theory. As the deposition temperature decreased, insufficient energy was delivered to the adatoms and promoted the growth of (111)-orientated grains. For the coatings deposited at 400 °C, the ion peening effect became intense with increasing nitrogen flow rate and thereby increasing electrical resistivity from 141.4 to 178.8 μΩ·cm. Furthermore, with increasing N/metal ratio, the hardness of N-series specimens decreased from 25.9 to 17.9 GPa, and compressive residual stress decreased from -3.66 to -1.43 GPa due to the decrease of nitrogen-vacancy hardening effect. In contrast, coatings deposited at temperature ranging from 200 to 350 °C showed no significant variation in N/metal ratio, indicating that nitrogen-vacancy hardening effect was not the primary factor that affected hardness and residual stress of T-series specimens. The results of X-ray diffraction confirmed the presence of a second phase at 350 °C and below, where the resistivity of the specimens substantially increased. The fraction of the second phase increased as deposition temperature decreased, which was correlated with increasing hardness and residual stress. The second phase may play a major role in influencing the properties of T-series specimens.

9:40am **MA2-2-WeM-6 Multi-Scale Investigation of Superior Mechanical Properties in Nitride Ceramics with Negative Stacking Fault Energy**, *Yong Huang, Zhuo Chen,* ***Zaoli Zhang [Zaoli.Zhang@oeaw.ac.at]***, Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

Introduction: Ceramics are widely used in various structural and functional applications; however, their intrinsic brittleness at room temperature remains a critical challenge, often leading to early-stage catastrophic failures. This brittleness arises primarily due to the high critical-resolved shear stress required to initiate dislocation movement and the limited number of operational slip systems. Addressing this limitation is crucial for the development of ceramics with improved mechanical properties.This study aims to develop a novel strategy for enhancing the deformability of ceramics by leveraging negative stacking fault energy (SFE). The approach seeks to reduce the energetic barriers to dislocation motion and expand the number of available slip systems, ultimately improving room-temperature plasticity while maintaining high strength and toughness. In this work,a TiN/TaN superlattice was fabricated and subjected to in-situ micro-mechanical testing to evaluate its mechanical response. Post-mortem transmission electron microscopy (TEM) was employed to analyze deformation mechanisms at the atomic scale, providing insights into the role of negative SFE in promoting dislocation activity, atomic plane faulting, and twinning.The TiN/TaN superlattice exhibited remarkable room-temperature compressive plasticity (~43%), attributed to extensive atomic plane faulting and twinning facilitated by negative SFE. This behavior enabled an exceptional combination of plasticity, strength, and toughness, demonstrating the feasibility of overcoming the brittleness barrier in ceramics.

References: Huang, Y., et al. (2025). "Harvesting superior intrinsic plasticity in nitride ceramics with negative stacking fault energy." Acta Materialia: 120774.

Acknowledgement: The authors would like to thank Dr. Christian Mitterer, Velislava Terziyska (Montanuniversität Leoben) for the film deposition. We sincerely thank Rainer Hahn and Helmut Riedl (TU Wien) for their invaluable assistance with the micropillar compression tests. We also appreciate Verena Maier-Kiener (Montanuniversität Leoben) for her support with the nanoindentation tests and Michael Meindlhumer (Montanuniversität Leoben) for his help with the microcantilever bending tests. Additionally, we acknowledge David Holec, Thomas Leiner, and Lukas Hatzenbichler (Montanuniversität Leoben)for their contributions to the DFT calculations. Also, thanks to Zequn Zhang (ESI) and Yonghui Zheng for their help with microscopy. The financial support (Y.H., Z.C., and Z.L.Z.) by the Austrian Science Fund (PAT 1946623) is highly acknowledged.

11:00am **MA2-2-WeM-10 TiNbN / AlTiNbSiN / CrN Multilayer Coatings Irradiated by 300 keV Ar^+ Ions: The Role of Nitrogen**, ***Kuan-Che Lan [kclan@mx.nthu.edu.tw]***, *Chun-Hung Hsiao,* National Tsing Hua University, Taiwan*; Yin-Yu Chang,* National Formosa University, Taiwan

To study the crystalline stability of nitride coating against heavy ion irradiation for nuclear-related applications,nitride multilayer coatings with the architecture of TiNbN/AlTiNbSiN/CrN of an average period of 25 nm deposited by cathodic arc deposition were irradiated with 300 keV Ar^+ ions at the initial of room temperature under vacuum to the damage levels upto 7 dpa (displacements per atom). The irradiation-induced the change in crystalline structure, composition, and mechanical properties and electrical properties were systematically investigated. Ar^+ ions irradiation, noticeable interdiffusion between adjacent layers was observed. The region of depth exhibited a decrease in nitrogen content after irradiation which is consistent with the prediction of SRIM simulation. The reduction in hardness, electrical conductivity of the coating has been monitored. Besides, post irradiation examination of TEM and APT were carried out to investigate the depth distribution of irradiation induced defects at atomic level resolution. The defects of the role of nitrogen behavior of the properties among a variety of nitride with in the multilayer coating.

11:20am **MA2-2-WeM-11 Extremely Versatile Coating Design Through Adjustable Magnetic Field Settings for Arc Sources Using the Advanced Arc Technology from Oerlikon Balzers**, ***Alexandre Michau [alexandre.michau@oerlikon.com]***, *Denis Kurapov,* Oerlikon Surface Solution AG, Liechtenstein

Magnetic fields play a critical role in cathodic arc deposition processes. Usually applied in the vicinity of the targets, they steer the arc spots and have a big impact on the plasma and subsequent coating properties [1-2]. While random arc motion might be desirable for specific applications, modern processes rely on steered arc motions because it significantly reduces the number of macroparticles incorporated in the coatings [3]. Few studies address magnetic field configurations because they are typically way more complex to implement and modulate compared to other conventional deposition parameters like temperature, pressure or bias voltage.

The optimal magnetic field depends on the coating material to evaporate and grow as well as on its targeted properties and performance. However, such versatility is rarely available at an industrial scale. The Advanced Arc Technology (AAT) from Oerlikon Balzers offers unprecedented capabilities for precise magnetic field tuning and thus versatile coating design in combination with high efficiency of deposition process as well as reduced surface roughness.

The maximum achievable magnetic field density is now twice as high as before, opening a new process window for target materials that are sensitive to high steering speeds. Furthermore, the magnetic field dynamicity, in other terms the speed at which the magnetic field can be changed, approaches the ms scale. This enables advanced strategies such as nanolayering with alternating antagonistic magnetic configurations, opening a new coating architecture window. Finally, the magnetic field flexibility has been improved, allowing its shape and intensity to match the ones from previous generations while introducing new features such as a controlled discharge voltage offering gain in reproducibility and operational simplification.

We will discuss the possibility to tune coating properties with different magnetic field configurations generated using the Advanced Arc Technology. The focus is be given on the magnetic field density (parallel and orthogonal components compared to the target surface) while working with different focused shapes. The versatility of the coating design is demonstrated using two material systems. (Al,Cr)N and (Al,Ti)N are deposited in an industrial scale coater (INVENTA kila from Oerlikon Balzers) using the reactive mode of the following metallic targets: AlCr targets with Al ≥ 70 at.% and AlTi targets with Al ≥ 67 at.%.

[1] A.B.B Chaar et al, Coatings, 9 (2019) 660.

[2] F.F. Klimashin et al., Materials and Design, 237 (2024) 112553.

[3] P.D. Swift, Journal of Physics D: Applied Physics, 29 (1996) 2025.

Protective and High-temperature Coatings
Room Palm 3-4 - Session MA3-3-WeM

High Entropy and Other Multi-principal-element Materials III

Moderators: Frederic Sanchette, Université de Technologie de Troyes, France, **Pavel Soucek**, Masaryk University, Czechia

9:00am **MA3-3-WeM-4 CrMoNbTaV Refractory High-Entropy Alloy: From Bulk Material to Films via a Synergistic Theoretical–Experimental Approach**, *Rafael Mendoza-Pérez, Ricardo González-Campuzano,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*; David E. Martínez-Lara,* 2Escuela Nacional Preparatoria No.7 “Ezequiel A. Chávez”, Universidad Nacional Autónoma de México*; Roxana M. Calderón-Olvera, Josué E. Romero-Ibarra, Ignacio A. Figueroa-Vargas,* ***Sandra E. Rodil-Posada [srodil@unam.mx]***, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México

High-entropy alloys (HEAs) have attracted significant attention since the initial findings by Cantor et al. and Yeh et al. in 2004. These alloys consist of five or more elements in equiatomic or nearly equiatomic proportions (5–35 at.%), resulting in high mixing entropy that reduces Gibbs free energy and promotes the formation of stable solid solutions. Their high configurational entropy originates from the multiple ways in which the different elements are arranged within the crystal lattice. This unique composition yields complex microstructures and outstanding mechanical properties, including corrosion resistance, high strength, toughness, and ductility. HEAs exhibit remarkable thermal stability and wear resistance, suggesting them as promising materials for multiple applications.

In this work, a synergistic theoretical-experimental approach was applied that simplified the planning, synthesis, characterization, and analysis of the atomic structure of custom-designed RHEA $Cr_8Mo_{25}Nb_{27}Ta_{16}V_{24}$composite coatings. The coatings were obtained by DC magnetron sputtering with a custom-designed RHEA target, meticulously produced through thermodynamic calculations, phase diagrams, and metallurgical processes. This ensured a single-phase, non-equiatomic composition that encompassed all the different predictors of the HEA. The samples were characterized using X-ray diffraction (XRD), Rietveld refinement, optical and mechanical profilometry, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), high-resolution transmission electron microscopy (HRTEM), high-angle annular dark-field (HAADF), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). The findings confirm a predicted body-centered cubic (BCC) crystal structure in the coatings. Detailed atomic structural analysis by Rietveld refinement and HRTEM revealed a primary β-phase with a BCC crystal structure, coexisting with a minor β'-phase that surprisingly exhibited a body-centered tetragonal (BCT) crystal structure. These coatings demonstrated highly desirable properties: they remained flat, exhibited low oxidation, and reduced mechanical stress.

9:20am **MA3-3-WeM-5 Effects of HiPIMS Plasma Ionization and Deposition Parameters on the Microstructure and Mechanical Properties of TiZrNbTaMo High Entropy Alloy Films***, **Chia-Lin Li [chialinli@mail.mcut.edu.tw]**,* Center for Plasma and Thin Film Technologies, Ming Chi University of Technology, Taiwan*; Bih-Show Lou,* Chemistry Division, Center for General Education, Chang Gung University, Taiwan*; Jyh-Wei Lee,* Department of Materials Engineering, Ming Chi University of Technology, Taiwan

TiZrNbTaMo high entropy alloys (HEAs) with a body-centered cubic (BCC) structure are well known for their excellent compressive yield strength and significant plasticity, which can be retained even in thin film form. These outstanding mechanical properties make them promising candidates for advanced applications. The deposition parameters play a critical role in determining the density, microstructure, and mechanical behavior of HEA thin films. In this study, TiZrNbTaMo high entropy alloy films (HEAFs) were deposited using high power impulse magnetron sputtering (HIPIMS), DC, and RF power sources to investigate the effects of deposition conditions on their structure and properties. HIPIMS, as an advanced physical vapor deposition (PVD) technique, enables a high degree of metal ionization and promotes dense film growth. To further understand plasma effects, the pulse frequency and duty cycle in HIPIMS were systematically varied while maintaining a constant average power. An ion meter was used to evaluate the degree of metal ionization under different peak discharge currents, and pulse-resolved optical emission spectroscopy (OES) was conducted to analyze the temporal evolution of excited species within each HIPIMS pulse, providing insights into discharge behavior and plasma–film interactions. The resulting films were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM) to analyze their crystallographic structure and microstructure, while nanoindentation was used to measure hardness and elastic modulus. The TiZrNbTaMo HEAFs deposited by HIPIMS exhibited increased hardness due to the higher peak power density, which induced the coexistence of amorphous and nanocrystalline structures. This study demonstrates that combining HIPIMS deposition with pulse-resolved plasma diagnostics provides an effective approach to control plasma activation and tailor the microstructure and mechanical properties of TiZrNbTaMo high entropy alloy thin films, highlighting their potential for high-performance coating applications.

9:40am **MA3-3-WeM-6 Phase Formation, Microstructure and Selected Properties of Magnetron Sputtered Cr-Ta, Cr-Nb and Cr-v-Ta Thin Films***, Jan-Ove Soehngen, Vincent Ott, Sven Ulrich, **Michael Stueber [michael.stueber@kit.edu]**,* KIT, Germany

Refractory alloy thin films, especially novel complex compositional and multiple principal element thin films, are of high interest in recent materials research. These materials can exhibit unique properties making them suitable candidates for a variety of high-load thermo-mechanical applications. Suprisingly, there is often a gap in the knowledge and data collection on thin film formation in more fundamental, simpler systems covering even binary or ternary refractory metals. In this study, we present results on phase formation, microstructure and selected properties on magnetron sputtered thin films in the systems Cr-Ta, Cr-Nb and Cr-V-Ta. The thin films were prepared by low-temperature, zero bias deposition from segmented targets to enable combinatorial studies of phase formation and microstructure evolution reflecting mainly the impact of the variation in chemical composition of the thin films. A major result is that by co-deposition from the segmented target single-phase solid solution b.c.c. structured thin films can be deposited in all systems under defined conditions. It is further of interest that the formation of a Laves phase, i.e. Cr_2Ta, Cr_2Nb or Art $(Cr,V)_2Ta$, can be suppressed by this approach. Finally, mechanical properties such as indentation hardness and modulus or electrical conductivity can be precisely controlled via tuning of the elemental composition of the thin films.

11:00am **MA3-3-WeM-10 Overcoming Strength-Plasticity Trade-Off in Complex Concentrated Alloy Thin Films by Engineering Their Atomic and Microstructure***, Davide Vacirca, Arjun Curam,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France*; Gregory Abadias,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France*; Andrea Li Bassi,* Nanolab, Departement of Energy, Politecnico di Milano, Italy*; Christian Ricolleau,* University of Paris, Laboratory of Matériaux et Phénomènes Quantiques, France*; Gerhard Dehm,* Max Planck institute for Sustainable Materials, Germany*; **Matteo Ghidelli [matteo.ghidelli@lspm.cnrs.fr]**,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France

The design of high-performance structural materials is always pursuing the combination of mutually exclusive properties such as mechanical strength and plasticity. Complex concentrated alloys (CCAs) have recently attracted attention due to their superior mechanical properties, emerging from their multicomponent nature. However, such atomic complexity often prevents a nanoengineering approach with limited control over composition and microstructure, especially in bulk form.

Here, we exploit thin film (TF) synthesis to produce model FCC CCA-TFs with precise control over composition and microstructure (crystalline phase, density of structural defects and grain size), leading to large and tailored mechanical properties. Moreover, our approach encompassed both commonly employed synthesis method (i.e., sputtering) as well as pulsed laser deposition (PLD), leading to the development of novel nanostructures with unique nanoscale features [1].

Firstly, I will demonstrate a simple defect-engineering pathway in sputter-deposited CoCrNi CCA-TFs by introducing Fe to form Fex(CoCrNi)100–x [2]. Increasing the Fe content drives a structural transition from a dual FCC-HCP phase to a single FCC phase, accompanied by a decrease in defect density (stacking faults, nanotwins) and lattice distortion. This results in increased mass density and dislocation mobility, reflected by a decrease in hardness (from 9.6 down to 7.4 GPa), and increment in activation volume (up to ~13 b3).

Then, I will focus on CoCrCuFeNi CCA-TFs by PLD, with unprecedented microstructural control [3]. I will show how to synthetize ultrafine grain structures with controllable size (down to 12 nm) which can be further tailored by post-thermal annealing treatments, resulting in high hardness (11 GPa) and yield strength (2.0 GPa) due to Hall-Petch strengthening, outperforming similar CCA-TFs while maintaining high plasticity (no fracture at 30% strain). Moreover, these ultrafine CCA-TFs show remarkable thermal stability, with grain growth initiating only at 49% of the melting temperature, while maintaining high hardness (9.1 GPa) after annealing for 1h at 460°C.

Overall, we established a comprehensive nanoengineering strategy to tailor structure-property relationships in CCA-TFs, offering new opportunities to overcome the strength-plasticity trade-off.

[1] F. Bignoli et al., Acta Materialia, 300, 121456, (2025).[2] A. Curam et al., Submitted to Acta Mater. (2025). [3] D. Vacirca et al., Submitted to Materials Today, (2025).

11:20am **MA3-3-WeM-11 Exploring the Microstructure and Mechanical Properties of CoCrFeNiMn Thin Films***, **Thomas Astecker [thomas.astecker@tuwien.ac.at]**,* TU Wien, Austria*; Peter Polcik,* Plansee SE, Austria*; Alexander Kirnbauer, Paul Heinz Mayrhofer,* TU Wien, Austria

Among high-entropy alloys, the equiatomic CoCrFeNiMn alloy, commonly known as the Cantor alloy, has emerged as a benchmark system due to its exceptional combination of strength, ductility, and thermal stability, stemming from its single-phase face-centered cubic structure and high-entropy effects. While the bulk properties of CoCrFeNiMn are well established, its behavior in thin-film form remains less explored, particularly under metastable synthesis conditions such as sputter deposition. In this work, we investigate the microstructure, thermal stability, crystal structure, and deformation mechanisms of CoCrFeNiMn thin films synthesized via magnetron sputtering. Films were deposited in an Ar atmosphere using a lab-scale PVD system at different substrate temperatures, with selected samples subjected to post-deposition thermal treatments. X-ray diffraction (XRD) was employed to assess crystal structure and phase formation, while mechanical behavior was probed using nanoindentation, in situ micropillar compression, and micro tensile testing, enabling direct comparison of plasticity and failure modes across multiple loading configurations. Chemical composition was analyzed by energy-dispersive X-ray spectroscopy (EDS), and transmission electron microscopy (TEM) provided insights into grain structure, defect evolution, dislocation activity, and potential deformation twinning. The results reveal the interplay between microstructure and mechanical response in sputtered CoCrFeNiMn thin films, demonstrating how microstructural features and size effects govern strength and ductility. These findings advance the understanding of deformation mechanisms in high-entropy alloys at small scales and inform their potential application as structural materials.

11:40am **MA3-3-WeM-12 Reactive Sputtering of CrMoNbWTiAgCx Carbide Films by High Power Impulse Magnetron Sputtering System: Effect of Ag and C Contents**, ***BengYan Lu [w2859562@gmail.com]***, *Yung-Chin Yang,* National Taipei University of Technology, Taiwan*; Chia-Lin Li,* Ming Chi University of Technology, Taiwan*; Bih-Show Lou,* Chang Gung University, Taiwan*; Jyh-Wei Lee,* Ming Chi University of Technology, Taiwan

High power impulse magnetron sputtering (HiPIMS) systems can produce thin films with dense microstructure compared with mid-frequency (MF) sputtering, due to the higher ion energy and plasma density. The combination of MF and HiPIMS has been reported to achieve higher deposition rates and reduced residual stress compared with HiPIMS alone. High entropy alloy (HEA) coatings, composed of multiple principal metallic elements forming carbides, borides, or nitrides, have attracted increasing attention for their exceptional mechanical and chemical stability.

In this study, CrMoNbTiWAg and CrMoNbTiWAgCx HEA carbide coatings were deposited using a superimposed HiPIMS–MF sputtering system. The Ag content was controlled by adjusting the power input to the Ag target, while the acetylene gas flow rate was tuned to control the degree of target poisoning during deposition. Microstructural evolution and phase formation were characterized using FE-SEM, XRD, TEM, and AFM, while mechanical properties such as hardness, adhesion, and wear resistance were evaluated by nanoindentation, scratch, and pin-on-disk tests. Electrochemical and oxidation behaviors were assessed via potentiodynamic polarization in 3.5 wt.% NaCl solution and thermogravimetric analysis (TGA) on X-750 superalloy substrates. Electrical properties were determined through four-point probe measurements, and antibacterial performance was evaluated via bacterial inhibition assays.

This study aims to elucidate the synergistic effects of Ag and C additions in improving the mechanical properties, corrosion protection, and multifunctional durability. The results are expected to provide valuable insights for developing durable and functional HEA carbide coatings through advanced HiPIMS technology.

Keyword: HiPIMS; high entropy alloy carbide; CrMoNbWTiAgCx coating; target poisoning; hardness; corrosion resistance.

Plasma and Vapor Deposition Processes
Room Town & Country B - Session PP2-1-WeM

HIPIMS, Pulsed Plasmas, and Energetic Deposition I

Moderators: Arutiun P. Ehiasarian, Sheffield Hallam University, UK, **Tetsushide Shimizu**, Tokyo Metropolitan University, Japan

8:00am **PP2-1-WeM-1 Alpha-alumina thin films at low temperature: how R-HiPIMS process parameters influence purity and crystallinity**, ***Célia Dieudonné [celia.dieudonne@icmcb.cnrs.fr]***, ICMCB, France*; Marjorie Cavarroc-Weimer,* Safran, France

Reactive High Power Impulse Magnetron Sputtering (R-HiPIMS) is emerging as a highly effective technique for the deposition of high-quality insulating metal oxide coatings. There are numerous process parameters. Some are similar to those of reactive conventional magnetron sputtering (working pressure, gas ratio, substrate temperature etc.), while others are similar to those of pulse use (frequency, time-off etc.). This study highlights the potential of R-HiPIMS to produce dense, homogeneous, and pure alpha-alumina (α-Al_2O_3). High ionization rates and peak power densities inherent to R-HiPIMS play a crucial role in promoting film densification and stabilizing the α-Al_2O_3 phase. The influence of other process parameters including oxygen partial pressure, working pressure, target power density, and substrate temperature on film microstructure is investigated. Special attention is given to the effect of the bias configuration of the steel substrate, comparing the presence of α-Al_2O_3 when the substrate is grounded or at a floating potential. This aspect constitutes a major focus of the study, as the substrate bias state significantly affects the energy and flux of incoming ions, as well as the overall plasma–substrate interaction during deposition. A mechanism to stabilize α-Al_2O_3 is proposed.

8:20am **PP2-1-WeM-2 Influence of Pulse Parameters in Multi-Pulse Hipims on Reactive Mode Transition for VO_2 Thin Film Deposition**, ***Erdong Chen [chen-erdong@ed.tmu.ac.jp]***, *Rina Watabe,* Tokyo Metropolitan University, Japan*; Stephanos Konstantinidis,* University of Mons, Belgiums, Belgium*; Daniel Lundin,* Linköping University, Sweden*; Tetsuhide Shimizu,* Tokyo Metropolitan University, Japan

Vanadium dioxide (VO2) undergoes a thermochromic phase transition around 68°C, changing from a tetragonal to a monoclinic structure accompanied by a substantial change in optical and electrical properties, which can be used in e.g., smart windows. However, synthesizing single-phase VO2 films via reactive sputtering remains challenging due to 1) the wide range of vanadium-oxygen (V-O) stoichiometries, and 2) the need to grow the proper crystalline phase, leading to a limited process window with a very narrow phase transition from VOx to VO_2.

In this study, these challenges were addressed by regulating the peak current (Ipk) in reactive multi-pulse High-Power Impulse Magnetron Sputtering (HiPIMS) to control the reactive mode transition. The number and on-time of micro-pulses were systematically varied to elucidate the relationship between the incident ion flux and Ipk evolution as a function of O_2 gas flow, using ion mass spectrometry.

With this approach, a linear increase in Ipk was achieved upon O_2 introduction, mitigating the abrupt current drop and reducing process hysteresis typically observed in single-pulse HiPIMS. This enabled more stable control over VO_2 deposition and improved the deposition rate within the transition regime.

As a result, VO_2 crystalline thin films were successfully deposited on ZnO/glass substrates. Thermochromic measurements revealed a resistivity change of over two orders of magnitude across the phase transition occurring at approximately 50 °C.

8:40am **PP2-1-WeM-3 Bipolar HiPIMS Discharges: Principles, Diagnosticsand Thin Film Deposition Strategies**, ***Jiří Čapek [jcapek@kfy.zcu.cz]***, *Tomáš Kozák, Andrea Dagmar Pajdarová, Mina Farahani, Tomáš Tölg,* University of West Bohemia in Pilsen, Czechia **INVITED**

The properties of thin films depend on their microstructure, crystal structure, and residual stress, which are influenced by the mobility of adatoms during growth. In magnetron sputtering, the adatom mobility can be enhanced via ion bombardment by applying a bias voltage. High-power impulse magnetron sputtering (HiPIMS) offers greater control by delivering high-power density pulses, producing a high fraction of ionized species and enhanced ion bombardment, even without a substrate bias. However, a bias voltage may still be needed to control low-energy ions. Recently, bipolar HiPIMS, where a positive voltage pulse follows the main negative voltage pulse, has been suggested to be used instead of a substrate bias voltage.

This presentation summarizes our research on bipolar HiPIMS. Plasma analyses using the Langmuir probe and mass spectroscopy revealed that plasma parameters evolve similarly regardless of positive pulse parameters or distance from the target, though their values differ. During the initial phase of the positive pulse, a large potential difference (up to 200 V), high electron temperature (up to 150 eV), and a significant drop in electron density were observed. After this part, the difference between the potentials and the electron temperature is low. The time-averaged spectra of ions exhibit a prominent high-energy peak. It is shown that the position of the peak can be varied by the positive pulse amplitude, its magnitude scales with the pulse length, and its width can be slightly influenced by the length of the delay interval.

Special attention is devoted to the deposition of films on insulating surfaces. Biasing such surfaces becomes ineffective because the plasma-substrate potential difference necessary for ion acceleration almost vanishes once the surface is charged by the incident plasma ions. We propose the utilization of chopped bipolar HiPIMS (featuring several short positive pulses replacing a single long positive pulse) to enhance energy flux to such insulating surfaces. Results show that for an insulated surface with low capacitance, bipolar pulse configurations do not significantly increase energy flux to the surface due to its rapid charging by plasma ions. Conversely, high surface capacitance facilitates an increase in energy flux even for a long positive pulse. For medium surface capacitance (tens of nF), chopping the positive pulse in bipolar HiPIMS effectively increases the energy delivered to the film by discharging the surface in the off-times. Optimal conditions for the deposition of thin films will be discussed based on this systematic study of various unipolar and bipolar pulse configurations.

9:20am **PP2-1-WeM-5 Synthesis-Dependent Phase Evolution in the W–N System: A Case Study with HiPIMS and N+ ion source***, **Oleksandr Pshyk [oleksandr.pshyk@empa.ch]**, Kerstin Thorwarth, Nathan Rodkey, Sebastian Siol,* Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Many nitride compounds exhibit relatively wide homogeneity ranges, which usually simplify their synthesis. However, some complex nitrides, such as W-N, contain numerous stable ground-state phases as well as metastable phases. Some of these phases have been computationally predicted to possess extraordinary properties, especially the nitrogen-rich compounds. In contrast, some of these phases have a very narrow homogeneity range, which, combined with variations in synthesis conditions, complicates their controlled synthesis. Exploring such a complex phase space becomes even more challenging when non-equilibrium synthesis methods, such as physical vapor deposition (PVD) methods, are employed. Therefore, understanding the phase evolution sequences within the W-N system under the exceptional synthesis conditions provided by high power impulse magnetron sputtering (HiPIMS) can help identify the conditions necessary for the synthesis of unique nitride compounds.

In this report, we present a comprehensive exploration of the basic synthesis parameter space for W-N thin films using HiPIMS. In addition to varying the nitrogen partial pressure (and thus the nitrogen-to-tungsten ratio), we investigate the effects of substrate temperature, substrate bias potential, and substrate-to-target distance on phase formation. We show how the phase fractions within each composition window change with variations in these process parameters. Furthermore, to elucidate the role of N_2 gas dissociation and ionization on phase evolution, we perform W-N thin film deposition assisted by an electron cyclotron wave resonance nitrogen plasma source. Our results reveal that the synthesizability of the two most commonly reported W-N phases synthesized using PVD methods - the NaCl-structured WN_x and WC-structured WN_x phases - strongly depends on the nitrogen concentration in the films set by substrate temperature or substrate bias. Furthermore, the boundaries between different phases are highly sensitive to the deposition rate, which is determined by the substrate-to-target distance. We analyze and discuss these results in the context of plasma characteristics at different nitrogen partial pressures and substrate-to-target distances.

The findings presented here can serve as a guide for synthesizing other compounds within complex phase diagrams that contain numerous stable and metastable phases within narrow homogeneity ranges.

9:40am **PP2-1-WeM-6 Development and Optimization of CrN and CrSiN Hipims Coatings for Enhanced Tool Performance in Cryogenic Machining of Ti6Al4V***, **Gaya CHETTOUH [gaya.chettouh@utt.fr]**,* University of Technology of Troyes (UTT), France*; Soufyane ACHACHE, Lamine GUEYE,* Université de Technologie de Troyes, France*; Yoann PINOT,* École Supérieure Nationale d'Arts et Métiers de Cluny, France*; Frederic SANCHETTE, Mohamed EL GARAH,* Université de Technologie de Troyes, France*; Corinne NOUVEAU,* École Supérieure Nationale d'Arts et Métiers de Cluny, France

Cryogenic machining is a sustainable alternative to conventional cutting fluids, reducing environmental impact while improving cooling efficiency at the tool–workpiece interface. This study develops protective coatings for cutting tools used in the cryogenic machining of Ti6Al4V titanium alloy. Although Ti6Al4V offers excellent mechanical strength and corrosion resistance, its poor machinability due to low thermal conductivity, high hardness at elevated temperatures, and strong chemical reactivity remains challenging.

Coatings are commonly applied to tungsten carbide tools to enhance their mechanical and tribological behavior. Lin et al. [1] showed that CrN deposited by modulated pulsed power magnetron sputtering (MPPMS) reached a hardness of 26 GPa and a Young’s modulus of 330 GPa, while Si addition (6.3 at. %) by pulsed DC sputtering increased hardness and modulus to 38 GPa and 395 GPa, respectively. This work reports on the enhancement of CrN and CrSiN coatings deposited by high power impulse magnetron sputtering (HiPIMS). Deposition parameters, including nitrogen flow, target duty cycle, bias voltage, and bias pulse synchronization (T_{on})—were optimized to improve film adhesion and density.

Microstructural and phase analyses were carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive spectroscopy (EDS). Nanoindentation revealed a maximum hardness of 33.2 GPa and modulus of 317 GPa at T_{on} = 110 µs. Tribological tests with a rotary tribometer showed friction coefficients between 0.51–0.53 against Ti6Al4V balls, with a minimum wear volume of 1.24×10^{-5} mm^3/Nm at T_{on} = 210 µs. Coatings deposited at T_{on} = 210 µs and 310 µs also exhibited superior adhesion, with critical loads (LC_3) of 4.5 N and 4.15 N, respectively. The CrN coating at T_{on} = 210 µs offered the best balance between mechanical and tribological performance, highlighting the key role of bias pulse synchronization in HiPIMS coatings.

Finally, the effect of Si incorporation was studied using a hybrid HiPIMS/pulsed DC mode to deposit CrSiN coatings containing 0–10 at. % Si. The influence of Si on microstructure and mechanical properties was compared with the optimized CrN reference. Coatings were then tested under cryogenic conditions to assess their machining performance. The corresponding results are presented.

[1] Lin et al. Surf. Coat. Technol., vol. 216, p. 251–258, 2013

11:00am **PP2-1-WeM-10 Nanopatterned Nanolayer TiN/NbN Coatings as Plasmonic and Wear Resistant Antimicrobial Materials***, **Arutiun P. EHIASARIAN [a.ehiasarian@shu.ac.uk]**, Arunprabhu Arunachalam Sugumaran,* Sheffield Hallam University, UK*; Ryan Bower, Ming Fu,* Imperial College London, UK*; David Owen, Ethan Muir, Yashodhan Purandare, Papken Ehiasar Hovsepian,* Sheffield Hallam University, UK*; Peter K. Petrov, Rupert Oulton,* Imperial College London, UK*; Thomas Smith,* Sheffield Hallam University, UK

Light-activated antimicrobial materials based on superhard nanoscale multilayer coatings are a novel class of materials which avoid eluting toxic heavy metals, are activated by visible light and are resistant to wear. High Power Impulse Magnetron Sputtering (HIPIMS) has been used to fabricate TiN / NbN nanoscale multilayers, whose surface was patterned into a nanoscale spike array using reactive ion etching to create features that amplify light-induced surface plasmon resonance. The film bilayer thickness was tailored and graded to enhance the toughness of the nanospikes and improve their resistance to sliding wear as evaluated in pin-on-disk tests and SEM observations. A highly activated plasma chemistry was observed in the HIPIMS environment with metal-to-gas ion momentum ratios reaching 4 for NbN and 2.7 for TiN at pulse duration of 200 µs. These conditions stabilised a (200) crystallographic texture for the nanolayer stacks. A high density microstructure observed in AFM curbed plasmon losses by reducing the density of scattering centres at grain boundaries. Preferential oxidation of NbN on the surface detected through XPS was responsible for deteriorating the plasmonic figure of merit of the films as observed through ellipsometry. Pump-probe laser measurements showed significant increases in the lifetime of active electron species in the films due to trapping of hot carriers by oxygen vacancies such as Nb^{3+} and Ti^{3+}, with Nb being more sensitive due to a higher enthalpy of its oxide. An enhanced Raman scattering was observed from nanospike regions. Antimicrobial activity of up to 4-log kill was observed *for Staphylococcus aureus* and *Pseudomonas aeruginosa* bacteria under UV illumination.

Keynote Lectures
Room Town & Country A - Session KYL2-WeKYL

Keynote Lecture II
Moderator: Sandra E. Rodil, Universidad Nacional Autónoma de México

1:00pm **KYL2-WeKYL-1 Nanoengineered Materials and Coatings for Medicine and Beyond***, Krasimir Vasilev [krasimir.vasilev@flinders.edu.au],* Flinders University, Australia **INVITED**

In this keynote talk, I will give an overview of recent progress from my lab on development of plasma polymer facilitated nanoengineered surfaces and materials that benefit many areas of application. Over the years, we developed a range of plasma-based methods with allows us to control that entire spectrum of material surface properties, including chemical, physical, mechanical and topographical. The main focus of our research is the design and surface modification of novel medical devices and biomaterials for applications in areas such as tissue engineering, controlling inflammation and infections, drug delivery and medical diagnostics. However, our surface modification technologies are not limited to medicine. We have demonstrated the utility of nanoengineered plasma polymers for solving problems in other areas such as environmental science and remediation, water treatment and even wine making. I will present the engineering and chemical concepts underpinning “plasma nanoengineering” and give a range of examples of application of the technology in various fields, including commercial applications.

Functional Thin Films and Surfaces
Room Palm 1-2 - Session MB1-WeA

Optical Materials and Thin Films

Moderators: Jiri Houska, University of West Bohemia, Czechia, **Juan Antonio Zapien**, City University of Hong Kong

2:00pm **MB1-WeA-1 Ultrafast Phenomena in Optical Materials with fs–ns Time-Resolved Spectroscopic Ellipsometry***, Shirly Espinoza* ***[shirly.espinoza@eli-beams.eu]***, ELI Beamlines. ELI ERIC, Czechia **INVITED**

Static, imaging, and time-resolved ellipsometry link microstructure and optical function in thin films. Using time-resolved spectroscopic ellipsometry (TRSE), we access amplitude and phase simultaneously (angles Ψ and Δ) to recover the complex dielectric function (ε) with femtosecond resolution, a capability that conventional transient probes do not provide directly and that is key to disentangling overlapping ultrafast processes. As complementary techniques, time-resolved X-ray diffraction (TR-XRD) correlates lattice strain and structural pathways with the optical response, while imaging ellipsometry maps, with spatial resolution, thickness and optical constants (n, k), assessing uniformity and device-level variability.

In ZnO thin films, TRSE separates bleaching by Pauli blocking, band-gap renormalization, and intra-valence-band absorption, together with the evolution of excitonic features under strong photoexcitation; this yields the full-time evolution (real and imaginary parts) of ε(ω,t) and clarifies electron–electron and electron–phonon coupling on sub-ps time scales.

In $LaCoO_3$ thin films, TRSE reveals a photoinduced insulator-to-metal transition with spectral-weight transfer to low energies, followed by an ultrafast relaxation and, between 1–30 ps, a second maximum whose kinetics and thickness dependence evidence coherent acoustic phonons that transiently modulate the optical constants.

Complementarily, imaging ellipsometry applied to spin-coated oxides demonstrates its utility for metrology and function: thickness/optical-constant mapping and fabrication of Co_3O_4/CeO_2 diodes with reproducible rectification, all within a low-cost deposition platform.

Finally, for layered chalcogenides, recent results obtained outside our TRSE setup show that GaS acts as a reconfigurable optical material: laser-induced structural modification persistently tunes the band structure and refractive index with low loss, enabling sub-wavelength patterning and programmable optical elements.

Taken together, TRSE, TR-XRD, and imaging ellipsometry form a quantitative toolbox to read and design ultrafast optical functionalities in oxides and chalcogenides, from fundamental dynamics to scalable device integration.

2:40pm **MB1-WeA-3 The Role of Contaminants in the Microstructural Evolution of Defects in Low-Emissivity Glazing at High Temperatures***, Phillip Rumsby* ***[phillip.rumsby@etud.polymtl.ca]****, Bill Baloukas, Oleg Zabeida, Ludvik Martinu,* Polytechnique Montréal, Canada

Silver-based coatings present exceptional optical and electrical properties, garnering them significant interest in applications requiring multifunctional optical filters. Amongst these are low-emissivity (low-E) windows. These dramatically reduce radiative heat transfer, improving the energy efficiency of window units while simultaneously providing highly transparent and aesthetically pleasing glass facades. However, Ag films present specific challenges in terms of their chemical and high-temperature stability, which must be managed with an appropriate combination of protective layers (hard coatings, diffusion barriers, metallic interface layers).

In this work, we investigate the processes by which minor mechanical defects in said protective layers evolve during glass tempering. This process, in which coated glass is heated at temperatures in excess of 650 °C, can cause small, practically invisible scratches, formed during glass cutting and handling, to develop into highly visible features. This can lead to entire panes of glass being rejected late in the fabrication process.

First, the multiple mechanisms participating in coating degradation are isolated and their interplay is analyzed: indeed, in addition to purely microstructural changes, disruption of the protective films allows diffusion of both atmospheric and substrate contaminants to the Ag layer, such as O_2, H_2O, and Na. The effect of different combinations of contaminants is thus evaluated by annealing partial stacks with various barrier layer configurations in controlled environments and on substrates of different composition, allowing one to control contaminant availability. Subsequent optical, electrical and microstructural analyses reveal key differences in the Ag dewetting behavior induced by O_2 and Na exposure.

Defects with repeatable morphological features are then generated using a microscratch tester with a diamond tip indenter. The effect of defect types and tempering conditions on scratch visibility is then compared quantitatively by image analysis of dark-field photographs. This reveals that atmospheric contaminants play a dominant role in scratch intensification. Investigation of the coating microstructural features leading to this increase in visibility is performed by both scanning and transmission electron microscopies; this indicates that large Ag particles (≈ 1 µm) formed at the scratched surfaces are not the main contributor. Rather, particles formed inside the coating, with restricted sizes (≈ 100 nm) contribute to scattering much more strongly, as evidenced by Mie scattering calculations.

3:00pm **MB1-WeA-4 Thermochromic VO_2-Based Coating for Energy-Saving Smart Windows: Design and Scalable Synthesis***, Jaroslav Vlcek* ***[vlcek@kfy.zcu.cz]***, University of West Bohemia, Czechia **INVITED**

Vanadium dioxide (VO_2) exhibits a reversible phase transition from a low-temperature monoclinic VO_2(M1) semiconducting phase to a high-temperature tetragonal VO_2(R) metallic phase at a transition temperature of approximately 68 °C for the bulk material. The automatic response to temperature and the abrupt decrease of infrared transmittance with almost the same luminous transmittance at the transition into the metallic state make VO_2-based coatings a promising candidate for thermochromic smart windows reducing the energy consumption of buildings.

We report two different types of high-performance thermochromic coatings synthesized on standard soda-lime glass at a low substrate temperature of 320-350 °C: three-layer YSZ/$V_{0.855}W_{0.018}Sr_{0.127}O_2$/$SiO_2$ coatings, where YSZ is yttria-stabilized zirconia, prepared using a scalable (proved by a successful transfer to a large-scale roll-to-roll deposition device with ultrathin flexible glass substrate) sputter deposition technique, and even higher-performing coatings with four layers of subwavelength W-doped VO_2 nanoparticles dispersed in SiO_2 matrix prepared using a two-step process, combining magnetron sputter deposition and postannealing in oxygen. The coatings exhibit a transition temperature of 22-33 °C with an integral luminous transmittance T_{lum} > 60% and a modulation of the solar energy transmittance ΔT_{sol} > 10%. Such a combination of properties, together with the low substrate temperature in both cases, fulfill the requirements for large-scale implementation on building glass (glass panes, or flexible glass and polymer foils laminated to glass panes) and have not yet been reported in the literature.

We present and explain the fundamental principles of both developed low-temperature (usually used temperatures are higher than 450 °C) preparation techniques and the design of these thermochromic coatings. Moreover, we explain the effect of Sr in the W and Sr co-doped VO_2 on the electronic structure and the enhanced thermochromic properties of the three-layer YSZ/$V_{0.855}W_{0.018}Sr_{0.127}O_2$/$SiO_2$ coatings, and the effect of the discontinuous W-doped VO_2 microstructure on the very promising thermochromic properties (ΔT_{sol} > 15%) of the coatings with four layers of W-doped VO_2 nanoparticles dispersed in SiO_2 matrix.

3:40pm **MB1-WeA-6 Designing Light-Active Thin Film Heterojunctions: Band Alignment and Layer Engineering for Efficient Photocatalysis***, Monserrat Bizarro* ***[monserrat@materiales.unam.mx]***, UNAM, Mexico **INVITED**

The design of functional thin films capable of harvesting visible light for photocatalytic processes relies critically on controlling charge transport and interfacial phenomena. While the formation of semiconductor heterojunctions in nanoparticles or powdered materials has proven to be a powerful approach to improve carrier separation and extend light absorption, the actual mechanisms that govern the performance of *thin-film* heterostructures—where photocatalysis is inherently surface-dominated—remain poorly understood.

In this work, we explore how stacking order and interfacial electric fields define the photocatalytic response in two representative systems: ZnO/Bi_2O_3 and BiOBr/BiOI thin-film heterojunctions prepared by spray pyrolysis. Each semiconductor was first deposited as an individual layer to establish its structural, optical, and electronic properties, and then combined in two configurations (A/B and B/A) to evaluate the influence of layer sequence. Detailed microstructural analyses confirmed the formation of well-defined physical junctions and excluded the presence of new ternary phases. Band positions, carrier concentrations, mobilities, and Fermi levels were determined to construct energy band diagrams that explain the observed photocatalytic trends.

Under blue or simulated sunlight irradiation, the heterostructures exhibited a pronounced dependence of activity on stacking order. Configurations in which the semiconductor with the wider band gap and less negative conduction band (ZnO or BiOBr) occupied the surface achieved superior photocatalytic efficiency toward dye degradation, attributed to favorable band alignment, internal electric fields that drive charge migration, and reduced recombination at the interface. Conversely, reversing the stacking sequence quenched the photocatalytic response, highlighting the delicate interplay between layer order, thickness, and interfacial charge transfer.

These findings demonstrate that thin-film heterojunctions can be rationally designed to enhance surface photocatalytic activity through precise control of band alignment and interface fields. Beyond their relevance for environmental photodegradation, such insights are broadly applicable to solar energy conversion, photoelectrochemical devices, and other light-assisted surface reactions, positioning thin-film heterostructures as a versatile platform for functional materials engineering.

Tribology and Mechanics of Coatings and Surfaces
Room Town & Country C - Session MC3-2-WeA

Tribology of Coatings and Surfaces for Industrial Applications II

Moderator: Osman Eryilmaz, Argonne National Laboratory, USA

2:00pm **MC3-2-WeA-1 Tailoring and Designing High-Performance Carbon Coatings - Insides in Recent Developments and New Approaches for Tribological Applications**, ***Dominic Stangier [dominic.stangier@oerlikon.com]***, Oerlikon Balzers Coating Germany GmbH, Germany **INVITED**

The deposition of diamond-like carbon coatings is an established approach to enhance the service life of tribologically stressed components and tools for industrial applications. Due to today's challenges of reduced lubrication, increased thermal and tribological loads as well as the demand for improved performance and service life, conventional and standardized existing thin films solutions are often limited in their wear-resistance and therefore provide insufficient protection. To overcome these challenges, tailored and application-specific coating systems have gained enormous interest in the field of carbon coatings. On the one hand the efficient deposition of these coating designs requires often a combination of advanced plasma technologies, as well as on the other side the possibility of chemically doping the amorphous carbon network to adjust the property profile. In this regard, the deposition of ta-C coatings by cathodic arc evaporation was found to be an excellent solution, which allows the adjustment of mechanical properties in a broad range as well as offers the possibility to combine different plasma technologies for the deposition of functional multi-layer designs. However, the key challenge is the evaporation of the carbon cathode, which was conducted by an industrial scale arc source (APA evaporator) using a dynamic controlled electro-magnetic field generated by a coil system to steer the arc spot motion and control the deposition conditions. This technology enables the modification of the tribological properties for the running-in phase and the "stationary" wear behavior by adjusting the coordination of the carbon network (sp^3/sp^2-ratio) as well as the chemical composition. In addition, the results reveal the possibility of controlling the intrinsic residual stresses of ta-C coatings to improve the coating adhesion. Furthermore, tailoring the properties was conducted by doping small amounts of Si in ta-C coatings for increasing the thermal stability, which therefore extends the application field of the coating systems.

2:40pm **MC3-2-WeA-3 Advanced Coating and Surface Techniques in Modern Automotive Tribology**, *Sung Chul Cha,* Hyundai Motor Group-Hyundai Kefico, Republic of Korea; *Kyoung Il Moon, Hae Won Yoon,* KITECH, Republic of Korea; *Jongkuk Kim,* KIMS, Republic of Korea; ***Gi-Hoon Kwon [kgh9900a@kitech.re.kr]***, KITECH, Republic of Korea

This paper presents low-friction coating technologies for automotive tribology applied over the past 20 years. In the era of eco-friendly vehicles, particularly electric vehicles (EVs), it is essential to develop suitable coating technologies. Hyundai Motor Group has forecasted mobility trends for 2035: strong HEVs will account for 23% in 2035 (16% in 2024), plug-in HEVs 26% (8%), and battery EVs 38% (13%). By 2035, eFuel capacity is expected to increase from 3 billion liters to 100 billion liters. Global coating companies are developing technologies using hybrid process, low temperature coating process for polymer material, high ionization and high speed. Oerlikon-Balzers has introduced ta-C coatings for polymer materials, as well as MoN and ta-C coatings for automotive components. As a major research institution, Fraunhofer IWS in Germany presented Si- and B-doped ta-C coatings for applications up to 500 °C. RWTH Aachen University's IOT developed coatings with a graded structure, consisting of S-rich and Mo-rich layers on CrAlN, to achieve low friction on plastic substrates. Recent developments in low-friction coatings presented at ICMCTF were analyzed, and the findings are included in this work. In Korea, R&D efforts focus on developing ultra-low friction coatings for extreme conditions, such as those found in EV components. Current coatings exhibit a coefficient of friction (CoF) of 0.05, while ultra-low friction coatings (CoF 0.01) include nitrides and ta-C doped with elements such as ZrCuSi, ZrMoTi, MoZrTiSi, and ZrMoTiCuSi. To address the corrosion issues of SiO-DLC caused by bioethanol fuels, ta-C coatings have been successfully applied, demonstrating high hardness (66 GPa), low friction (CoF 0.05), thermal resistance up to 500 °C, and excellent corrosion resistance. Furthermore, to enhance the frictional performance of coatings, electrochemical polishing technique (DLyte) has been employed, resulting in a significant reduction in surface roughness (Ra from 0.4 µm to 6 nm).

3:00pm **MC3-2-WeA-4 Development and Evaluation of TiAlVSiCN Coatings for Automotive Applications**, ***Jianliang Lin [jlin@swri.org]***, Southwest Research Institute, San Antonio Texas, USA

To increase the fuel efficiency of diesel engines or enhance the performance of racing vehicles, reducing the friction of moving components, such as piston rings and valvetrain parts, is critical, particularly at low engine speeds and loads. Therefore, there is a strong need to develop novel, low coefficient of friction (COF), and robust tribological coatings. In this research, low friction titanium–aluminum–vanadium–silicon–carbon–nitride (TiAlVSiCN) nanocomposite coatings were developed by sputtering Ti-6Al-4V targets in a reactive gas mixture using high power impulse magnetron sputtering (HiPIMS). The chemistry and microstructure of the TiAlVSiCN coatings were tuned by varying the gas flow rate. The tribological behavior of the coatings deposited on stainless steel coupons was evaluated using ball-on-disk and block-on-ring wear tests in SAE 10W-30 engine oil (no additives). The TiAlVSiCN coatings with thicknesses in the range of 6-10 µm exhibited tunable hardness in the range of 15–35 GPa, and the lowest COF of 0.03 and wear rate of $4.8x10^{-9}$ $mm^3N^{-1}m^{-1}$ under lubricated conditions. The optimized coating, offering the best combination of low COF and wear resistance, was deposited on piston rings and further evaluated using a TE 77 bench test. Its performance was compared with an OEM diamond-like carbon (DLC) coating and a traditional low friction TiSiCN coating. The TiAlVSiCN coating demonstrated superior performance compared to both the OEM DLC and TiSiCN coatings in terms of sliding friction, smooth run-in behavior, galling resistance, and wear resistance. The TiAlVSiCN coating was subsequently applied to piston rings and tested in an internal combustion engine. The results of the engine tests, in comparison with OEM DLC coatings, will be updated.

3:20pm **MC3-2-WeA-5 New Carbon High Productivity / Low Temperature Coater with New Temperature Measurement and New Colour Coating**, ***Markus Esselbach [markus.esselbach@oerlikon.com]***, Oerlikon, Liechtenstein

Despite the long legacy of carbon coatings in the PVD world, there are still many possibilities to stretch the boundaries of what is possible. With the new coating platform INSPIRA Carbon Mega we were able to develop a new PVD / PACVD coating machine reducing significantly machine production costs and coating temperature at the same time. A new, fast temperature measurement that allows an accurate in situ temperature indication on the turning part during process will be presented and gives a new dimension of insights in the design of coating process ensuring not to overheat sensitive substrates even in short periods of the process. The machine can provide the whole range of smooth carbon coatings from WCC to DLC to hydrogen free DLC coatings with up to 40 GPa hardness with low dependence on loading geometry. Additionally, a new black coating with extremely low L-Value and high hardness is available on this machine and will be presented.

3:40pm **MC3-2-WeA-6 Evaluation of Boriding as a Post-Treatment to Improve the Thermal Stability and Tribological Performance of Weld-Repaired Tool Steels**, ***Cesar Resendiz Calderon [resendiz.cesar@tec.mx]***, *Leonardo Farfan Cabrera,* Tecnologico de Monterrey, Mexico; *Enrique Campos Silva,* Instituto Politecnico Nacional, Mexico; *Edgar Ravelo Santos, Mateo Roux Reyna, Sebastian Garcia Barragan,* Tecnologico de Monterrey, Mexico

Metal deposition processes for component repair are gaining attention as a practical alternative to replacement. Yet, welding-based methods can alter microstructures and reduce mechanical integrity, especially in high-carbon steels. Such effects are critical in components exposed to elevated temperatures and demanding service conditions. In this study, the effectiveness of boriding as a post-conditioning treatment to improve wear resistance and reduce tribological heterogeneity is investigated, with special attention to its stability under long-term high-temperature exposure. A repair process based on welding was simulated on AISI H13 tool steel. AISI 308L austenitic stainless steel and ERNiFeCr-2 alloys were used as filler materials for the restoration using the GTAW technique. After metal deposition, a pack-boriding treatment was applied to form a continuous boride layer over the repaired surfaces. Half of the borided samples were exposed to 700 °C for 240 h to evaluate their thermal stability. Surface hardness, coating adhesion, and tribological performance were characterized before and after thermal exposure, both in the repaired and non-repaired regions, using nanoindentation, scratch testing, and dry reciprocating sliding tests. Surface damage and wear mechanisms were analyzed by scanning electron microscopy, and the wear volume was quantified through optical profilometry. Boriding proved effective in reducing mechanical property mismatches between the base and repaired regions and in enhancing the tribological performance of repaired H13 steel, even after prolonged high-temperature exposure. The treatment was particularly beneficial for samples repaired with stainless steel filler metal.

Plasma and Vapor Deposition Processes
Room Town & Country B - Session PP2-2-WeA

HiPIMS, Pulsed Plasmas, and Energetic Deposition II

Moderators: Arutiun P. Ehiasarian, Sheffield Hallam University, UK, **Tetsushide Shimizu**, Tokyo Metropolitan University, Japan

2:00pm **PP2-2-WeA-1 Understanding the Hyper-Power Impulse Magnetron Discharge and related Arc Transition***, **Tiberiu Minea [tiberiu.minea@universite-paris-saclay.fr]**, Erwan Morel, Zakaria Belkaid, Adrien Revel,* University of Paris-Saclay, France **INVITED**

High-power impulse Magnetron Sputtering (HiPIMS) has already proven its advantages over conventional magnetron discharge. Using refractory metals or graphite as target materials paved the way for much higher current densities in HiPIMS exceeding 10 A cm^{-2} [1]. In addition, replacing the argon with helium leads to even higher currents, despite the discharge transition from glow to arc, under certain conditions.

The experimental findings suggested the crucial role played by self-sputtering at high voltage (~1 kV) and gas recycling at a lower pulse voltage [2]. Recent global modeling proved this scenario and unveiled microscopic information on the He/Mo HiPIMS discharge [3]. A cross-correlation with a high-speed gated camera and optical emission spectroscopy measurements revealed the plasma evolution [2]. The electron density is highly dependent on the presence of metal vapor in the plasma.

Gas preionization (low DC current) significantly improves the current rise to 1 kA when a high voltage pulse is applied, even for long pulses of 1,000 µs. Five times more power can be transferred into the plasma compared to the HiPIMS without preionization. Consequently, this operation mode has been referred to as the Hyper-Power Impulse Magnetron (HyPIM) [4]. The metastable gas states effectively sustain this high-density plasma in glow mode [5].

The glow-to-arc transition is known to be triggered by very high current densities impinging on the target or high plasma densities. Both are present in the new HyPIM discharge. The early stage of cathodic spot formation, observed as bright dots, can preserve the glow mode or turn into a hot spot. The energy of cohesion and sublimation of the target material certainly play a key role in the transition to arc [6].

Finally, the co-existence of an arc with a diffusive glow discharge, initiated by a HiPIMS pulse, shows a hybrid glow-arc regime with interesting properties. [7]

[1] E. Morel et al., PSST 30 (2021) 125001; https://doi.org/10.1088/1361-6595/ac3341

[2] E. Morel et al., J. Appl. Phys. 133 (2023) 153301; https://doi.org/10.1063/5.0145547

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2:40pm **PP2-2-WeA-3 Plasma Characteristics, Microstructure, and Mechanical Properties of Tetrahedral Amorphous Carbon Thin Films Deposited by Time-Resolved High-Power Impulse Magnetron Sputtering with Synchronized Bias Control***, **Fu-Sen Yang [D11103004@mail.ntust.edu.tw]**, Yu-Lin Kuo,* National Taiwan University of Science and Technology, Taiwan*; Chi-Lung Chang,* Ming Chi University of Technology, Taiwan, Republic of China

Time-resolved ionization analysis of graphite plasma discharges was conducted using optical emission spectroscopy (OES) and plasma mass spectrometry (PSM) during high-power impulse magnetron sputtering (HiPIMS). During the pulse-on period, the generation sequence of argon and carbon ions is synchronized with the HiPIMS target power supply through the bias control system. The timing of the bias output is then regulated to adjust the incident flux and kinetic energy of these ions, thereby enabling the deposition of a tetrahedral amorphous carbon (ta-C) thin film. The effects on plasma characteristics, microstructure, chemical composition, and mechanical properties were studied. Plasma characteristics were analyzed using time-resolved OES and PSM on a graphite target.Time-resolved analysis revealed that argon ions were generated first, followed by carbon ions. By setting synchronization (Syn.) and delay times (TD = 0, 25, 50, 75, 100, 125, and 150 µs) at the bias trigger, the attraction and arrival sequence of argon and carbon ions at the substrate were controlled, thereby regulating the incident ion flux and energy to facilitate the deposition of the tetrahedral amorphous carbon (ta-C) thin film. The thin film analysis results indicate that all ta-C thin films deposited under different trigger synchronization and delay times exhibit an amorphous structure. However, transmission electron microscopy (TEM) analysis reveals that the crystallinity of carbon nanocrystals improves progressively with increasing delay time. The density of the ta-C thin film was determined using X-ray reflectivity (XRR) analysis, and the results showed that the thin film reached a maximum density of 2.95 g/cm^3 at a trigger delay time of 125 µs. The chemical and mechanical analyses revealed that in the synchronous mode, the maximum compressive stress reached -5.6 GPa, the I_D/I_G ratio was 0.52 at a trigger delay time of 125 µs, the sp^3 content was 70%, the hardness reached 48 GPa, and the Young's modulus was 263 GPa. This is primarily because a longer trigger delay time allows more carbon ions to be attracted for bombardment while reducing argon ion bombardment, thereby preventing the conversion of sp^3 to sp^2 bonds caused by thermal effects.

3:00pm **PP2-2-WeA-4 Carbon Discharge Dynamics by Pulse Sequencing: Pulse Parameter Control in Multipulse Hipims***, Ryo Sakamoto,* ***Tetsuhide Shimizu [simizu-tetuhide@tmu.ac.jp]***, Tokyo Metropolitan University, Japan

Amorphous carbon (a-C) thin films exhibit excellent mechanical properties. However, a-C films formed by sputtering often show reduced density and hardness due to the low ionization rate of carbon species. The High-Power Impulse Magnetron Sputtering (HiPIMS) technique employs high-density plasma generated by applying short, high-power pulses to the target. A major issue in HiPIMS, however, is ion back-attraction, in which ionized sputtered species are drawn back toward the target by the applied voltage. To address this issue, the multipulse HiPIMS approach applies a train of ultra-short pulses to enhance discharge efficiency through pre-ionization and suppress ion back-attraction, thereby promoting the transport of carbon ions toward the substrate. In this study, the effects of pulse parameters, specifically pulse width and pulse interval on HiPIMS carbon discharge were investigated using energy-resolving time-of-flight mass spectrometry (ETOFMS) during multipulse HiPIMS discharges of a graphite target in an argon atmosphere. The discharge conditions included varying the pulse width to 20, 30, and 50 µs, and the pulse interval to 10, 20, and 50 µs, with the number of sequential pulses fixed at five. Under these conditions, ion energy distribution functions (IEDFs) were measured for Ar^+, Ar^{2+}, C^+, and C^{2+} ions in both time-averaged and time-resolved modes. As results, a high-energy tail was observed in the C^+ion energy distribution at shorter pulse width (t_{on}), while both C^+ and Ar^+ion fluxes increased with a higher number of pulses at longer t_{on}. In contrast, shortening the pulse-off time (t_{off}) led to a significant increase in the ion energy of C^+ ions. Furthermore, time-resolved measurements revealed that the C^+ ion intensity continued to increase with the number of pulses when t_{off} was reduced to 10 µs, indicating enhanced pre-ionization in after-glow plasma by short pulse interval.

3:20pm **PP2-2-WeA-5 Understanding the Impact of Kinetic and Potential Ion Energies on Thin Film Structure Toward Low-Temperature Deposition***, Dmitry Kalanov, Andre Anders,* ***Yeliz Unutulmazsoy [yeliz.unutulmazsoy@iom-leipzig.de]****,* Leibniz Inst. of Surface Eng. (IOM), Germany **INVITED**

Over recent years, we have investigated how energetic thin film deposition techniques can reduce conventional substrate temperature requirements, focusing on pulsed filtered cathodic arc deposition. Our work investigates the effect of ion potential energy on thin film structure. The main research questions are: How can the influence of ion kinetic energy, ion potential energy, and ion flux on film structure be studied while decoupling these parameters as much as possible? What is the isolated effect of ion potential energy?

Decoupling these effects is challenging because ion kinetic and potential energies are inherently coupled in cathodic arc plasmas. We applied an external magnetic field to preserve multiply charged ions and conducted comparative studies. The results demonstrate that an increased fraction of multiply charged ions enables the formation of crystalline films without conventional substrate heating. Crystalline, dense, and macroparticle-free metallic (V-Al) and ternary nitride (V-Al-N) films were successfully deposited at room temperature, facilitated by the ion potential energy provided by multiply charged ions[1,2], due to a mechanism known as *"atomic-scale heating."*

These insights could help to reduce or partially replace conventional substrate heating in various energetic deposition processes, lowering energy consumption and enabling thin film deposition on temperature-sensitive substrates. This approach can be critical for sustainable surface engineering across various materials systems.

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Topical Symposium on Sustainable Surface Engineering Room Palm 5-6 - Session TS2-1-WeA

Coatings and Surfaces for Renewable Energy Technology I

Moderators: Arnaud Le Febvrier, Uppsala University, Sweden, **Marcus Hans**, RWTH Aachen University, Germany

2:20pm **TS2-1-WeA-2 Strain Engineering of ScN Thin Film by HiPIMS and Its Effect on Optical, Electrical and Thermoelectric Properties***,* ***Arnaud le Febvrier [arnaud.lefebvrier@kemi.uu.se]****, Sanath Kumar Honnali,* Uppsala University, Angstrom Laboratory, Sweden*; Charlotte Poterie,* Universite de Poitiers-CNRS, France*; Tiago V. Fernandes, Robert Frost,* Uppsala University, Angstrom Laboratory, Sweden*; Vladyslav Rogoz,* Linköping University, Sweden*; Martin Magnuson,* Linkoping University, Sweden*; Fabien Giovannelli,* Université de Tours, France*; Joaquim P. Leitão,* Universidade de Aveiro, Portugal*; Jean Francois Barbot,* Universite de Poitiers-CNRS, France*; Per Eklund,* Uppsala University, Angstrom Laboratory, Sweden

Scandium nitride (ScN) is a cubic NaCl-structured, degenerated narrow-bandgap n-type semiconductor with an indirect bandgap of ∼0.9 eV and a direct band gap estimated at around 2.6 eV. It has remarkable semiconducting phonon-polariton application, electrical, thermoelectric and piezoelectric application. The physical properties of ScN nitride are sensitive to defects such as crystal defect, morphology, intentional or unintentional doping. In this work, the impact of strain on the electrical transport properties and optical properties has been investigated. For the purpose of reducing the deposition temperature of ScN, High power impulse magnetron sputtering (HIPIMS) technique was used to produce a series of film on c-sapphire in a 250-850 °C temperature range. The composition and overall crystal structure of the film remained relatively the same in the sample series while its optical and electrical properties were deteriorated upon temperature decrease. Using in depth XRD, optical and electrical characterization, the effect of strain and dislocation on the semiconductor properties of ScN was evaluated. A reduction of deposition temperature from 850 °C to 450 °C yield a slow degradation of the electrical, and optical properties to a drastic change for a film deposited below 450 °C. Below 450 °C, the films present a high dislocation density (10^{11} m^{-2}) along with a rhombohedral distortion of ScN cell (α: 90° → 88.6°) being the main cause of electrical transport deterioration (σ/10000; n/100, µ/100). The presence of dislocation / crystal defect in the film creates defect states near the valence and conduction bands which impact the electron density, hence their correlated electrical transport and thermoelectric properties. To the best the ScN shows promising thermoelectric properties and having an orange appearance when grown at high temperatures while behaving like a poor semiconductor with a black appearance when grown at low temperature.

2:40pm **TS2-1-WeA-3 1D & 2D Material-Based Electronic Devices for Energy Harvesting and Sustainable Technology***,* ***Elisabetta Dimaggio [elisabetta.dimaggio@unipi.it]****,* University of Pisa, Italy **INVITED**

As we move toward a greener economy, sustainability must be at the core of any technological advancement. In a future filled with smart devices and driven by the Internet of Things (IoT), the design of integrated electronic circuits requires new approaches that target environmental friendliness, and renewable energy sources for power. Our efforts in this direction focus on harvesting energy from sustainable sources following standard Integrated circuits (IC) techniques. In the talk, innovative approaches for on-chip thermoelectric devices (TED) will be presented, exploiting silicon nanostructures as core components, and based on classic IC fabrication technologies[1,2]. The reason for using silicon nanostructures stems from their distinctive properties in terms of electrical conductivity and Seebeck coefficient, which can be tailored with technological solutions, and low thermal conductivity. Two strategies will be discussed. The first focuses on enhancing the Seebeck coefficient via the energy filtering effect, achieved by introducing multiple energy barriers, each tens of nanometers wide, through selective doping of silicon nanomembranes. The second involves the development of a prototype on-chip TED that integrates numerous silicon nanobeams into a compact device measuring only a few square millimeters. These devices can generate several milliwatts of power from hot surfaces, enabling low-power electronic systems, such as sensor nodes, to operate in a battery-less mode.

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[2] A.Masci, E.Dimaggio, N.Neophytou, D.Narducci, G.Pennelli, *Large Increase of the Thermoelectric Power Factor in Multi-barrier Nanodevices*, **Nano Energy** 132, 110391, 2024

3:20pm **TS2-1-WeA-5 Harnessing the mechanical and magnetic energy with PMN-PT/Ni-Mn-In-based flexible piezoelectric nanogenerator***,* ***Satyam Shankhdhar [satyam_s1@ph.iitr.ac.in]****,* Indian Institute of Technology Roorkee (IIT R), India

Multifunctional piezoelectric nanogenerators (PENG) hold significant potential in developing smart sensing technologies for the military, healthcare, and industrial sectors. Here, we present the efficient energy harvesting from mechanical and magnetic stimuli in 0.67Pb $(Mg_{1/3}Nb_{2/3})O_3$-0.33$PbTiO_3$ (PMN-PT) / $Ni_{50}Mn_{35}In_{15}$ (Ni-Mn-In)-based PENG fabricated on a flexible nickel substrate using the DC/RF magnetron sputtering technique. The performance of the device has been assessed by imparting forces in the range of 0.12 to 0.61 N using various weights, finger tapping, bending, and magnetic fields. The device generates the maximum open circuit voltage (V_{oc}) of 9.3 V and 6 V with 0.61 N of force and finger tapping, respectively. The corresponding short circuit current (I_{sc}) has been obtained as 1.33 µA (0.61 N) and 0.9 µA (finger tapping). The device shows a maximum V_{oc} of 10.6 V and I_{sc} of 1.51 µA at the bending angle of 120°. Furthermore, the V_{oc} and I_{sc} have increased from 0 mV and 0 nA to 240 mV and 35 nA under the presence of 0 Oe to 500 Oe of DC magnetic field, respectively. The fabricated device exhibited a power density of 2.7 µW/cm^2 with a high mechanical stability of 2500 cycles. Additionally, LEDs of green, red, yellow, and white colour have been illuminated. The receptiveness of the fabricated PENG towards mechanical and magnetic stimuli highlights its potential in areas such as tactile sensing, wearable electronics, human-machine interfaces, and biomedical devices

3:40pm **TS2-1-WeA-6 High Power Impulse Magnetron Sputtering of CoCrFeNiV High Entropy Alloy Thin Films for Enhanced Supercapacitor Applications***,* ***Krishnakant Tiwari [KRISHHH0901@GMAIL.COM]****,* Ming Chi University of Technology, Taiwan*; Bih Show Lou,* Chang Gung University, Taoyuan, Taiwan*; Jyh Wei Lee,* Ming Chi University of Technology, Taiwan

In this study, CoCrFeNiV high entropy alloy (HEA) thin films were successfully deposited on nickel foam substrates using a high power impulse magnetron sputtering (HiPIMS) system for application as advanced electrode materials in supercapacitors. The use of HiPIMS enabled precise control over film composition and enhanced adatom mobility, promoting uniform growth and strong adhesion of the HEA coating on the porous Ni foam surface. Comprehensive materials characterization, including morphological, structural, and compositional analyses, was conducted to understand the evolution of film microstructure during deposition and the elemental distribution across the coating. The electrochemical performance was systematically evaluated through cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy. The CoCrFeNiV HEA electrode exhibited a remarkably high specific capacitance and excellent rate capability, demonstrating superior energy storage characteristics. Furthermore, long-term cyclic stability tests confirmed outstanding charge–discharge durability, highlighting the potential of HiPIMS-deposited CoCrFeNiV HEA thin films as promising electrode materials for next-generation high-performance supercapacitors.

Awards Ceremony and Honorary Lecture
Room Town & Country A - Session HL-WeHL

Bunshah Award Honorary Lecture

5:45pm **HL-WeHL-1 “Chameleon” Adaptive Tribological Coatings: Lessons Learned and Future Outlook***, Andrey A. Voevodin [Andrey.Voevodin@unt.edu]*[1], University of North Texas, USA **INVITED**

Tribological contact surfaces, which can operate in oxidative and high temperature environments are of a practical importance for aerospace applications, where extremes of temperature, pressure, and environments limit liquid lubrication and requires solid lubricants and robust wear-protective coatings. This presentation discusses surface engineering concepts for preparing self-adaptive coatings and contact surfaces, called “chameleon”, for friction and wear reduction under oxidative environments and high temperatures. Several key mechanisms which can be self-evoked by the tribological contact mechanical, chemical and temperature stimuli are discussed, including straining, re-orientation, phase transformations, diffusion, and oxidation, and how these mechanisms can be guided to reduce friction and wear of contacts in environments with variable and cycled environments and temperatures. Surface engineering concepts and coating designs which may allow for such mechanism operations are used as examples for the discussion. These include composite coatings made of hard nano-crystalline carbide, nitride and oxide matrices with nano-sized inclusions of solid lubricants and transition metals capable of surface diffusion or forming high-temperature lubricating oxides, duplex coatings based on plasma electrolytic oxidation with controlled surface morphology and embedded adaptive lubricants, solid lubricants made of intrinsically layered solids allowing hexagonal plane reorientation and self-assembly, and other. Lessons learned in exploring and testing such conceptual mechanisms are applied to outline future perspectives and opportunities for engineering self-adaptive tribological surfaces.

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[1] **R.F. Bunshah Awardee Honorary Lecture**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

In this framework, unsupervised learning algorithms are applied to analyze the high-speed indentation dataset, identifying clusters of mechanical behavior. These mechanically defined clusters guide targeted investigations into microstructural and micromechanical properties. The analysis utilizes micropillar compression data from over 200 pillars across different regions of interest to directly assess yield strength and strain-hardening behavior.

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

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

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

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

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

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

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

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

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

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

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

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

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3. Y. Matsuda et al, Wear, **259**, p. 1497–1501 (2005)

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Surface Engineering - Applied Research and Industrial Applications
Room Palm 1-2 - Session IA3-ThM

Innovative Surface Engineering for Advanced Cutting and Forming Tool Applications

Moderators: Markus Esselbach, Oerlikon Balzer, Liechtenstein, **Fan-Yi Ouyang**, National Tsing Hua University, Taiwan

8:20am **IA3-ThM-2 Tool–Embedded Piezoresistive Thin–Film Sensors for Guide–Pad Normal Force Measurement in Deep Hole Drilling**, ***Martin Rekowski [martin.rekowski@ist.fraunhofer.de]**,* Fraunhofer IST, Germany*; Lucas Brause, Sebastian Michel,* TU Dortmund University ISF, Germany*; Anna Schott, Christoph Herrmann,* Fraunhofer IST, Germany*; Dirk Biermann,* TU Dortmund University ISF, Germany

Deep hole drilling is essential for producing long, high-quality bores in safety–critical components such as hydraulic cylinders, turbine shafts, and fuel injectors. Its asymmetrical tool design and guide pad support enable excellent straightness and surface finish, but the contact zone experiences severe thermo–mechanical loads and steep temperature gradients followed by rapid oil quenching. These conditions can induce residual stresses and micro-structural alterations (e.g., white etching layers), directly affecting surface integrity and fatigue performance. Because the contact zone is inaccessible, workpiece-side measurements are limited and often require post-process analysis. Miniaturized thin-film sensors integrated directly into the tool's guide pad offer a robust and space-saving way to measure temperature, normal force, and wear in the force flow in real time. This paper details the design, fabrication, and characterization of a tool–embedded piezoresistive thin–film sensor system for measuring guide pad normal force with integrated temperature compensation. A 6 µm hydrogenated carbon DiaForce® (DLC) layer is deposited on a polished and hardened high-speed steel substrate (Rz = 0.1 µm) using plasma enhanced chemical vapor deposition (PECVD) process. Electrodes and conductive tracks are applied in a 0.2 µm thick chromium layer, which is deposited using physical vapor deposition (PVD) and patterned with photolithography and wet chemical etching. The stack is insulated and protected with SICON® layers. Three sensor structures (F1–F3) are positioned in the force flow to resolve normal loads, while additional unloaded DiaForce® electrodes act as temperature references to decouple thermoresistive drift from the force signals. Two overlapping thin steel washers (t = 150 μm) ensure uniform electrode loading. The overlap and thus the area of the loaded surface was determined in preliminary tests and can be adapted to the respective measurement conditions. Shielded leads were soldered to the base body and provide connectivity to a telemetry system. Calibration is done by recording resistance changes versus temperature and pressure. The DiaForce® reference electrodes show a decreasing exponential temperature dependency modeled by the Steinhart–Hart equation, enabling real–time compensation of the force signal, while pressure sensitivity is linear to quadratic over the investigated range. Servo–press experiments confirm stable signal deflection under combined mechanical loading and dynamic thermal transients. The thin-film sensor system is applied to both single–lip drilling (SLD) and BTA deep hole drilling

8:40am **IA3-ThM-3 Development of in-Situ Cleaning Processes and Customized Coatings on Numismatic Coinage Dies for Minting Industry**, *João Coroa, Alexander Gorupp, Parnia Navabpour, Giuseppe Sanzone,* ***Hailin Sun [hailin.sun@teercoatings.co.uk]***, Teer Coatings, UK **INVITED**

The minting industry is responsible for the design, production, and distribution of coins and medals both for national currencies and for commemorative purposes. The design and fabrication of coin dies combine expert craftsmanship with state-of-the-art technology which preserves value and celebrates heritage by producing coins of beauty and enduring worth.

The coin dies typically comprise of both highly-polished and frosted areas to create distinct visual contrasts and intricate images. The surface of dies needs to be coated with hard, wear resistant coatings for the die to withstand the force and repeated impact exerted on it during coin production. Physical vapour deposition (PVD) is an environmentally-friendly method used for the deposition of coatings on dies. Some of the processes, such as laser engraving, used in the minting industry during the production of dies have created new challenges for the PVD coatings.

Currently, Teer coatings PVD systems used in the minting Industry are capable of producing coatings for numismatic, proof or circulation coin dies using the PVD magnetron sputtering technique. To overcome the new challenges, an in-situ linear ion source device has been integrated in the coating equipment. It generates a wide, collimated plasma beam for treating large substrates. It is used to pre-clean surfaces by removing the surface oxides and hydrocarbons in order to improve the adhesion of the deposited thin films. At the same time, the process is tailored to ensure that the original features such as roughness, etc. are retained.

This study presents some of the developments which achieve the industrial demands, both through optimised coating design, and through equipment developments that enable the combination of different treatment and deposition technologies to improve the coating performance.

9:20am **IA3-ThM-5 Machining of Hardened Steels under Dry Conditions: Wear Mechanisms of AlTiSiN and AlTiXN-TiSiZN (X, Z= nonmetal elements) Coatings**, ***Rong Zhao [rong.zhao@eifeler-vacotec.com]****, Simon Evertz, Alexander Fehr, Markus Schenkel,* voestalpine eifeler Vacotec GmbH, Germany

To obtain more environmentally friendly and cost efficient production processes, lubricants in milling applications are either removed completely or reduced to a minimum. Thereby, protective coatings for tools gain even more importance. Dry machining of hardened steels presents significant challenges due to elevated temperatures and the simultaneous occurrence of abrasive and adhesive wear. AlTiSiN based coating systems have been the state of the art for milling applications under these demanding conditions. In this study, milling tests were conducted to evaluate the performance of milling tools with different coatings. The coated tools exhibited varying degrees of wear and service life. Hence, understanding the underlying wear mechanisms is decisive for the development and selection of next-generation coatings, as wear is closely linked to tool longevity. Two types of coating systems were investigated: one AlTiSiN coating and one AlTiXN-TiSiZN coating. Wear was analyzed using confocal microscopy, scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy. Distinct wear patterns and mechanisms were identified for each of the coatings. The results demonstrate that the AlTiXN-TiSiZN coating exhibits superior wear resistance, which makes it particularly suitable for milling of hardened steels with a hardness higher than 55 HRC.

9:40am **IA3-ThM-6 Improving Injection Molding Process Performance of Recycled Plastics**, ***Yavor Sofronov [ysofronov@tu-sofia.bg]****, Georgi Todorov, Milko Angelov, Boyan Dochev, Antonio Nikolov, Valentin Mishev, Krum Petrov, Rayna Dimitrova, Milko Yordanov,* Technical University of Sofia, Bulgaria; *Krassimir Marchev,* Technical University of Sofia, USA

The forthcoming European Union Packaging and Packaging Waste Regulation mandates that nearly all plastic packaging incorporate at least 30% post-consumer recycled (PCR) content, creating significant technological challenges for injection molding manufacturers. In particular, the use of recycled polyethylene terephthalate (rPET) is associated with pronounced adhesion to polished mold core surfaces and progressive polymer smearing, leading to frequent production interruptions for mold cleaning and reduced process stability. This study characterizes a functional Ti/TiN/(CrN/TiN)ml low-wettability coating deposited by unbalanced magnetron sputtering on injection mold cores from 1.2343 steel as a mitigation strategy. The coated surfaces exhibit reduced interfacial adhesion between rPET melt and metallic tooling, effectively suppressing polymer smearing and facilitating reliable part release. Peel strength according to ASTM D903 exhibits decreasement from 22.5N for uncoated core to 7.5N for coated which is 3 times reduction. As a result, the injection molding process demonstrates improved operational stability and a measurable increase in productivity. Industrial validation shows that the implementation of the proposed coating solution enables an increase in hourly production rate of approximately 20%, without altering processing parameters or material formulation. The results confirm that surface engineering of mold tooling represents a robust and industrially scalable approach to overcoming rPET-related processing limitations under emerging regulatory requirements.

11:00am **IA3-ThM-10 Over 30 Years of PVD Aluminium-Oxide Based Hard Coatings in Demanding Industrial Applications**, ***Philipp Immich [pimmich@hauzer.nl]****, Louis Tegelaers, Julia Janowitz, Daniel Barnholt,* IHI Hauzer Techno Coating B.V., Netherlands; *Rolf Schäfer, Tobias Radny,* Robeko GmbH & Co. KG, Germany; *Thomas Schütte,* PLASUS GmbH, Germany

Over the past six decades, the requirements for hard coatings in protective applications have increased significantly. The progression from simple TiC monolayer coatings deposited via Chemical Vapor Deposition (CVD) in the 1960s to today's sophisticated multilayer systems has been driven by several key factors: enhanced reliability of industrial coating equipment, continuous optimization of substrate materials and new pre- and post-treatment processes.

Among the most notable advancements are aluminium oxide (Al_2O_3) coatings, which have become a benchmark in modern cutting applications. Their unique phase structures offer performance benefits that are difficult to replicate with other coating systems. Alumina's high hardness, electrical insulation, chemical inertness, and thermal stability make it exceptionally well-suited for demanding environments.

Beyond cutting tools, aluminium oxide is widely used across various industrial sectors. Its mechanical strength and thermal resilience support its role in protective coatings, while its excellent insulating properties are essential for sensor technologies. Additionally, its optical transparency and chemical resistance make it ideal for advanced protective layers.

In cutting tool applications, CVD remains the established method for depositing aluminium oxide. However, over the past 30 years, Physical Vapor Deposition (PVD) has gained increasing relevance, because of the lower deposition temperatures compared to CVD —initially driven by high-temperature cutting applications and more recently expanding into low-temperature applications such as insulating coatings for sensors.

Despite its versatility, scaling the PVD deposition of alumina thin films for industrial use presents several challenges. RF sputtering from compound targets can produce stoichiometric, high-quality coatings, but its low deposition rate limits its practicality for mass production. PVD techniques—particularly dual magnetron sputtering (DMS) from metallic targets—offer significantly higher deposition rates and effectively address issues such as the disappearing anode.

In this presentation, we will highlight ongoing developments in PVD oxide coatings—including innovations in coating equipment and advanced deposition technologies—that are opening new possibilities for enhanced cutting performance and broader industrial applications. We will compare various regulation strategies, examine the properties of alumina films deposited at different temperatures, and discuss future technological improvements that could further optimize deposition processes.

11:20am **IA3-ThM-11 Sputtered CrN-based coating concepts for plastic injection molding**, ***Alexander Fehr [alexander.fehr@eifeler-vacotec.com]***, Voestalpine eifeler Vacotec, Germany

Typical demands in plastic processing are minimized material adhesions, better deformability as well as a certain gloss level of the produced plastic parts. Therefore, surfaces in plastic processing often require mirror-like polishing to produce very smooth plastic parts. Furthermore, there is a challenge with very complex structured plastic molds when it comes to the reproduction of textures on the plastic part. These applications do not only require a wear resistant but also a near net shape surface solution to guarantee a conservation of the gloss level as well as a persistent surface quality of the produced plastic parts. Since plastic injection mold steels typically have a low annealing temperature, a sputtered, low-temperature coating represents a well-suited approach. In this context, the CHROME-X coating solution from voestalpine eifeler Vacotec will be presented with regard on the application on textured surfaces. It will be shown why a sputtered Cr based coating delivers more advantages for PIM applications when compared to an arc Cr based film. Furthermore, the influence of the sputtered coating on the gloss level of the plastic part will be addressed.

11:40am **IA3-ThM-12 Study on Multilayer Thick ta-C Coating Process on Cutting Tools for CFRP Machining Using Filtered Cathodic Vacuum Arc Deposition**, ***Jongkuk Kim [kjongk@kims.re.kr]***, *Jae-Il Kim, Young-Jun Jang,* Korea Institute of Materials Science, Republic of Korea

Carbon fiber reinforced plastic (CFRP) is a composite material consisting of a polymer matrix and carbon fibers, which requires excellent mold release, low friction, and high wear resistance during cutting. To meet these demands, cutting tools are often coated with high-hardness carbon-based films. Among these, tetrahedral amorphous carbon (ta-C) coatings exhibit outstanding hardness and low friction while minimizing chipping and substrate damage due to their nanolayer structure. However, the high intrinsic stress of ta-C limits its achievable thickness, hindering its application as a thick, durable coating.

In this study, a filtered cathodic vacuum arc (FCVA) system was employed to deposit thick ta-C coatings (>2.5 µm) on cutting tools. The effects of substrate bias voltage and process temperature on internal stress were investigated through multilayer film design. The deposition system consisted of an anode-layer ion source, a magnetron sputtering source, and a 90°-bent magnetic FCVA source. Stainless steel strips (100 µm) were used for stress analysis, and WC–Co inserts (15 × 15 mm) were used as substrates.

Prior to deposition, the substrate surface was cleaned using Ar ion etching at 2.5 kV and 400 mA, followed by deposition of a 500 nm Ti buffer layer via magnetron sputtering (6 A). The ta-C films were deposited using the FCVA source with alternating high-hardness (–70 V) and low-hardness (–200 to –500 V) layers, each 250 nm thick, yielding a total thickness of 2.5 µm. Additionally, the low-hardness layer (–500 V) was fixed at 100 nm, while the ratio between high- and low-hardness layers (1:2, 1:3, 1:4) was varied to optimize stress control.

The optimized multilayer structure (–500 V/–70 V, 1:3 ratio) produced a 63 GPa hardness and 4.5 GPa residual stress, enabling stable and uniform deposition even on the cutting edge of the inserts. These results demonstrate that proper stress control through multilayer engineering allows the formation of thick, high-hardness ta-C coatings suitable for CFRP machining applications, offering a promising route to improve tool performance and durability.

Keywords:

ta-C (tetrahedral amorphous carbon); Filtered Cathodic Vacuum Arc (FCVA); Cutting Tool; Hardness; DLC (Diamond-Like Carbon); Wear Resistance

12:00pm **IA3-ThM-13 Enhanced Fe and Ni bonded NbC Laser Surface Engineered Hardmetals: Alternative Cutter Materials for Electric Vehicle Applications**, *Rodney Genga,* University of the Witwatersrand, South Africa*; Suzan Conze, Lutz-Michael Berger, Johanes Pötschke,* IKTS Fraunhofer Institute, Germany*;* ***Julien Witte [julien.witte@bam.de]****, Dirk Schroepfer,* BAM Berlin, Germany*; Adam Čermák, Pavel Zeman,* Czech Technical University in Prague, Czech Republic*; Sinoyolo Ngongo, Arno Janse van Vuuren,* Nelson Mandela University, South Africa

The substitution of tungsten carbide (WC) and cobalt (Co) in hardmetals has gained increased attention in recent years due to the reclassification of Co as a carcinogenic substance and the designation of both Co and W as critical raw materials by the European Union and under the U.S. National Toxicology Program. Thus, this study investigates the development and performance of advanced NbC-based hardmetals utilizing nickel (Ni) and iron (Fe)-based binders as sustainable alternatives for metal machining applications within the electric vehicle (EV) manufacturing sector.

The materials were developed using a Machining Property Led Tailored Design (MPLTD) approach, a reverse engineering strategy that leverages machining performance data to guide the optimization of microstructural, mechanical, and tribological properties. Four novel NbC-based hardmetals were synthesized, two with Ni-based binders and two with Fe-based binders. These were benchmarked against two reference materials: a standard WC-Co composition and a conventional NbC-12Ni grade. Comprehensive material characterization was conducted using field emission scanning electron microscopy (FE-SEM), annular dark-field scanning transmission electron microscopy (ADF-STEM), Vickers hardness testing, fracture toughness measurements, and elastic modulus evaluations.

Cutting tool inserts were manufactured from these hardmetals were further enhanced via femto-second laser surface engineering (Fs-LSE), which was employed to form laser induced chip breakers and modify cutting edge morphology. The microstructural effects of Fs-LSE were examined through ADF-STEM and selected area electron diffraction (SAED) analyses. The performance of both untreated (blank) and Fs-LSE-modified inserts was evaluated through interrupted face milling tests on AZ31 automotive grade magnesium alloy. As AZ31 is considerably lighter than both steel and aluminum, its use in EV components significantly improves power-to-weight ratios and operational efficiency. The laser enhanced Fe- and Ni-bonded NbC inserts demonstrated machining performance comparable to industrial WC-Co benchmark grades. Furthermore, the Fs-LSE process resulted in over 100% reductions in flank wear and up to 80% decreases in resultant cutting forces. The inserts' performance in this study provided valuable insights into the suitability of alternatives to WC and Fs-LSM for automotive industrial applications

Functional Thin Films and Surfaces
Room Palm 3-4 - Session MB2-3-ThM

Thin Films for Emerging Electronic and Quantum Photonic Devices III

Moderators: Jiri Capek, University of West Bohemia, Czechia, **Spyros Kassavetis**, Aristotle University of Thessaloniki, Greece

8:40am **MB2-3-ThM-3 From Passive to Active Structurally Controlled Optical Coatings for Energy, Eyewear and Sensor Applications**, *Bill Baloukas, Martin Crouan, Brandon Faceira, Aleksandra Pajak,* ***Phillip Rumsby [phillip.rumsby@polymtl.ca]****, Oleg Zabeida, Jolanta Klemberg-Sapieha, Ludvik Martinu,* Polytechnique Montréal, Canada

Control of energetic interactions at the surface of the growing thin films allows one to selectively adjust their micro- and nanostructure. This is particularly important when synthesizing optical films by vapor-based techniques such as reactive sputtering (including HiPIMS), evaporation (including Glancing Angle Deposition), Plasma-Enhanced Chemical Vapor Deposition, Atomic Layer Deposition, Ion Beam Assisted Chemical Vapor Deposition, and Gas Agglomeration Cluster formation. As a result, this has become increasingly attractive for judicious fabrication of nanostructured optical filters with controlled film porosity, crystallinity, anisotropy, plasmonic effects, thermo-mechanical properties and other features of both passive as well as active (dynamic – e.g., electrochromic or thermochromic) coating materials with new functionalities.

This presentation will illustrate the progress and new opportunities in structurally controlled passive and active optical coating systems using a holistic approach from design to fabrication and device performance. This will specifically be highlighted by our work on high-performance low-emissivity and smart windows for energy saving in the building sector, energy control in micro/nanosatellites, hybrid (organic-inorganic) coatings and switchable electrochromic systems for ophthalmic lenses including novel transparent flexible electrodes, plasmonic optical filters for gas sensing, and other advanced optical coating devices.

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9:00am **MB2-3-ThM-4 Glancing Angle Deposition of WOx and Cu-doped TiO2 Thin Films for Improved Conductometric Gas Sensing*, Akash Kumar [akashkumarneutronics@gmail.com],*** University of West Bohemia, NTIS, India*; Stanislav Haviar,* University of West Bohemia, NTIS, Czechia*; Nirmal Kumar,* University of West Bohemia, NTIS, India

The emerging hydrogen industry is stimulating efforts in developing new materials for various purposes, including the quest for efficient, sustainable, and low-power hydrogen detectors. Many such devices rely on metal oxide semiconductor materials, which are easily integrable into devices and relatively cheap but suffer from some challenges, such as low sensitivity and selectivity.

This study explores the possibility of exploiting a Glancing Angle (GLAD) sputter deposition of Cu-doped TiO_2 and WO_x films, targeting the enhancement of active surface area and, therefore, sensor sensitivity improvements.

Cu-doped TiO_2 and WO_3 films were deposited using conventional reactive DC magnetron sputtering, employing circular titanium and tungsten targets in a mixture of argon and oxygen. Cu-doping was achieved by using a composite target.Films were post-annealed prior to sensing characterization. The Glancing Angle Deposition (GLAD) technique was employed to induce a characteristic columnar nanostructure, thereby increasing the films' porosity and so leading to a desired increase in active surface area. Multiple parameters were tuned to enhance the sensing response, including the angle of deposition (80°, 85°, 88°), thickness (50–300 nm), and reactive sputtering parameters.

Synthesized films were thoroughly analyzed by SEM and XRD. Sensing response measurements revealed an interesting fact: that neither the surface roughness nor the surface area improves the response to the sensing gas monotonically. In the presented paper, we discuss the geometrical reasons as well as the synthesis parameters that influence the sensing characteristic. The comparison of the two materials, WO_3 and TiO_2, is also given.

9:20am **MB2-3-ThM-5 Sputter Coating of High-Quality Vo2 Metal-Insulator Transition Films for Flexible Electronics*, Juan Andres Hofer [juhofer@ucsd.edu],*** University of California San Diego, USA*; Ali C. Basaran,* General Atomics, USA*; Tianxing Damir Wang, Ivan K. Schuller,* University of California San Diego, USA

The metal-insulator transition (MIT) in vanadium dioxide (VO_2) thin films is a topic of great interest for applications in smart windows, memristors, and neuromorphic computing applications. VO_2 thin films are accompanied by substantial changes in the electronic and optical properties across the MIT, and these changes can be induced by external stimuli such as voltage, strain, or temperature. While several studies have shown that flexible and freestanding VO_2 films can be achieved, complex pre- or post-growth processing is required. In this work, we show that direct sputter deposition of VO_2 on flexible Kapton substrates results in a straightforward methodology to achieve flexible MIT films. A pre-deposited Al_2O_3 layer on Kapton enhances film adhesion, and the resulting flexible VO_2 films show up to 4 decades of change in resistance across the MIT. Temperature and substrate-induced strain during growth affect substantially the quality of the films. The resulting VO_2 flexible devices show ultra-low power consumption for resistive switching, up to two orders of magnitude lower than in samples grown on traditional substrates. We also demonstrate that the VO_2 MIT characteristics can be governed by mechanical deformation, resulting in a novel method to induce resistive switching and decrease power consumption. This study reveals a straightforward approach for direct growth of high-quality flexible VO_2 films exhibiting robust MIT, with promising applications in tactile sensors and electromechanical devices.

Funding Acknowledgment: This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-22-1-0135.

10:20am **MB2-3-ThM-8 - In Situ Electron-Beam-Induced Selective-Area Growth of Tellurium Films by Molecular Beam Epitaxy*, Ossie Douglas [dro3@usf.edu],*** University of South Florida, USA*; Peter Snapp,* NASA Goddard Space Flight Center, USA*; Ali Ashraf,* University of South Florida, USA

Recently, thin films of elemental tellurium (Te) have gained increasing attention due to their intrinsically anisotropic crystal structure and morphology-dependent semiconducting properties. Molecular beam epitaxy (MBE) is an established technique for producing chemically pure, wafer-scale Te films with high morphological precision. However, post-processing of Te films for device fabrication typically relies on masked lithographic techniques, which can inadvertently degrade film quality and electrical performance. While selective-area growth approaches have been explored to mitigate these effects, mask-based methods introduce additional pre-processing complexity and crystallographic constraints. An in situ selective-area growth technique offers a pathway to reduce fabrication complexity while preserving intrinsic film properties.

Here, we demonstrate an in situ process for selective-area growth of Te thin films on muscovite mica (MuM) dielectric substrates using an electron beam generated by a reflection high-energy electron diffraction (RHEED) gun integrated within an MBE system. Spatially selective growth is achieved without physical masking, resulting in millimeter-scale lateral patterning of nanometer-thick Te films, confirmed by optical characterization. Directional control of film growth is realized through azimuthal alignment of the substrate relative to the incident electron beam. The resulting feature dimensions are found to depend strongly on electron beam voltage, exposure duration, and substrate temperature. This approach demonstrates controllable Te film shape and thickness during growth, highlighting new opportunities for direct-write epitaxial patterning within MBE systems.

10:40am **MB2-3-ThM-9 High Tunability in Crystallographic Design of Thin Films Enabled by Atomic Imprint Crystallization*, Koichi Tanaka [ktanaka@anl.gov],*** Argonne National Laboratory, USA*; Xella Doi, Connor Horn, Chloe Tsang, Supratik Guha,* University of Chicago, USA

In general, properties of thin films are dependent on their crystal orientation, and the most common approach to control the crystal orientation of thin films is to utilize epitaxial growth on single-crystalline substrates. Although a variety of materials have been synthesized on single-crystalline substrates using chemical and physical vapor deposition (CVD, PVD), epitaxial growth methods allow us to grow materials into only one fixed orientation predetermined by the substrate orientation, and typically with limited tunability in terms of area or orientation.

In this talk, we report area-selective, orientation-tunable crystallization processes of amorphous Si utilizing atomic imprint crystallization (AIC), where an amorphous Si layer is crystallized by solid phase epitaxy from an external single-crystal Si template. Using a flat template, the top surface of an amorphous Si is crystallized following the crystal orientation of the template wafer up to 5 mm diameter, indicating that the crystallization of the amorphous Si can be initiated by an external template wafer. Using micro-patterned single-crystalline Si templates, limited areas (~50 µm diameter) of an amorphous Si film, where the film surface and patterned template surface are in contact, are crystallized via SPE to create an array of crystallographically aligned dots embedded in amorphous matrix. Combining the AIC from the top surface and conventional SPE from the substrate, we developed new crystallization processes to fabricate unique microstructures such as a twisted interface with a tunable twist angle and an array of crystalline dots embedded in single-crystalline matrix with tunable in-plane rotation angle. The results demonstrate the area-selective, orientation-tunable crystallization process enabled by AIC, controlling crystallographic properties of thin films, which can open up new materials design capabilities for variety of applications in materials science including but not limited to electronics and quantum device applications.

11:00am **MB2-3-ThM-10 Thin Film Processing Strategies for High-Throughput Autonomous Materials Discovery and Development*, Christopher Muratore [cmuratore1@udayton.edu],*** University of Dayton, USA*; Brian Everhart, Drake Austin, Nicholas Glavin,* US Air Force Research Laboratory, USA

The talk highlights automated experimental tools enabling synthesis and characterization of hundreds of samples per day. This approach, where experimentation is much faster than simulation has the potential to flip the traditional 'order of operations' for materials discovery where experiment feeds model during initial iterations.One high-throughput format relies on scanning lasers with broad ranges of power, scan rates, and focal positions to induce physical and chemical transformations within materials. Laser heating parameters may be set to approximate quasi-equilibrium heating as in a furnace, or induce extreme heating and cooling rates, thereby broadening the range of accessible compositions and crystal structures dictated by kinetics of both chemical reactions and crystallization. Deposition tools may also be used to create a broad range of compositions on the sample surface. Once a combinatorial sample with a desired range compositions and laser illumination conditions is processed, it can be manually or autonomously subjected to the combination of high-throughput characterization tools required for evaluation of the properties specified by the user. Autonomous systems enable users to specify a desired property and the system iterates processing and characterization data to 'make decisions' about optimization of conditions to realize the user-specified input.For example, an automated Raman spectroscopy system enables rapid collection of key data points (grain size, defect density, thickness, etc.) for technologically important optical, electronic, and energy materials.Some specific case studies include fundamental kinetics studies showing migration-limited crystallization kinetics amorphous materials can be directly observed.Pre-cursor materials for downstream processing can be converted directly into reaction intermediates with the appropriate non-equilibrium laser energy input to reduce process activation energy and process temperature required for high-quality materials. For photocatalysis materials rapid, non-equilibrium process conditions were identified demonstrating optimized performance with mixtures of phases.

11:20am **MB2-3-ThM-11 Designing Porosity for Function: Polymer-Templated Metal Oxides for Catalysis and Broadband, Wide-Angle Optics***, **Elena V. Shevchenko [eshevchenko@anl.gov]**,* University of Chicago, Argonne National Laboratory, USA*; Diana Berman,* University of North Texas, USA **INVITED**

Nanostructuring metal oxides through controlled porosity provides a powerful route to simultaneously enhance surface reactivity and tailor optical response. By introducing interconnected nanoscale voids into inorganic frameworks, it becomes possible to maximize accessible surface area while engineering light propagation, scattering, and refractive index profiles. Such materials are increasingly important for catalytic, electrocatalytic, sensing, and photonic technologies. This talk will present polymer-directed strategies for fabricating nanoporous metal oxide coatings with precisely controlled architecture and composition. In this approach, sacrificial polymer scaffolds define pore morphology prior to oxide formation. Inorganic precursors infiltrate the template from solution or vapor phases, yielding conformal oxide networks that preserve structural integrity after template removal. The method is compatible with single- and multicomponent systems, enabling the formation of hierarchical structures and functional heterointerfaces.

By tuning pore size, connectivity, and composition, we demonstrate how nanoscale architecture directly governs catalytic activity, charge transport, and light–matter interactions. In particular, controlled refractive index gradients and tailored pore distributions enable broadband antireflective coatings that maintain excellent optical performance across a wide range of incident angles. The resulting materials combine high catalytic efficiency with angularly robust optical functionality, illustrating how rational porosity design transforms metal oxides into multifunctional platforms for energy and photonic applications.

Surface Engineering of Biomaterials, Devices and Regenerative Materials: Health, Food, and Agriculture Applications

Room Town & Country B - Session MD2-2-ThM

Coatings and Sensors for Health, Food and Agriculture: Antibacterial, Bioactive, and Flexible Interfaces II

Moderators: Valentim A.R. Barão, University of Campinas (UNICAMP), Brazil, **Jean Geringer**, Ecole Nationale Superieure des Mines, France

8:00am **MD2-2-ThM-1 Surface Modification of AZ31B by Oxygen-Plasma Immersion Ion Implantation to Promote Schwann Cell Interaction for Peripheral Nerve Regeneration***, **Luciana Malvestiti [luciana.malvestiti.1@ulaval.ca]**, Carlo Paternoster, Francesco Copes,* LBB, CHU de Quebec research center, Laval University, Canada*; Paolo Mengucci, Giani Barucca,* Department SIMAU, Università Politecnica delle Marche, Ancona, Italy*; Silvia Ceré,* INTEMA-CONICET, Mar del Plata National University, Argentina*; Andranik Sarkissian,* Plasmionique Inc., Varennes, QC, Canada*; Diego Mantovani,* LBB, CHU de Quebec research center, Laval University, Canada

Their biocompatibility, electrical conductivity and biodegradability properties, make Mg-based alloys a potential biomaterial for peripheral neuropathy. Even if these alloys release Mg^{2+} cations, fundamental in neurological functions, their high corrosion rate triggers implant failure and tissue damage. To control the degradation pattern, and improve the biological response, a plasma-based technique (oxygen-plasma immersion ion implantation, O-PIII) was used on a Mg-based substrate (AZ31B) to generate a thin MgO layer. In addition, other modified surface properties such as roughness and surface energy, improved the general biological response of the material

O-PIII was performed in a PBII-300 system (Plasmionique) on the surface of chemically polished (CP) AZ31B (Al 3 wt.%, Zn 1 wt.%, Mg bal.) specimens. Pressure (5 to 10 mTorr), and pulse repetition rate (200 to 1000 Hz) were working parameters. The morphological, chemical and electrochemical characterization was performed with scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), static drop contact angle, and polarization curves in Hanks' solution. The cytotoxicity of the corrosion products toward Schwann cells (SC), and the interaction between the modified alloy and SC were studied through an indirect test and adhesion test, respectively.

Plasma treatment introduced different surface features depending on the used parameter values, which affected the morphology, roughness, chemical composition, and corrosion resistance. After O-PIII, XPS revealed an increase in MgO content, accounting for the ~70% total detected oxygen. The hydrophilicity of the treated surfaces decreased, from ~40° for CP to ~75°-100° after O-PIII, being within the range that promotes protein adsorption[2]. Applying O-PIII, the corrosion rate was reduced, improving also the corrosion pattern of the material. SC exposure to 10% and 1% extracts did not show a relevant cell viability reduction. After 6 h of incubation, SC were adhered on the modified surfaces exhibiting an elongated morphology, which could be compatible with a regenerative phenotype.

O-PIII modified the AZ31B surface topography, chemical composition (Mg oxide/hydroxide related species), and wettability, enhancing its corrosion resistance. Low concentration of corrosion products did not affect SC viability, moreover, the modified surface allowed SC attachment. These results support the use of O-PIII technique as a potential surface modification for AZ31B, constituting a valid approach for peripheral nerves regeneration.

8:20am **MD2-2-ThM-2 Multifunctional PEO–PPy/Zn Coatings Combined with Electrical Stimulation for Enhanced Antimicrobial and Osteogenic Titanium Surfaces***, **Valentim A. R. Barão [vbarao@unicamp.br]**, Maria Helena R. Borges, Samuel Santana Malheiros, Julia M. Teodoro,* University of Campinas (UNICAMP), Brazil*; João Gabriel S. Souza,* Guarulhos University (UNG), Brazil*; Elidiane C. Rangel,* Sao Paulo State University (UNESP), Brazil*; Ana Paula Souza, Bruna Egumi Nagay,* University of Campinas (UNICAMP), Brazil

Dental implant failure often results from polymicrobial biofilm infections and poor osseointegration, underscoring the need for multifunctional surface modifications of titanium (Ti). Here, we developed a plasma electrolytic oxidation (PEO) coating followed by the electrodeposition of the conductive polymer polypyrrole (PPy) and the antimicrobial agent zinc (Zn), combined with osteogenic stimulation through electrical therapy (ES). We systematically investigated the surface, mechanical, physicochemical, tribological, electrochemical, antimicrobial (mono- and polymicrobial biofilms), and biological properties, as well as osteogenic activity using MC3T3-E1 cells. Ti discs were prepared as four groups: (1) machined, (2) PEO, (3) PEO+PPy, and (4) PEO+PPy/Zn, each evaluated with or without ES. The PEO+PPy and PEO+PPy/Zn surfaces exhibited enhanced mechanical strength, tribocorrosion resistance, reduced wear, and increased hardness ($p<0.05$). Zn incorporation imparted pronounced antimicrobial effects, significantly decreasing biofilm viability and metabolic activity ($p<0.05$), while promoting protein adsorption ($p<0.05$). Moreover, ES further improved cell proliferation, osteogenic differentiation, and mineralized nodule formation ($p<0.05$). Collectively, the multifunctional PEO+PPy/Zn coating, particularly when combined with ES, shows strong potential to enhance implant longevity by strengthening substrate resistance, preventing microbial colonization, and stimulating osteogenesis.

8:40am **MD2-2-ThM-3 Effect of Zirconium Addition on Zn- and Mg-Based Thin Film Properties Deposited by Magnetron Sputtering for Intravascular Biodegradable Materials***, **Fatiha Challali [fatiha.challali@univ-paris13.fr]**,* *Cristiano Poltronieri,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France*; Vinicius De Oliveira F. Sales, Carlos Henrique Michelin Beraldo, Carlo Paternoster,* Université Laval, Canada*; Frédéric Chaubet,* Université Sorbonne Paris Nord, France*; Philippe Djemia,* Laboratoire des Sciences des Procédés et des Matériaux (LSPM) – CNRS, France*; Diego Mantovani,* Université Laval, Canada

Intravascular medical devices allow the treatment of internal vessel-related diseases circumventing open-surgery, in daily-hospital treatment, and with great benefits for patients. The thickness of the devices is inversely proportional to how far in vascular bed diseased sites can accessed, especially for cerebrovascular applications. Unhappily, the fabrication of thin and ultrathin (hundreds to tens of microns) metallic implants remains a key challenge for these applications. Moreover, biodegradable metals are now a reality for adding the degradability components to these devices. For thin intravascular applications, zinc-based alloys are promising candidates due to their moderate degradation rates compared to magnesium-based materials, despite mechanical properties and corrosion rate still need to be investigated. The uniformity of the expected degradation also constitutes a main bottleneck, and metallic glasses, being exempted by surface defects like grain joints, provide a new insight, as recently shown on amorphous Zn–Mg–Ca. Thin film metallic glasses (TFMGs), characterized by a disordered atomic structure, exhibit exceptional mechanical properties, including a large elastic limit (>2%), high hardness, and yield strength (>2 GPa). Their homogeneous atomic arrangement promotes uniform corrosion with tunable rates depending on alloy composition.

This work aimed to enhance the glass-forming ability (GFA) and achieve tunable corrosion rates in Zn- and Mg-based thin films through the addition of Zr. Incorporating Zr as a glass-forming element is an effective strategy to extend the compositional ranges of amorphous or nanocrystalline alloys. The addition of Zr enables precise control over the microstructure and crystallinity, facilitating the design of biodegradable materials with improved performance. Thin films of Zn–Zr and Mg–Zr binary alloys were synthesized by magnetron co-sputtering onto silicon substrates using pure metallic targets, with thicknesses ranging from 300 to 900 nm, covering a wide composition range. The film microstructure and chemical composition were analyzed by XRD and SEM/EDS, respectively. Corrosion behavior was evaluated through electrochemical measurements performed at room temperature, while biodegradability was assessed by immersion tests in simulated body fluid at 37 °C for up to eight weeks. XRD results showed that Mg–Zr films exhibited a nanocrystalline structure, while amorphous Zn–Zr films were obtained for Zn contents between 26 and 88 at.%. Immersion tests revealed premature cracking and delamination in Zn- and Mg-rich films after one week, whereas Zr-rich films remained adherent even after eight weeks of immersion.

9:00am **MD2-2-ThM-4 Swelling Effect on Uhmwpe Cup: Long Term Consequences on Malfunctioning the Junction Head-Cup-Metal Back***, **Jean Geringer [geringer@emse.fr]**,* *Albert Boyer,* Mines Saint-Etienne, France*; Bertrand Boyer,* Hopital Edouard Herriot - Hospices Civils de Lyon, France*; Frederic Farizon,* CHU Saint-Etienne, France

Objectives

Hip arthroplasty is nowadays a successful surgical operation. 90% of patients, generally speaking, are satisfied and with time (after 10 years) this success rate is decreasing to 80% and less. Some factors are responsible for this decrease: infection, impingement, some pain due to joint blocking. The swelling effect of the cup polymer, UHMWPE, should be one of the factors. 0,2% is not a big deal...

In any case, swelling effect should have a minor effect or no effect. Long term action should have an impact and has an effect. On 10cm, we are talking about 2mm, roughly, of dimension change. Let's imagine a quotation change of 2mm on any dimension, radius of sphere, clearance between cup and metal back... The manufacturing lab of any organisation should fire any member if he is saying: 'don't care, pay attention on next...'

Materials and Methods

The cup sample was issued from the SERF™, now Stryker™, It was manufactured in 2019 with traditional manner . The material was UHMWPE polymer, polyethylene was the based material. UHMWPE was real cup. PEEK material was used, under disc. The first weight measurement was in 2008, less than 20 years. A balance with 5 digits was used. The control and the maintenance were always under survey.

New results

UHMWPE is gaining mass with time, after more than 8000 weeks. It means that adsorption is increasing with time. About PEEK material, one may say that stabilisation does occur after 100 weeks, i.e a bit less than 2 years. Thus the mass is stabilized after 2 years.

Conclusions & significance

UHMWPE is constantly increasing his mass with time. PEEK material was maintaining the mass after 2 years. Cup dimensions were changing with time when the material was UHMWPE. On the contrary, PEEK was constant after 15 years.

Acknowledgements

The authors are grateful to Mr. J-L. Aurelle for providing cup samples, ex. Serf company.

9:20am **MD2-2-ThM-5 Effect of Thermal Evaporation Deposited Silver Nanoparticles on the Antibacterial Behavior of Plasma Electrolytic Oxidation Coated AZ31B Magnesium Alloy***, **Ming-Hsuan Chang [tom0935802018@gmail.com]**,* *Chuan-Ming Tseng,* Ming Chi University of Technology, Taiwan

In this study, porous $MgO-Mg_2SiO_4$ bioceramic composite coatings were successfully fabricated on AZ31B magnesium alloy by using plasma electrolytic oxidation (PEO) under a bipolar pulsed power mode in alkaline sodium phosphate ($Na_3PO_4 \times 12H_2O$), sodium silicate ($Na_2SiO_3 \times 5H_2O$) and potassium titanium fluoride (K_2TiF_6) solutions. The $MgO-Mg_2SiO_4$ composite coatings exhibited higher hardness and better adhesion, serving as stable scaffolds for subsequent functionalization. In order to enhance antibacterial efficiency, silver nanoparticles (Ag NPs) deposited onto PEO coatings were employed via thermal evaporation deposition with various deposition durations (5~15 min). The effect of silver particle size on the antibacterial behaviors of Ag NPs deposited PEO coatings was also investigated in this study. The microstructural characteristics of Ag NPs deposited PEO coatings using XRD, SEM-EDS and EPMA show that the particle size of Ag NPs is increased parabolically from ~56 nm to ~220 nm as increasing deposition duration from 5 min to 15min, respectively. However, the prolonged evaporation gives rise to the aggregation of Ag NPs and the formation of larger island-like structures on PEO coatings. The antibacterial properties of Ag NPs deposited PEO coatings were carried out by measuring the numbers of *Escherichia coli* bacterial colony after various incubation durations (30~90 hr). The experimental results show that the antibacterial effect of the Ag NPs deposited PEO coatings is significantly improved with decreasing particle size of Ag NPs on PEO coating. Moreover, the Ag NPs deposited PEO coating after deposition duration with 5 min exhibits a 100% antibacterial efficiency to *Escherichia coli* after incubation in 90 min. The PEO coating with smaller size of Ag NPs (~56 nm) deposited exhibits a significantly larger specific surface area, and 100% antibacterial efficiency after incubation in 90 min can be achieved due to the facilitated rapid silver ion release.

Keywords: Plasma electrolytic oxidation (PEO), Thermal evaporation deposition, AZ31B magnesium alloy, Silver nanoparticles (Ag NPs), Antibacterial behavior.

10:20am **MD2-2-ThM-8 Dislocation-Mediated Plasticity and Strain Localization in Transition Metal Nitrides: Insights from Micropillar Compression***, **Rainer Hahn [rainer.hahn@tuwien.ac.at]**,* CDL-SEC, TU Wien, Austria*; Peter Polcik, Szilard Kolozsvari,* Plansee Composite Materials GmbH, Germany*; Klaus Boebel,* Oerlikon Surface Solutions AG, Liechtenstein*; Helmut Riedl,* CDL-SEC, TU Wien, Austria **INVITED**

Transition metal nitrides are key materials in advanced protective and functional coatings, yet their mechanical response is often constrained by intrinsic brittleness. Recent studies show that defect engineering and electronic structure control can fundamentally alter this behavior, enabling metallic-like plasticity in selected compounds. In this work, we employ in-situ micropillar compression to investigate the deformation mechanisms of epitaxial TiN, CrN, and WN thin films. Despite their structural similarity, these nitrides exhibit strikingly different responses under load. TiN and CrN deform through slip-band formation and early strain localization, indicating limited dislocation mobility and a strong tendency toward brittle failure. In contrast, WN displays pronounced metal-like plasticity, sustaining large plastic strains through dislocation glide and interaction processes more typical of metallic systems. These findings demonstrate how compositional tuning and bonding character influence the transition from brittle to ductile behavior in refractory nitrides. The results establish in-situ micropillar compression as a powerful tool to uncover intrinsic deformation pathways and identify WN as a key model system bridging metallic and ceramic mechanical responses.

11:00am **MD2-2-ThM-10 Biofunctional Zinc Phosphate-Loaded Membranes as a Potential Anti-Biofilm and Remineralizing Approach for Caries Management**, ***Gina Prado-Prone [gpradoprone@comunidad.unam.mx]**, Lorena Reyes-Carmona, Lizeth A. González-Vargas,* Laboratorio de Biointerfases, DEPeI, Facultad de Odontología, Universidad Nacional Autónoma de México*; Phaedra S. Silva-Bermudez,* Unidad de Ingeniería de Tejidos, Terapia Celular y Medicina Regenerativa; Instituto Nacional de Rehabilitación Luis Guillermo Ibarra Ibarra, Mexico*; Sandra E. Rodil,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*; Nicola Cioffi,* Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Italy*; Camila A. Zamperini Zamperini,* Department of Restorative Dentistry, College of Dentistry, University of Illinois Chicago, USA*; Argelia Almaguer-Flores,* Laboratorio de Biointerfases, DEPeI, Facultad de Odontología, Universidad Nacional Autónoma de México

Introduction: Dental caries is the most common oral disease, mainly caused by persistent cariogenic biofilm on dental surfaces. The acidic environment created by acid-producing and acid-tolerant bacteria leads to dental demineralization and, ultimately, caries formation. The most important strategies in cariology currently focus on preventing caries and treating early-stage lesions by inhibiting biofilm formation and optimizing tooth health remineralization. Therefore, developing novel antibiofilm and remineralizing anti-caries biomaterials has great potential to enhance caries prevention and treatment.

Objectives: To develop zinc phosphate (ZnP)-loaded membranes and evaluate their capacity to prevent dental caries-related biofilms and promote dental remineralization.

Methods: ZnP microparticles were synthesized via chemical precipitation. Membranes were synthesized via electrospinning a polycaprolactone-gelatin blend (1:1) incorporating ZnP microparticles at 1%, 2%, and 5% (w/w) concentrations. The micro-morphology, chemical composition, wettability, and thermal properties were analyzed using SEM, EDS, FTIR, WCA, TGA, and DSC. The *in vitro* anti-biofilm effect was evaluated by turbidity and Alamar Blue assays using four bacteria associated with caries: *Streptococcus mutans* (25175™ATCC®), *Streptococcus sanguinis* (110556™ATCC®), *Lactobacillus acidophilus* (4356™ATCC®), and *Veillonella parvula* (17745™ATCC®). To assess the remineralization potential of the experimental membranes in *in vitro* root caries lesions, human root dentin specimens were slightly demineralized and exposed to the membranes under remineralization cycling. The mineral density, depth, and porosity of the final root caries lesions were assessed by computer microtomography and confocal scanning laser microscopy after rhodamine infiltration.

Results: Membranes exhibited a microfibrillar structure with interconnected porosity and desirable physico-chemical properties for clinical applications. Antibacterial testing showed 44-80% inhibition of biofilm formation of the four bacterial strains on the ZnP-membrane surfaces; the antibiofilm effect appears to depend on the ZnP concentration. The 5% ZnP-loaded membranes exhibited a more favorable pattern of remineralization for *in vitro* root caries treatment, but there were no statistically significant differences in caries depth and porosity among groups ($p \geq 0.05$).

Conclusions: ZnP-loaded membranes can potentially be used as an anti-biofilm and remineralizing approach for dental caries management.

Acknowledgements: This work was funded by the UI System/UNAM Joint Research Partnership Program, and the UNAM-PAPIIT #TA100424 and #IN207824 projects.

11:20am **MD2-2-ThM-11 Growth Mechanism and Cellular Response to Film Thickness Variations of Nanoporous Alkaline Titanate-Converted, Magnetron Sputtered Ti Thin Films**, ***Matthew Wadge [m.wadge@mmu.ac.uk]**,* Manchester Metropolitan University, UK*; Kozim Midkhatov,* University of Manchester, UK*; Jonathan Wilson, Louise Briggs, Timothy Cooper, Zakhar Kudrynskyi,* University of Nottingham, UK*; Reda Felfel,* University of Strathclyde, UK*; Ifty Ahmed, Colin Scotchford, David Grant,* University of Nottingham, UK*; Justyna Kulczyk-Malecka,* Manchester Metropolitan University, UK*; Mahetab Amer,* University of Manchester, UK*; Peter Kelly,* Manchester Metropolitan University, UK

The standard process for improving bioactivity of implant surfaces for natural fixation is reliant on high temperature (>1500 K) plasma spraying of hydroxyapatite (HA) [1]. However, these surfaces have been shown to spall due to their brittle nature, high internal stresses, and weak mechanical adhesion [1]. Bioactive titanate surfaces have been developed as a low-temperature, more simplistic alternative, however, their applicability is limited to titanium (Ti) and its alloys only via chemical conversion routes [1]. The present authors previously demonstrated the applicability of titanate surfaces generated from PVD Ti coatings [2], however, assessment of thickness variation on cellular performance is still required, due to potential unwanted effects such as poor cellular proliferation. This paper highlights for the first time the cellular performance of titanate films generated on various thicknesses of Ti coating. By varying the thickness of the PVD deposited Ti coating, one can influence the formation mechanism of the wet-chemically derived titanate surface produced, since the mechanism is diffusion dependant and material limited.

Magnetron sputtering was employed to generate the Ti coatings (ca. 50, 100, 200, 500 nm) owing to its excellent step coverage, relatively quick deposition rate, ability to coat onto, and from, a wide variety of materials. In the conversion process, Ti coatings are treated in NaOH (5 M; 60 ^{o}C; 24 h) to generate sodium titanate structures [1]. The resultant materials were characterised using SEM, EDX, XPS, XRD, as well as cellular assessments, in order to understand the formation mechanism, the resultant morphological (Fig.1&2), structural (Fig.3) and chemical (Fig.4) properties, as well as influence on cellular response. It was clear that the Ti coatings exhibited good step coverage. Following titanate formation, only the 200 and 500 nm coatings produced the characteristic nanoporous 'webbed' titanate structures, due to the lack of free Ti in the coating, as opposed to the conventional diffusion limitation (Na and O) of the titanate mechanism. Both XPS and XRD analyses confirmed the formation of titanate on all of the coatings tested, despite the morphological differences and irrespective of thickness. Through utilising sputtering, the applicability of these titanate materials in a biomedical context can be significantly improved due to its ability to coat most materials and matching the subsequent wet-chemical temperature conditions.

References

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11:40am **MD2-2-ThM-12 Antibacterial Performance of Electrodeposited Copper Coatings on Titanium Alloy Surfaces for Biomedical Applications**, ***Bryan Angel Zárate Verduzco [1629251c@umich.mx]**,* Universidad Michoacana de San Nicolás de Hidalgo, Mexico*; Victor Manuel Solorio García, Miguel Ivan Dávila Perez,* Tecnologico Nacional de México/ Instituto Tecnológico de Morelia, Mexico*; Roberto Guerra González, Sandra Edith Lopez Castañeda, Alfonso Lemus Solorio, Maria Guadalupe Carreon Garcidueñas,* Universidad Michoacana de San Nicolás de Hidalgo, Mexico

The increasing incidence of implant-associated infections underscores the urgent need for effective antibacterial surface modifications that prevent biofilm formation without compromising the mechanical integrity of metallic implants. In this study, copper (Cu) coatings were electrodeposited onto Ti6Al4V alloys fabricated by powder metallurgy to impart bacteriostatic functionality and inhibit microbial colonization. Controlled deposition was performed at varying durations (1 min, 5 min, 15 min, 1 h, and two h). Surface morphology and composition were characterized by scanning electron microscopy (SEM) and energy-dispersive spectroscopy (EDS), revealing dense, adherent Cu layers whose thickness increased proportionally with deposition time. Microbiological assays against Staphylococcus aureus (MRSA) and Escherichia coli demonstrated over 99% reductions in bacterial viability after 24 h, along with marked suppression of biofilm development and maturation on the coated surfaces. The antibacterial mechanism was attributed to the controlled release of Cu^{2+} ions, which induces an oligodynamic effect on bacterial membranes and interferes with early-stage adhesion and extracellular matrix formation. These results confirm that electrodeposited Cu films on Ti6Al4V represent a cost-effective, scalable, and environmentally responsible route toward infection-resistant implants. This approach provides a promising alternative to conventional antibiotic prophylaxis, supporting the development of next-generation biomaterials designed to reduce post-surgical infections and improve the long-term safety and performance of metallic implants.

12:00pm **MD2-2-ThM-13 Low-Pressure Plasma Processes for the Deposition of Adherent Diamond-Like Carbon Coatings on Titanium Alloys for Biomedical Applications***, Chloé Audet,* ***Pascale Chevallier [pascale.chevallier@crchudequebec.ulaval.ca],*** Laboratory for Biomaterials and Bioengineering, (CRC-Tier I), Dept Min-Met-Materials Eng., & Regenerative Medicine, CHU de Quebec, Laval University, Canada*; Sandra Rubio,* Laboratoire Interdisciplinaire de Spectroscopie Electronique, Namur Institute of Structured Matter, University of Namur, Belgium*; Andranik Sarkissian,* Plasmionique Inc, Canada*; Laurent Houssiau,* Laboratoire Interdisciplinaire de Spectroscopie Electronique, Namur Institute of Structured Matter, University of Namur, Belgium*; Diego Mantovani,* Laboratory for Biomaterials and Bioengineering, (CRC-Tier I), Dept Min-Met-Materials Eng., & Regenerative Medicine, CHU de Quebec, Laval University, Canada

Titanium and its alloys are widely recognized as the gold standard for bone contact implants due to their suitable mechanical properties and biological performances. However, their long-term clinical performance remains impaired, mainly due to insufficient integration with surrounding tissues and the risk of infection. In order to enhance their performance, surface modification through coatings are explored. Among these coatings, diamond-like carbon (DLC) has emerged as a promising material due to its superior mechanical properties, chemical inertness, and stability, as well as its ability to integrate antibacterial agents such as Ag, ZnO, etc., resulting in a multifunctional coating. However, due to the high intrinsic stresses of DLC compared to the native oxide layer, the adhesion of DLC to metallic surfaces remains rather low. Therefore, this work focuses on improving DLC adhesion to the Ti alloy surface using plasma-assisted chemical vapor deposition (PECVD), by optimizing different surface pretreatments prior to coating. The results showed that the nature and duration of the pretreatment significantly influenced the chemical composition and topography of the substrate prior to deposition, which in turn had an impact on the thickness, structure and morphology of the DLC. Short methane carburizing, particularly for 10 min, appeared to be the most effective pretreatment, as it removed the native oxide layer, enhanced carbon implantation, led to thick, adherent DLC coatings with a diamond-like structure, and stable even after 7 days of aging in pseudo-physiological conditions. In contrast, argon etching alone was ineffective, and combining both treatments yielded thinner films.

Controlled plasma carburization prior to DLC deposition significantly improves coating adhesion and stability on Ti alloys, paving the way for improved implant performance. The addition of antibacterial agents within the DLC matrix could further improve clinical outcomes of implants and reduce implant-associated infections.

Keywords: Surface modification, plasma-enhanced chemical vapor deposition, diamond-like carbon, Ti-alloy medical implant.

Topical Symposium on Sustainable Surface Engineering
Room Town & Country D - Session TS2-2-ThM

Coatings and Surfaces for Renewable Energy Technology II

Moderators: Arnaud le Febvrier, Uppsala University, Sweden, **Marcus Hans**, RWTH Aachen University, Germany

8:00am **TS2-2-ThM-1 Energy-Efficient Hydrogen Production via Urea-Assisted Electrolysis Enabled by Linker-Engineered NiCo MOFs***,* ***Thi Xuyen Nguyen [nguyenxuyen1511@gmail.com]****, Hui-Chuan Chen, Jyh-Ming Ting,* National Cheng Kung University, Taiwan **INVITED**

Hydrogen (H_2) is widely recognized as a promising sustainable energy carrier for addressing the global energy crisis and achieving the net-zero carbon emission target. Among the various H_2 production strategies, urea-assisted electrochemical water splitting offers an energy-efficient route for H_2 production; however, the inherently sluggish six-electron urea oxidation reaction requires highly active electrocatalysts. Herein, we report a linker-engineering strategy in which the benzene dicarboxylate (BDC) linker of a NiCo-BDC metal-organic framework (MOF) is partially replaced by a redox-active dicarboxylferrocene (DFc) ligand to construct NiCo-MOF-DFc. The strongly coordinated DFc linker effectively modulates the electronic structure, enriching Ni^{3+} species, generating abundant oxygen vacancies, and inducing coordination asymmetry, thereby markedly enhancing urea oxidation activity. The NiCo-MOF-DFc catalyst delivers 100 mA cm^{-2} at a low potential of 1.33 V with excellent durability. Operando characterizations reveal that DFc facilitates rapid electron transfer, accelerates the transformation of the MOF into the catalytically active metal (oxy)hydroxide phase, and stabilizes the active sites. Density functional theory calculations further demonstrate that DFc weakens CO_2 adsorption and lowers the energy barrier of the rate-determining desorption step. An anion exchange membrane electrolyzer employing NiCo-MOF-DFc as the anode achieves 1000 mA cm^{-2} at a low cell voltage of 1.83 V and sustains stable operation for 500 h. Notably, the system requires only 48.6 kWh to produce 1 kg of H_2, representing over 10% lower energy consumption than conventional OER-based electrolysis, highlighting its strong potential for energy-efficient hydrogen production.

8:40am **TS2-2-ThM-3 Low-Cost, High-Performance Flexible Supercapacitors Based on Vanadium Oxynitride Reactively Sputtered on Porous Polymeric Substrate for Sustainable Energy Storage Applications***,* ***Habeebur Rahman [habeeb.physics10@gmail.com]****, Davinder Kaur,* Indian Institute of Technology Roorkee, India

This work presents an air bubble method to fabricate a porous polyvinyl alcohol (PVA) substrate for room-temperature (RT) reactively sputtered vanadium oxynitride (VON)-based high-performance, eco-friendly flexible supercapacitor. The air was inserted into the aqueous PVA solution, and controlled stirring was performed to form micron-sized air bubbles, which, upon drying in a mould, formed the porous substrate. Further, vanadium pentoxide (V_2O_5) was reactively sputtered at RT on the Ag current collector coated plane and porous substrates. The supercapacitor device fabricated on the porous PVA substrate demonstrated drastically enhanced performance in 1M Na_2SO_4 electrolyte due to remarkably higher surface area. For further improvement, the VON-based supercapacitor was fabricated that exhibited 377 F/g specific capacitance (areal capacitance of 18.9 mF/cm^2 and volumetric capacitance of 196.35 F/cm^3), 1.2 V potential window, 27.8 Wh/kg energy, and 3.0 kW/kg power density. It demonstrated 100 % capacitance retention after 5,000 charging-discharging cycles. For real applications, five devices connected in series glowed different colored light-emitting diodes (LEDs) for more than 180 seconds, and 10 red LEDs together for 60 seconds. Further, it showed no performance degradation upon bending and twisting, and illustrated fast disposal in normal water and moist soil. The fabricated materials were studied employing various characterising tools.

9:00am **TS2-2-ThM-4 Optimization of Tunable Interfacial Engineering in WOx/α-Fe_2O_3 Heterostructures via Dc Magnetron Sputtering for Enhanced PEC Activity and Carrier Transport Efficiency***,* ***Carlos Gomes [c.e.gomes@ifsp.edu.br]****, Mariane Murase Murase, Matheus Torres, Douglas Leite, Rodrigo Pessoa, Argemiro Sobrinho, André Pereira,* Instituto Tecnológico de Aeronáutica, Brazil

Transition metal oxide heterostructures are crucial for advancing sustainable energy technologies, demanding precise control over interfacial charge dynamics and long-term chemical stability. This work presents a systematic study on the fabrication and optimization of an Iron Oxide (α-Fe_2O_3) a visible-light absorber heterojunction with a Tungsten Oxide (WO_x) as an electron-transport layer, serving as a band alignment at the interface. Junction formation is a powerful strategy to overcome intrinsic limitations like poor charge transport and high surface recombination in semiconductors [1]. The staggered band alignment creates an internal electric field that promotes efficient separation of photogenerated electron(e^-)/hole(h^+) pairs and facilitates electron extraction, significantly reducing surface charge recombination [1,2].

The structures were fabricated using scalable DC Magnetron Sputtering, depositing the α-Fe_2O_3 layer over FTO glass (SnO_2/F) followed by the WO_x transport layer. The study investigates tunable surface engineering by systematically varying the WO_x deposition time to precisely control the layer's thickness and potentially its stoichiometry (WO_{3-x}), thereby modulating the electronic band alignment and transport efficacy.

Comprehensive characterization, including XRD, SEM, EIS, and CV, was employed to correlate layer thickness with interfacial structure. Analysis confirmed WO_x crystallization at 550°C, showing a direct relationship between peak intensity and deposition time. Deposition of an optimal WO_x layer enhanced Fe_2O_3 optical modulation, resulting in a 15% lower visible transmittance minimum (at ≈ 600 nm).

Functional performance such as stability and charge transfer dynamics was assessed, revealing that the WO_x (180s) sample's highest carrier number and lowest flat band voltage directly correlate with superior electrochemical performance (Specific Power under light and Specific Energy in the dark), suggesting that the improved electronic structure drives enhanced charge storage and transfer capabilities.

This research presents valuable insights into controlled thin film deposition and advanced surface engineering of robust oxide structures. These findings support the development of next-generation photoelectrochemical cells (PEC) for water splitting.

Keywords: WOx/α-Fe_2O_3, Heterojunction, DC Magnetron Sputtering, Thin Film Deposition, Advanced Surface Engineering.

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9:20am **TS2-2-ThM-5 Thermal Treatment Effects on the Structural and Optoelectronic Properties of Nb2O5 Thin Films Deposited by DC Magnetron Sputtering***, Rodrigo Prado Medeiros Leite da Silva, Natali da Silva Barbosa, Bianca Sartori,* Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Brazil*; Lucas Diniz Araujo,* Aeronautics Institute of Technology (ITA), Brazil*; Carlos Eduardo Gomes,* Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Brazil*; Filipe Caldatto Dalan, André Luis de Jesus Pereira,* ***Argemiro Soares da SIlva Sobrinho [argemiro@ita.br]****,* Aeronautics Institute of Technology (ITA), Brazil

The development of efficient semiconductor oxides for solar-driven energy conversion is a key step toward achieving a sustainable hydrogen economy. Transition-metal oxides such as TiO_2, WO_3, and Nb_2O_5 have emerged as promising photoactive materials due to their chemical stability and suitable band-edge alignment for photoelectrochemical (PEC) water splitting. Among them, niobium pentoxide (Nb_2O_5) is particularly attractive for its abundance, low toxicity, and tunable optoelectronic properties associated with oxygen-vacancy engineering. Understanding how deposition and post-treatment conditions affect its structure and charge-transport characteristics is therefore essential for optimizing its functional performance. In this work, Nb_2O_5 thin films were deposited by DC magnetron sputtering onto Si, glass, and FTO substrates and subsequently annealed at 300 °C, 400 °C, 500 °C, and 600 °C for eight hours under two controlled atmospheres: air at atmospheric pressure and vacuum (~10^{-2} Torr). The films were characterized by X-ray diffraction, Raman spectroscopy, UV–Vis transmittance, and electrochemical techniques to evaluate the influence of temperature and ambient on crystallization, defect formation, and electronic behavior. Structural analyses revealed a transition from amorphous to orthorhombic (Pbam) Nb_2O_5 above 500 °C, while vacuum-treated samples exhibited more pronounced oxygen-vacancy-related Raman features and a narrower optical band gap. Electrical impedance and cyclic-voltammetry results indicated reduced charge-transfer resistance for oxygen-deficient films, evidencing the beneficial role of substoichiometry in enhancing carrier mobility. These results demonstrate that both annealing temperature and atmosphere strongly modulate the structural and optoelectronic properties of sputtered Nb_2O_5, providing valuable guidelines for tailoring its performance in PEC and photocatalytic applications.

10:20am **TS2-2-ThM-8 Interface-Driven Evolution and Electrochemical Behavior of CuO/WO_X Heterostructures Deposited by Magnetron Sputtering***, Rafael Leal, Giovana Fazenda, Helen Barros, David Graves, Filipe Dalan, Mariane Murase, Marcilene Gomes,* Aeronautics Institute of Technology (ITA), Brazil*; Douglas Leite,* Aeronautics Institute of Technology, Brazil*; Argemiro Silva-Sobrinho,* ***André Pereira [andreljp@ita.br]****,* Aeronautics Institute of Technology (ITA), Brazil

Heterostructures composed of copper and tungsten oxides have drawn increasing attention for solar-driven photoelectrochemical (PEC) hydrogen generation due to their complementary optical and electronic properties [1]. The interface between p-type CuO and n-type WO_x plays a critical role in charge separation and carrier transport; however, its efficiency strongly depends on the structural order and chemical composition of the WO_x layer [1,2]. In this work, CuO/WO_x heterostructures were fabricated entirely by DC magnetron sputtering. CuO films were first deposited onto FTO substrates and annealed at 450 °C for 2 h to promote crystallization and improve adhesion. WO_x overlayers were then deposited for 1, 5, and 10 min, followed by post-annealing at 450 °C for 2 h to obtain crystalline layers; as-deposited samples were kept amorphous. The WO_x layer thickness, determined by profilometry and ellipsometric modeling, increased linearly with deposition time (~15 nm min^{-1}), while the refractive index was slightly higher for crystalline samples, indicating greater density and lower porosity. Structural and vibrational analyses revealed distinct interface behaviors. For crystalline WO_x layers, Raman and XRD showed that samples with 5 and 10 min deposition underwent interdiffusion at the interface, forming $CuWO_4$, whereas the 1 min sample exhibited a substoichiometric WO_x layer. In contrast, amorphous WO_x overlayers preserved only CuO peaks. Electrochemical measurements confirmed the correlation between structure and functionality. Cyclic voltammetry and impedance spectroscopy revealed that crystalline samples containing $CuWO_4$ exhibit lower charge-transfer resistance and higher photocurrent under illumination, while amorphous heterostructures display slower carrier dynamics and greater capacitive behavior. The electrochemically active surface area (ECSA), estimated from non-faradaic capacitive current, was significantly larger for crystalline samples, particularly those with $CuWO_4$, indicating an increased density of electroactive sites and enhanced charge accumulation capability. Overall, the controlled formation of $CuWO_4$ or substoichiometric WO_x interlayers offers a promising strategy to improve PEC efficiency and long-term stability of CuO-based photoelectrodes for sustainable hydrogen generation.

Acknowledgments
We acknowledge the financial support from FAPESP (Grant No. 2022/02994-2) and CNPq (Grant No. 302823/2025-5).

[1] X. Wen et al., ACS Appl. Nano Mater. 7 (2024) 14936–14945. DOI: 10.1021/acsanm.4c00769.

[2] M. Castaneda Mendoza et al., Materials 18 (2025) 2896. DOI: 10.3390/ma18122896.

10:40am **TS2-2-ThM-9 Unlocking the Potential of Medium-Entropy Prussian Blue for Superior Electro-Fenton Oxidation***,* ***Sheng-Wei Lin [alec97622964@gmail.com]****, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Electro-assisted advanced oxidation processes, such as the electro-Fenton (EF) process, are gaining intensive attention recently. This work investigates the application of a medium-entropy Prussian blue analogue (designated as 3M-PBA) as a heterogeneous EF catalyst for the removal of organic pollutants from water. EF process can overcome the drawbacks of conventional Fenton process, such as the limited pH range and poor reusability. In this work, the 3M-PBA catalyst further enhances the EF performance by providing multiple redox-active sites, which accelerate electron transfer and improve structural stability during operation.

The phase, morphology, oxidation state, charge-transfer behaviour, hydroxyl-radical generation efficiency, and EF degradation performance were characterized using several techniques. UV-Vis spectroscopy analysis shows a continuous decrease in the characteristic TC absorption peak at 357 nm with time, confirming the molecular breakdown. The 3M-PBA catalyst achieves a high TC removal within a short time under an applied potential (0.6 V vs. Ag/AgCl). Iron leaching remains below 0.4 ppm throughout the five cycles, indicating strong structural integrity and environmental safety.

Keywords: electro-Fenton, high-entropy PBA, charge transfer, catalyst stability, wastewater treatment

11:00am **TS2-2-ThM-10 Non-Precious Metal Phosphide/Sulfide Heterostructure Electrocatalyst for SOR***,* ***Jian-An Wu [tommy772222@gmail.com]****, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

With the increasing discharge of wastewater containing sulfur compounds from various industries, the need for efficient sulfur removal and recovery is becoming more urgent. The Sulfion Oxidation Reaction (SOR), which converts sulfide ions (S^{2-}) into elemental sulfur (S_8), which is common for industrial use. Unlike the conventional oxygen evolution reaction (OER), which is thermodynamically challenging and energy-consuming, SOR operates at a much lower potential (-0.48 V vs. RHE), making it a more energy-efficient alternative for sulfur oxidation. Furthermore, the added economic value makes SOR an attractive option for wastewater treatment, as it reduces the need for costly disposal methods while turning a pollutant into a resource.

Herein, we have synthesized a non-precious metal phosphide/sulfide heterostructure catalyst with conductive backbone and abundant active site on the surface. The catalyst demonstrates an exceptional SOR performance in 1M KOH with 1M Na_2S, achieving a low potential of 0.278V at 100 mA cm^{-2} and 0.368V at 300 mA cm^{-2}, and a lower onset potential.

Keywords:Sulfion Oxidation Reaction (SOR), transition-metal based catalyst, heterostructure

11:20am **TS2-2-ThM-11 Defect-Engineered Copper-Based Materials for Electrocatalytic Nitrate Reduction***, Ting- Chun Hung* ***[jim8965976@gmail.com]****, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Electrochemical nitrate reduction reaction (NO_3RR) has emerged as a promising strategy for simultaneously addressing nitrate pollution and producing valuable ammonia via a carbon-free process. Ammonia is an important chemical feedstock, widely used in fertilizer production, and offers advantages such as an alternative energy source for replacing hydrogen due to its ease of storage and transport.

For NO_3RR, copper-based materials are known to be highly active catalysts by facilitating the conversion of nitrate (NO_3^-) to nitrite (NO_2^-), which is the rate-determining step. In this study, novel Cu-based heterostructure nanosheets rich in oxygen vacancies (Ov) were investigated as an effective electrocatalyst for NO_3RR. The catalyst was synthesized via a hydrothermal method, followed by chemical reduction for controlled creation of Ov. The catalyst exhibits excellent NO_3RR performance, achieving a Faradaic efficiency of ~95% at -0.2 V vs. RHE, a high ammonia yield rate of 0.92 mmol h^{-1} cm^{-2}, and outstanding stability over 1000 hours, demonstrating both superior activity and long-term durability. Density functional theory calculation was performed to support the experimental data.

Keyword: Electrochemical nitrate reduction, heterostructures, oxygen vacancy, high ammonia yield rate

Keynote Lectures
Room Town & Country B - Session KYL3-ThKYL

Keynote Lecture III
Moderator: Sandra E. Rodil, Universidad Nacional Autónoma de México

12:40pm **KYL3-ThKYL-1 Compressive Stress as Creative Force: Engineering Ultrahard Hydrogen-Free Carbon for a Diamond-Like Properties***, David R. McKenzie [david.mckenzie@sydney.edu.au],* University of Sydney, Australia **INVITED**

Hydrogen-free amorphous carbon films, which I first termed as "tetrahedral amorphous carbon (ta-C)", which my colleagues recently colloquially termed 'McKenzie Material' in recognition of my early identification and continued research of this metastable phase, exhibit extreme hardness, chemical inertness, optical transparency and tunable electronic properties. These properties are all attractive for tribological coatings, biomedical implants and microelectronic devices. Despite these advantages, scalable synthesis of dense, sp^3-rich films with sufficient thickness and adhesion has long been limited by intrinsic compressive stress and shortcomings of conventional deposition methods. Here I review recent advances in high-power impulse magnetron sputtering (HiPIMS) and its advanced variants that include mixed-mode, bipolar, hybrid-arc and multi-pulse configurations that achieve sp^3 fractions exceeding 80 %, hardness approaching 75 GPa and markedly reduced noble-gas incorporation. Precise control of pulse parameters, substrate bias and sputtering atmosphere enables tailored ion energy and flux, promoting dense tetrahedral bonding while suppressing macroparticle contamination and micro-arcing. I highlight with insights from state of the art molecular dynamics how stress generation and relaxation mechanisms operate, including sublayer implantation combined with intermittent thermal or excimer-laser annealing to relieve multi-gigapascal compressive stresses without compromising sp^3 content. Integrated strategies enable the deposition of adherent, µm-thick ta-C coatings on diverse substrates, facilitating industrial-scale deployment in wear-resistant tooling, biocompatible surfaces, and energy systems. The synergy of HiPIMS processes with targeted stress-management protocols establishes hydrogen-free amorphous carbon as a versatile platform for next-generation ultrahard, functional thin films.

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

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

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

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

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

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

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

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

1. Fébba, D. M. *et al.* Autonomous sputter synthesis of thin film nitrides with composition controlled by Bayesian optimization of optical plasma emission. *APL Materials* **11**, 071119 (2023).
2. Schaefer, S. *et al.* Rapid screening of molecular beam epitaxy conditions for monoclinic (InxGa1−x)2O3 alloys. *J. Mater. Chem. A* (2024) doi:10.1039/D3TA07220G.
3. Fébba, D., Egbo, K., Callahan, W. A. & Zakutayev, A. From text to test: AI-generated control software for materials science instruments. *Digital Discovery* **4**, 35–45 (2025).

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

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

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

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

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

References:

[1] Szymanski, N.J., *et al.* An autonomous laboratory for the accelerated synthesis of novel materials. *Nature* **624**, 86–91 (2023)

[2] Szymanski, N.J., *et al.* Autonomous and dynamic precursor selection for solid-state materials synthesis. *Nat Commun* **14**, 6956 (2023)

[3] Giunto, A., *et al.* Harnessing Automated SEM-EDS and Machine Learning to Unlock High-Throughput Compositional Characterization of Powder Materials, 14 October 2025, PREPRINT [https://doi.org/10.21203/rs.3.rs-7837297/v1]

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

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

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

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

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

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

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

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Surface Engineering - Applied Research and Industrial Applications

Room Town & Country D - Session IA2-2-ThA

Surface Modification of Components in Automotive, Aerospace and Manufacturing Applications II

Moderators: Miha Cekada, Jozef Stefan Institute, Slovenia, **Satish Dixit**, Plasma Technology Inc., USA

1:40pm **IA2-2-ThA-2 From Development to Series Production in Automotive – The Role of Coating Characterization**, ***Nazlim Bagcivan [nazlim.bagcivan@schaeffler.com]***, Schaeffler Technologies GmbH & Co. KG, Germany **INVITED**

Coatings have contributed significantly to performance improvements in automotive applications in various ways, such as friction reduction, extended service life through wear protection, and increased corrosion resistance. Meeting specified properties plays a central role in achieving these goals.

The verification of these properties and the characterization process differ greatly between research and development (R&D) and industrialization. While R&D focuses on the pure verification of achieving the specified property, industrialization and subsequent series production aim to ensure that these properties are reliably achieved through robust coating processes while maintaining quality characteristics.

This presentation highlights the role of coating property characterization in both R&D and industrialization. It presents and discusses both commonalities and differences. The goal is not only to illustrate selected characterization methods with examples but also to provide insight into methodological approaches, such as the Production Part Approval Process (PPAP) or the determination of process capability.

2:20pm **IA2-2-ThA-4 Investigation of Salt Solution Drying Behavior to Improve Coating Performance for Marine Turbomachinery**, ***Sadikshya Pandey [pande224@umn.edu]***, *David Poerschke,* University of Minnesota, USA

Salt deposition and fouling in compressors contributes to performance degradation of gas turbines operating in marine environments. These deposits accumulate over time as seawater mist enters with the intake air and evaporates during operation. Developing effective coating strategies that limit salt accumulation is essential to improve operational reliability. Although antifouling coatings are proposed for such applications, the mechanisms linking surface properties to salt deposition behavior are not well understood. In this study, we performed salt solution misting experiments on substrates with distinct surface chemistries to investigate how the surface properties influence salt deposition dynamics. Observations from these experiments reveal key relationships between wetting, drying conditions, and deposition patterns. These insights provide a foundation for the rational design of engineered coatings with enhanced antifouling performance, aimed at reducing salt-induced performance losses in marine turbomachinery.

2:40pm **IA2-2-ThA-5 Enhancing Mechanisms for the Increased Performance of Nuclear Energy and Aerospace Coating- and Solid-RHEA Components**, ***Sal Rodriguez [tayloreddydk1@gmail.com]***, 11251 Pino Ave. NE, USA; *Satish Dixit,* Plasma Technology Inc., USA; *Nima Fathi,* Texas A&M University, USA **INVITED**

Refractory high-entropy alloys (RHEAs) are composed of multi-principal elements typically having near-equiatomic proportions. RHEAs are formed from refractory elements such as Nb, Ta, Mo, W, Hf, and Zr, which offer outstanding mechanical strength at elevated temperature, corrosion resistance, irradiation tolerance, and thermal stability. Hence, this provides a materials class ideal for harsh-environment applications often encountered in aerospace and nuclear energy applications. For example, NbTaTiV offers an exceptional 23% strain-to-failure and yield strength in excess of 1,300 MPa at room temperature, while some RHEAs have reached a yield strength of 375 MPa at 1,873 °C. Moreover, an alloy has good machinability performance if its engineering strain is greater than 5% at room temperature, which NbTaTiV far exceeds.

We present examples design, synthesis, and performance, with emphasis on thermal spray coatings based on high velocity oxygen fuel, advanced atmospheric plasma spray, high velocity air fuel, and cold spray suitable for RHEAs. In addition, we demonstrate the advanced manufacturing of industry-grade solid (bulk) RHEA components via spark plasma sintering (SPS) and subsequently machined to net shape via computer numerical control (CNC).

We investigate key properties of the RHEA coatings and solids, including hardness, modulus, ductility, machinability, wear resistance, and friction, as well as corrosion- and radiation-resistance behavior. But most importantly, we show leading-edge examples of industrial-grade RHEA and refractory-element based coated components, including turbine diffusers. Moreover, the CNC of a 3.5 kg solid NbTaTiV RHEA generated a 140-mm turbine diffuser, a 0.5-mm thick turbine blade, and small plates with flow channels for compact heat exchangers, all without visible microcracks at 30X magnification—a world's first. Case studies for NbTaTiV and other RHEAs demonstrate exceptional ductility, machinability, and protective performance when applied as coatings on stainless steels and Inconels under molten-salt and high-temperature environments.

These advances corroborate RHEAs as transformative materials for key industries, including energy, aerospace, electronics, and defense. As a result of their high-strength, high-temperature, and harsh-environment survivability, some applications include advanced nuclear reactors, plasma facing fusion components, compact heat exchangers, high-temperature jet turbines, hypersonics, quantum computer hardware, radiation-resistant electronics, high-temperature combustion, concentrated solar, missile defense, and biomedical devices.

3:20pm **IA2-2-ThA-7 Element-Resolved Investigation of Zr-Based Conversion Coatings on Aluminum and Zinc Alloy Substrates by AESEC and GD-OES***,* ***Suyeon Lee [suyeon.lee@horiba.com]****, Alice Stankova, Patrick Chapon,* HORIBA Europe Research Center, France*; Kayvon Savadkouei,* HORIBA, USA*; Junsoo Han,* Sorbonne University, France*; Dominique Thierry, Dan Persson,* Research Institutes of Sweden*; Kevin Ogle, Borhan Sultan,* Chimie Paris Tech, France

Zirconium-based conversion coatings (ZCC) have been considered in the last decades as environmentally friendly alternatives to chromate systems and are widely used in applications of corrosion protection of alloys.

Here, the formation and growth mechanisms of ZCC were investigated on two distinct alloy systems which are aluminum and zinc alloys using a combination of atomic emission spectroelectrochemistry (AESEC) and glow discharge optical emission spectroscopy (GD-OES).

For zinc-based alloy coatings, the effects of Cu(II) and NO_3^- additives in a Zr conversion coating bath (based on H_2ZrF_6) were investigated. Cu(II) ions underwent a displacement to form Cu(0) which acted as local micro-cathodes. In parallel, this accelerated NO_3^- reduction and hydroxide generation, thereby enhancing ZrO_2 film (i.e., ZCC) formation. The interplay between alloying elements in the presence/absence of additives was monitored in real-time by AESEC. The synergy between Cu(II) and NO_3^- resulted in the highest Zr incorporation in the coating, as confirmed by GD-OES depth profiling.[1]

For aluminum alloys, the influence of acid pickling pretreatment and bath additives (F^-, NO_3^-) on the dissolution kinetics of alloying elements and subsequent Zr deposition was quantitatively resolved by combining *in situ* AESEC and *ex situ* GD-OES. The results showed that nitro-sulfuro-ferric pickling homogenized surface reactivity and promoted the congruent dissolution of Al and Mg during subsequent exposure to the ZCC bath, leading to more uniform ZCC films.[2]

By correlating *in situ* elemental dissolution kinetics (AESEC) with *ex situ* depth-resolved composition (GD-OES), this comparative study demonstrates how to govern the balance between dissolution and precipitation in ZCC processes. The combination of two techniques provides a quantitative solution for optimizing Cr-free conversion coatings across different alloy systems.

[1] J. Han, D. Thierry, K. Ogle, Surface and Coatings Technology,402, 126236, 2020.

[2] B.B.M. Sultan, D. Persson, D. Thierry, J. Han, K. Ogle, Electrochimica Acta, 503, 144820, 2024.

4:00pm **IA2-2-ThA-9 DLC Coatings for Space Applications***,* ***Konrad Fadenberger [konrad.fadenberger@oerlikon.com]****,* Oerlikon Balzers Coating Germany GmbH, Germany*; Roland Holzbauer,* Aerospace & Advanced Composites GmbH, Austria*; Giulio Feliziani,* Oerlikon Balzers Coating Italy S.p.A., Italy*; Sebastien Guimond, Martin Drabik, Andreas Stadlberger, Julien Keraudy,* Oerlikon Surface Solutions AG Pfäffikon, Liechtenstein*; Igor Larranaga,* Oerlikon Balzers Coating Spain S.A.U, Spain

Carbon–based coatings such as amorphous carbon (a–C) and hydrogenated amorphous carbon (a–C:H) offer low friction, high wear resistance, and chemical stability, making them well suited for space mechanisms. In vacuum environments, the absence of ambient passivation amplifies the influence of material transfer, structural modification, and hydrogen concentration on tribological performance. Understanding how hydrogen content, bonding structure, and wear behavior interact under space–relevant conditions is therefore crucial for designing durable coating systems for long–term missions.

Tribological performance was assessed using high–vacuum pin–on–disk testing to characterize steady–state friction and long–duration wear, complemented by reciprocating sliding tests that simulate oscillatory motion typical for actuators and deployment mechanisms, including the associated risk of cold welding. The coatings were deposited using industrial PVD methods on metallic substrates. After testing, wear tracks and counter bodies were examined using SEM and optical techniques. Hydrogen content was determined through Elastic Recoil Detection Analysis (ERDA), providing depth–resolved hydrogen profiles, and results were benchmarked against Raman spectroscopy to evaluate sensitivity and correlations with structural parameters such as the sp^2/sp^3 ratio.

The experiments revealed pronounced differences in tribological response depending on hydrogen concentration and test configuration. ERDA enabled precise quantification of hydrogen distribution within the coating. This integrated approach allowed a comprehensive evaluation of coating performance in conditions representative of space mechanisms, linking vacuum tribology with accurate hydrogen measurement to support the development of reliable carbon–based coatings for space applications.

4:20pm **IA2-2-ThA-10 Solid Particle Erosion Mechanisms of Organic Matrix Composites With and Without Protective Coatings***,* *Veronika Simova,* ***Etienne Bousser [etienne-2.bousser@polymtl.ca]****,* Polytechnique Montréal, Canada*; Marjorie Cavarroc,* Safran Tech, France*; Juan Manuel Mendez,* MDS Coating Technologies, Canada*; Ludvik Martinu, Jolanta Ewa Klemberg-Sapieha,* Polytechnique Montréal, Canada

Organic matrix composites (OMCs), such as carbon fibre–reinforced polymers (CFRPs), have become widely used in the aerospace industry due to their low density, excellent strength-to-weight ratio, stiffness, aerodynamic smoothness, and resistance to fatigue and corrosion. In modern aircraft design, composite materials are employed extensively in both primary and secondary structures to reduce savings and improve fuel efficiency. In engines, they are mainly used in the cold section, such as the fan blades, fan cases, nacelles, and acoustic liners.

When subjected to solid particle erosion (SPE), CFRPs exhibit wear rates more than an order of magnitude higher than those of metallic materials. As any aircraft surface can be exposed to SPE, understanding the erosion mechanisms is crucial.

The erosion behavior of an uncoated OMC, consisting of carbon fibers (CF) embedded in an epoxy matrix (EP), was first examined by evaluating the effects of the erodent particle type, size and velocity, impingement angle, and CF orientation. Erosion rates were determined based on volume losses measured by optical profilometry, with SEM used to understand the failure mechanisms. It has been found that the SPE of the CFRPs arises from two competing erosion mechanisms: brittle erosion of the fiber, and ductile-like wear of the epoxy matrix. Composites with fibers oriented parallel to the erosion direction showed lower erosion rates than those with fibers oriented perpendicularly, especially at low impingement angles (30°).

Given that the erosion rates of uncoated OMCs are significantly higher compared to traditional metal materials, applying erosion resistant coatings is essential to enhance their lifetime and enable their extensive use in aerospace applications.

Therefore, protective TiAl and TiAlN coatings were deposited by pulsed DC magnetron sputtering from a rotating cylindrical TiAl target, in low (9.1%) or high (91%) duty cycle modes. Prior to deposition, short plasma etching was performed to activate the surface and promote the coating adhesion on the OMC substrate. The use of a cylindrical target, which enables high deposition rates, allowed for the preparation of thick coatings (up to 50 µm), with low substrate heating (~100°C) and RF biasing (−100 V). Erosion testing was performed with 50µm Al_2O_3 particles at angles of 30° and 90°, and the results were compared with uncoated OMCs. The 50µm-thick TiAl coating enhances the erosion resistance of OMCs at 75 m/s and 90° up to a factor of 6, providing a solid foundation for further optimization of coating properties, adhesion, and thickness to achieve even greater improvements in the erosion performance of OMCs.

Tribology and Mechanics of Coatings and Surfaces
Room Palm 3-4 - Session MC1-1-ThA

Friction, Wear, Lubrication Effects, & Modeling I

Moderator: Klaus Boebel, Oerlikon Surface Solution AG, Liechtenstein

1:20pm **MC1-1-ThA-1 Tribological Behavior of New and Green Surface Treatments of Anodized Aluminum Alloys***, Marc Schmittbuhl,* Ecole Centrale de Lyon - LTDS, France*; Gilles Auregan, Jacoboni Alex,* Safran Landing Systems, France*; Joffrey Tardelli,* IRT-M2P, France*; **Marjorie Cavarroc-Weimer [marjorie.cavarroc@safrangroup.com]**,* Safran Tech, France*; Vincent Fridrici,* Ecole Centrale de Lyon - LTDS, France

Light and high-performance aluminum alloys are widely used in aeronautical equipments manufactured by Safran Landing Systems. Many parts require sulfuric anodic oxidation surface treatments combined with a sealing step to protect them from corrosion during service. Compliance with chemicals regulations has led to the replacement of traditional sealing baths using chromates (hexavalent chromium) or nickel salts [1] with a combination of an impregnation bath consisting of trivalent chromium (Cr(III)) and fluorozirconates (Zr(IV)), followed by sealing bath with silicates additives [2]. Although these new treatments maintain good corrosion resistance, their tribological behavior differs and thus raises new issues, particularly with regard to friction in screw assemblies.

The objective of this study is to understand friction behavior and wear mechanisms of the new treatments through tribological tests and characterizations of the aluminum oxide layer.

Various configurations of surface treatments were studied, all on 2024 aluminum alloy oxidized by sulfuric anodization:

-Historical treatments sealed with water containing nickel salts

-New-generation treatments including Cr(III)/Zr(IV) impregnation and sealing with water containing silicate salts

-New-generation treatments including only the impregnation step or the sealing step

Flat samples are treated with each configuration and then tested in linear reciprocating tribological conditions in contact with the flat face of a cylindrical 100Cr6 steel pin. The experimental conditions are defined to approximate the conditions of screw fastening assemblies (number of cycles, contact conditions, kinematics, etc.).

The evolutions in friction coefficient for the different configurations are analyzed. Different features of the initial treatment and wear scars on both samples are characterized by means of topography (interferometry and roughness), microscopy (optical and SEM), chemistry (EDX and Raman spectroscopy), and mechanics (hardness). It allows us to identify the parameters influencing friction behavior and wear mechanisms.

Differences in coefficient of friction are related to changes in interface features. Examination of the wear tracks reveals different wear patterns, which can be explained by the effect of the impregnation of new generation treatments on friction.

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1:40pm **MC1-1-ThA-2 Mapping Property Spaces of Combinatorially Deposited Nanocrystalline Alloy Coatings***, John Curry, Frank DelRio, **Tomas Babuska [tfbabus@sandia.gov]**, Justin Hall, Kyle Dorman, David Adams, Nathan Brown, David Montes de Oca Zapiain, Scotty Bobbitt, Michael Chandross,* Sandia National Laboratories, USA*; Filippo Mangolini, Camille Edwards,* University of Texas at Austin, USA **INVITED**

Nanocrystalline alloys continue to gain interest as a promising class of alloys with exceptional mechanical, tribological and catalytic properties among many other intriguing functional properties. Even within simpler binary metallic alloy systems, relative pairings and composition ratios of each alloy can be varied to produce a wide range of alloys with different microstructures/phases and performance characteristics. The ability to rapidly screen the properties and performance of these alloy systems enables the discovery of new alloy compositions tailored to diverse application spaces. This work outlines test methodologies and results for rapidly assessing friction coefficients, tribofilm/wear scar topography, alloy hardness/modulus, resistivity, composition, and structure/density of binary alloy systems. Pt-Au, Pt-Ni and Cu-Ag alloy systems are the focus of current studies, each deposited through combinatorial deposition methods with ~ 336 individual samples per alloy spanning their full range of binary composition space. DFT and EAM-X calculations of adsorption and segregation energies are also discussed. Results show many compositions exist with diverse mechanical properties, tribological performance and mechanochemical phenomena. Application of FAIR data principles during data generation and organization will also be discussed. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

2:20pm **MC1-1-ThA-4 From Green Lubricant to Liquid Precursor for Hard, Multi-Functional Coatings***, **Mohammad Eskandari [mohammadeskandari@my.unt.edu]**, Diana Berman, Ali Zayaan Macknojia,* University of North Texas, USA

The development of sustainable, high-performance protective coatings via simple, scalable, and environmentally harmless methods is a significant challenge in materials science. This study introduces a new approach for surface engineering by polymerizing very-high viscosity Orychophragmus violaceus (OV) seed oil into a hard, multifunctional coating directly on a steel surface. OV seed oil, noted for its exceptional thermal stability, due to its unique triglyceride (TAG) estolide fatty acid structure, was used as a liquid precursor to form a hard protective film on 52100 bearing steel. The coating was synthesized in-situ through a simple, thermal curing process at moderate temperatures (200-250°C). Optimization of the steel-oil interface using surface activation was found to be advantageous for achieving excellent adhesion and film smoothness.

Comprehensive characterization revealed the formation of a uniform, amorphous, carbonaceous thin film with a controllable thickness. The coating exhibited a great hardness and an elastic modulus, as measured by nanoindentation, and demonstrated excellent adhesion through scratch testing. Under pin-on-disk reciprocal tribological testing against 52100 counterbody, the coating provided a low and stable coefficient of friction and specific wear rate, showing around an order of magnitude improvement in the tribological performance. Furthermore, potentiodynamic polarization tests in a 3.5% NaCl solution revealed a dramatic improvement in corrosion resistance compared to the uncoated 52100 steel.

This study presents a successful, cost-effective method for creating a hard, lubricious, and corrosion-resistant coating from a sustainable, green precursor. This in-situ formation process offers a promising alternative to conventional vacuum deposition techniques and opens new insight for the development of next-generation materials for high-performance lubrication and surface protection.

2:40pm **MC1-1-ThA-5 Promise and Pitfalls of Tribological Coatings in Electric Vehicle Applications***, **Ali Erdemir [aerdemir@tamu.edu]**, Gugyeong Sung, Seungjoo Lee, Merve Komurlu, Henry Papesh, Cagatay Yelkarasi,* Texas A&M University, USA*; Leonardo Farfan,* Tecnologico de Monterrey, Mexico **INVITED**

Electric vehicles (EVs) hold great promise for a green, reliable, and economically viable mobility for this century and beyond [1]. However, their long-term reliability is threatened by significant challenges related to critical materials and severe tribological issues triggered by higher torque, load, speed, and temperature conditions [2]. In particular, the shift to a torque-centric drivetrain, combined with extreme contact pressures and shear forces, can accelerate wear, fatigue, and scuffing failures. This situation is further exacerbated by the presence of frequent electrical discharges at the rolling/sliding contact interfaces, which cause severe surface damage and lubricant breakdown. In this talk, we will give a comprehensive overview of these critical issues and stress the need for more advanced materials and coatings that can significantly improve tribological performance and, consequently, the reliability of future EV systems. Specifically, we will highlight the crucial roles of highly electrically insulating Diamond-Like Carbon (DLC) [3] and/or conducting transition metal nitride coatings in enhancing the friction, wear, and scuffing performance of future EV drivetrains.

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3:20pm **MC1-1-ThA-7 Behavior of Nb-Doped Molybdenum Disulfide Coatings Under Electrified Tribological Tests***, Miguel Rubira Danelon,* University of São Paulo, Brazil*; Newton Kiyoshi Fukumasu,* Institute of Technological Research, Brazil*; **Roberto Martins de Souza [robertosouza@usp.br]**, André Paulo Tschiptschin,* University of São Paulo, Brazil

Adaptive coatings have been shown to extend the lifespan of mechanical systems exposed to magnetic, thermal, and electrical disturbances by modulating their properties. In electric vehicle powertrains, stray currents are known to accelerate the degradation of bearings and gears. Coatings based on transition-metal dichalcogenides, such as molybdenum disulfide, provide excellent solid lubrication and wear resistance. However, structural defects can facilitate the formation of MoO_3in humid environments, thereby undermining low-friction performance. Doping TMDs with transition metals enhances their mechanical properties, promotes the formation of amorphous structures with greater integrity, and allows bandgap tuning, enabling modulation of their properties via an electric current. In this study, Nb-doped MoS_2 coatings were deposited onto H13 tool steel substrates using balanced pulsed DC magnetron sputtering. Tribological testing involving electro-stimulation employed a reciprocating ball-on-plane apparatus with an AISI 52100 sphere, a normal load of 30 N, a 5 mm stroke, and a frequency of 0.28 Hz. Three electrical conditions (positively and negatively charged, and no current) were evaluated under both continuous and intermittent current-contact modes, with applied currents ranging from 100 to 1500 mA. Coating morphology and composition were characterized by scanning electron microscopy with energy-dispersive spectroscopy (SEM/EDS), and Raman spectroscopy was used to analyze the films before and after testing. Mechanical properties were assessed through instrumented nanoindentation. Results indicated that passing current reduced the coefficient of friction under both continuous and intermittent modes, achieving reductions of up to 50% relative to the non-electrified condition. This reduction is attributed to recrystallization of Nb:MoS_2 during sliding with an electrified contact. Wear behavior, however, was influenced by current direction, with positively charged counterbodies exhibiting greater wear than negatively charged counterbodies. It is proposed that opposite current polarities induce distinct tribolayer formation and elemental segregation (Mo, S, Nb), which maintains low friction but differentially affects wear. Overall, Nb-doped MoS_2 demonstrates current-responsive tribological behavior characterized by friction reduction and polarity-dependent wear mechanisms.

4:00pm **MC1-1-ThA-9 Calibrated Friction Measurements Using a New Interferometric Atomic Force Microscope***, **Joel Lefever [joel.lefever@oxinst.com]**, Aleksander Labuda, Roger Proksch,* Oxford Instruments, USA

Measuring lateral force is critical for friction measurements on tribological materials ranging from bearings in engines to 2D materials. The atomic force microscope (AFM) is one important tool for frictional measurement on the scales of both microns and nanometers. Conventional optical beam deflection (OBD)-based AFMs are difficult to calibrate, with most calibration methods requiring cumbersome sample exchanges which may disturb the alignment of the chip and detection beam, while simultaneously introducing substantial uncertainty.

We introduce a method for performing lateral force measurements using an AFM with a quadrature phase differential interferometer (QPDI) detector in addition to a traditional optical beam detector (OBD), which furthermore provides a new means to perform a direct calibration of the lateral sensitivity. The detection spot may be placed on the centerline of the cantilever, using QPDI for height feedback while using OBD for friction measurement. In this configuration crosstalk from the lateral signal into the normal signal is eliminated, which reduces the effects of friction and topography on the applied load and is useful for macroscopic relief. Alternatively, by positioning the interferometric detection spot along one edge of the cantilever, the AFM takes advantage of the detector’s low noise floor to observe stick-slip friction at scan rates that would be difficult or impossible with optical beam AFMs The results demonstrate clearly resolvable stick-slip friction over a range of tip speeds up to 2 μm/s and additionally show the variation of friction with applied load. Because this calibration technique can be performed *in situ* without sample exchanges, it also allows calibration to be performed in enclosed environments, for example to enable changing humidity. Furthermore, with some modifications, all of these methods can also be performed in liquid, which is useful for characterizing tribofilm growth and other phenomena.

4:20pm **MC1-1-ThA-10 Effects of Mo–N–Cu Doping on Microstructural, Mechanical, and Tribological Properties of Thick Ta-C Coatings for Cryogenic Applications***, **Young-Jun Jang [yjjang@kims.re.kr]**, Jae-Il Kim, Ji-Woong Jang, Jongkuk Kim,* Korea Institute of Materials Science (KIMS), Republic of Korea **INVITED**

The introduction of environmental regulations and the growing use of renewable energy have altered the operating temperature (111 K) of mechanical components used for transporting cryogenic fluids such as hydrogen, liquid nitrogen, and liquefied natural gas. In cryogenic environments, where lubrication fluids or special lubricants are unavailable, adhesive, abrasive, fatigue, and delamination wear can occur; hence, suitable materials for such conditions are essential. Various solutions have been proposed, including hybrid ceramic bearings combining hard ceramics and alloy steel, or protective coatings such as diamond-like carbon. Among these, tetrahedral amorphous carbon coatings exhibit excellent hardness and wear resistance, yet their performance in cryogenic environments is limited due to difficulties in forming low-friction tribo-films, which are hindered by thermal and chemical reactions in atmospheric conditions. Furthermore, ta-C coatings with surface hardness above 40 GPa can cause severe wear imbalance due to hardness differences with base materials (e.g., SUS 316L stainless steel, 1.75 GPa). The mismatch between the thermal expansion coefficients of the coating and substrate also increases delamination wear at lower temperatures. Excessive hardness additionally leads to reduced fracture toughness, low-temperature brittleness, fatigue, and fracture, thereby degrading coating functionality. For sliding components such as valves or bearings to maintain efficiency under cryogenic conditions, a modified ta-C coating that preserves the mechanical and tribological advantages of ta-C while accommodating thermal and structural stresses is required. This study explores Mo–N–Cu-doped tetrahedral amorphous carbon (Mo–N–Cu–ta-C) coatings synthesized using simultaneous filtered cathodic vacuum arc and unbalanced magnetron sputtering under air (296 K) and liquid nitrogen (77 K) environments. The resulting 1 μm-thick coating comprised nanocomposite Mo carbide and nanolayered Cu structures. Compared with undoped ta-C, Mo doping reduced counterpart wear by 82%, Cu doping enhanced fracture toughness by 22%, and decreased disk wear by 86%. Nitrogen addition promoted phase separation, strengthening the synergistic effects of Mo and Cu to achieve balanced wear. Cu and N_2 further minimized thermal expansion and strain mismatches between the coating and substrate at reduced temperatures, mitigating thermal stress and improving cryogenic reliability. At 296 K, the Mo–N–Cu–ta-C coating exhibited superior adhesion, controlled toughness, and stable wear behavior while maintaining reliable performance in LN_2.

Plasma and Vapor Deposition Processes
Room Town & Country B - Session PP3-ThA

CVD, ALD, and Laser-based Deposition & Microfabrication Technologies

Moderators: Carles Corbella, National Institute of Standards and Technology (NIST)/ University of Maryland, College Park, USA, **Frederic Mercier**, CNRS, Grenoble-INP, University Grenoble Alpes, SIMaP laboratory, France

2:00pm **PP3-ThA-3 Unveiling the Potential of Transparent Conductive Materials by Atomic/Molecular Layer Deposition: From Process Synthesis to Functionalization***, **Abderrahime Sekkat [abderrahime.sekkat@toulouse-inp.fr]**,* Univ. Toulouse, CNRS, Toulouse INP, LGC, Toulouse, France., France **INVITED**

From powering renewable energy systems to transforming lighting and data storage technologies, solar cells, electroluminescent displays (ELDs), organic light-emitting diodes (OLEDs), sensors, and printed electronics are driving the next wave of technological innovation. Transparent conductive materials (TCMs) play a key role in enabling and improving the performance of these devices by offering unique advantages for human–device interfaces and information processing. Today, transparent conducting indium tin oxide (ITO) remains the most widely used TCM, thanks to its excellent optical transparency (>90%) and low sheet resistance (<30 Ω/sq)1,2. It currently holds about 55% of the transparent conductive electrode (TCE) market in 20243. However, ITO is brittle, which limits its use in flexible devices, and its dependence on indium, a critical and scarce resource, raises sustainability concerns. To address these limitations, several alternative TCMs are being actively explored, covering inorganic, metallic, and organic material families.In this presentation, I will give an overview of our ongoing work on developing alternative TCMs using different vapor-phase deposition (VPD) methods. I will first focus on the growth of oxide films using atmospheric pressure spatial atomic layer deposition (AP-SALD), an innovative alternative to conventional ALD4. Unlike traditional ALD, AP-SALD relies on the spatial separation of precursors within a 3D manifold head rather than sequential gas injection. This approach enables faster deposition over large areas, making it well suited for scalable manufacturing. I will present some recent results on p-type oxides obtained by this method5–7. I will then show how oxide coatings can be used to improve the stability of transparent electrodes based on silver nanowire networks8,9. Finally, I will discuss the development of conjugated conductive polymers using oxidative VPD, with examples of their integration into real devices10. Overall, this work illustrates a comprehensive approach, from process synthesis to device functionalization, aimed at advancing the next generation of transparent conductive materials.References1. Nanomaterials 14, 2013 (2024).2. APL Mater. 9, 021121 (2021).3. https://www.imarcgroup.com/transparent-conductive-films-market. (Accessed: 24th July 2025)4. Adv. Mater. Technol. 2000657, 1–8 (2020).5. Nat. Commun. 2022 131 13, 1–11 (2022).6. Commun. Mater. 2, 78 (2021).7. J. Mater. Chem. A 9, 15968–15974 (2021).8. Adv. Mater. Technol. 8, 2200563 (2022).9. Adv. Mater. Technol. 8, 2301143 (2023).10. ACS Appl. Polym. Mater. 5, 10205–10216 (2023).* Corresponding author e-mail: abderrahime.sekkat@toulouse-inp.fr

2:40pm **PP3-ThA-5 In-Plasma XPS: a New Metrology Tool for Semiconductor Process Development and Control***, Andrei Kolmakov [andrei.kolmakov@nist.gov]***, NIST-Gaithersburg, USA **INVITED**

Modern ambient pressure X-ray photoelectron spectroscopy (AP-XPS), in addition to its real-time sub-monolayer sensitivity, now covers the pressure range typical of standard plasma processing applications, naturally expanding the capabilities of AP-XPS for operando plasma-assisted control. We recently demonstrated that XPS spectra can be successfully collected under plasma conditions, extending the application of XPS to plasma-surface-liquid-vapor interactions [1]. In previous work [2], we highlighted the importance of plasma chamber wall reactions on sample surface chemistry and showed that plasma-XPS can capture plasma chemistry both at the surface and in the gas phase. We recently applied plasma-XPS to industry-relevant and realistic poorly conducting surfaces, where we observed anomalous XPS binding energy shifts due to sample charging during an AC plasma exposure. We propose mechanisms that explain these plasma-induced shifts. Additionally, we noted plasma-induced binding energy shifts and peak splitting when measuring XPS from the plasma gas phase. The latter can be used for local diagnostics of the local plasma environment.

Overall, plasma-XPS metrology is a new emerging tool that offers significant potential for advancing real-time diagnostics of plasma-assisted deposition processes, and immediate mitigation strategies to reduce the damage of wafers, which is a well-known challenge in semiconductor fabrication [3].

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3:20pm **PP3-ThA-7 Ultrathin SiN_X Membrane Stability Under Energy Fluxes from Non-Thermal Plasma Discharges Monitored via Nanocalorimetry***, Carles Corbella [carles.corbellaroca@nist.gov]***, National Institute of Standards and Technology (NIST)/ University of Maryland, College Park, USA*; Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST), USA

Freestanding ultrathin silicon nitride (SiN_x) membranes are widely used as an electron, X-ray, and light transparent windows for environmental spectromicroscopy, separation membranes, and in microelectronics, e.g., as in MEMS devices and nanocalorimeters. However, their stability in the plasma environment requires further studies. Here, suspended 100 nm-thick SiN_x membranes have been wafer-scale fabricated on 15 mm^2-silicon frames using lithography. A platinum lithographically defined resistive microsensor of 100 nm thickness is deposited on the backside of the membrane, and it is calibrated for thermometry and calorimetry. This energy flux sensor (nanocalorimeter) has been exposed to cold plasmas in a custom-made research reactor equipped with a remote inductively coupled plasma (ICP) discharge source, Langmuir probe, retarding field energy analyzer, and optical emission spectroscopy (OES) channel. Energy fluxes (ions, electrons, energetic neutrals, and photons) from plasma plume are registered via sensor temperature evolution upon variations in the plasma parameters. The power carried by plasma species can be estimated from a simple energy balance model in measurements using sensor temperature variations up to a few hundred Kelvin with time resolution below 40 ms [Diulus et al, J. Vac. Sci. Technol. B 43, 020601 (2025)]. Additionally, the measurement setup allows for decoupling of the heating contributions by ions and VUV/UV-Vis-IR photons. It was found that the lifetime of the sensor is defined by the SiN_x sputtering rate combined with thermally induced mechanical stress. Ultrathin SiN_x membranes appear to be very robust even when immersed in the RF plasma plume region, manifesting low sputtering yield under typical electrically grounded experimental conditions. To investigate the chemical stability of the ultrathin membranes, nanocalorimetry experiments in argon plasma have been followed by preliminary tests using reactive gases such as oxygen and hydrogen.

Plasma and Vapor Deposition Processes
Room Palm 1-2 - Session PP4-ThA

Greybox Models for Wear Prediction

Moderator: Philipp Immich, IHI Hauzer Techno Coating B.V., Netherlands

1:40pm **PP4-ThA-2 Integrating Tribological Descriptors and Physics-Informed Modelling for Tool Wear Prediction in PVD Coated Milling Tools***, Amod Kashyap [amod.kashyap@kit.edu]***, Institute for Applied Materials (IAM-ZM), Micro-Tribology Centre (µTC), Karlsruhe Institute of Technology, Germany*; Amirmohammad Jamali,* Institute of Production Science (wbk), Karlsruhe Institute of Technology, Germany*; Finn Rümenapf, Nelson Filipe Lopes Dias, Wolfgang Tillmann,* Institute of Materials Engineering (LWT), TU Dortmund University, Germany*; Johannes Schneider,* Institute for Applied Materials (IAM-ZM), Micro-Tribology Centre (µTC), Karlsruhe Institute of Technology, Germany*; Michael Stueber,* Institute for Applied Materials (IAM-AWP), Karlsruhe Institute of Technology, Germany*; Volker Schulze,* Institute of Production Science (wbk), Karlsruhe Institute of Technology, Germany

Accurate prediction of tool wear in milling remains a major challenge due to the complex interplay between process parameters, coating properties, and local tribological phenomena at the cutting interface. Conventional approaches, whether based on extensive machining experiments or purely data-driven algorithms, often struggle to generalise across coatings and lack physical interpretability. This work includes a descriptor from tribological tests that connects generalised wear characteristics obtained through streamlined, indicative testing protocols, yielding a concise, physics-oriented model that flexibly adjusts to changes in operational parameters and contextual influences.

Building on this foundation, a hybrid model is introduced that merges the descriptor with process variables and perspectives derived from numerical simulations, thereby creating a more comprehensive depiction of wear evolution that aligns empirical patterns with conceptual frameworks. Predictions involving the range of coating variants (pulsed DC to HiPIMS) confirm the descriptor's ability to mirror the wear results from the real-world milling experiments. In essence, this approach establishes a flexible, understandable platform for wear forecasting applicable across diverse tool setups and everyday workpieces, dramatically reducing reliance on resource-intensive testing and characterisation.

2:00pm **PP4-ThA-3 Discovering Hard, Conductive Films via Combinatorial High-Throughput Multimodal Characterization and Machine Learning***, Brad Boyce [blboyce@sandia.gov]***, Sandia National Laboratories, USA **INVITED**

Hard, electrically conductive films with low friction and high wear resistance are relevant to electrical contact applications. Here we augment traditional process-structure-property investigations with an accelerated workflow to detect material structure/composition, prognose associated properties, and adapt the associated process to achieve improved product outcomes.This accelerated detect-prognose-adapt cycle is aided by four key elements: (1) automated combinatorial synthesis to enable rapid parameter sweeps, (2) high-throughput evaluation of both conventional and surrogate indicators of material chemistry, structure, and properties, (3) machine learning algorithms to unravel correlations in high-dimensional spaces beyond expert cognition, and (4) batchwise Bayesian optimization strategies to balance efficient exploration and exploitation.Unlike other ML-driven materials exploration campaigns that focus on variations in the composition of the material, here our primary emphasis is on variations in deposition conditions.We identify particular deposition conditions that produce metallic thin films with exceptional hardness (>9 GPa), low friction (m<0.1), and low electrical resistivity on par with commercial electrical contact alloys. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

2:40pm **PP4-ThA-5 Influence of Temperature- Dependent Mechanical Properties on Tool Load in Cutting***, **Christian Kalscheuer [kalscheuer@iot.rwth-aachen.de]**, Kirsten Bobzin, Xiaoyang Liu,* Surface Engineering Institute - RWTH Aachen University, Germany*; Benjamin Bergmann, Berend Denkena, Nico Junge,* Institute of Production Engineering and Machine Tools, Hannover, Germany

Hard physical vapor deposition (PVD) coatings are widely applied to protect cutting tools against wear. Simulating the thermomechanical load of coated tools is an important approach to understand wear mechanisms. In previous studies, the PVD coating in finite element chip formation simulations has typically been treated as a rigid body, or its properties were assumed to remain constant in the simulation. However, the mechanical properties of PVD coatings vary with temperature during cutting. Assuming constant properties may therefore reduce simulation accuracy. In this study, the temperature-dependent mechanical properties of a TiAlCrN coating are determined using high temperature nanoindentation, while thermal diffusivity is measured at different temperatures using the laserflash method. These experimentally determined coating properties were integrated in the simulation for the coating. Based on the experimental results the thermomechanical load is then simulated for cutting of C45 steel in a finite element chip formation simulation. The study compares the results of temperature-dependent mechanical coating properties with constant properties. The results show that simulations with temperature-dependent coating properties are different to simulations with fixed coating properties. This represents an advance in the research direction of understanding the thermomechanical tool load during cutting.

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

Advanced Characterization, Modelling and Data Science for Coatings and Thin Films Poster Session

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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CM-ThP-11 Investigation of Epitaxial Silicon Growth Mechanisms from Chlorosilane–H2 Systems on Si(100) Substrates*, Seokmin Oh [min12002@yonsei.ac.kr], Dongmin Yoon, Seonwoong Jung, Hyerin Shin, Jungwoo Kim, Dae-Hong Ko,* Yonsei University, Republic of Korea

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

Acknowledgment

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CM-ThP-12 Machine-Learning Based Prediction of Carbon Quantum Dot Fluorescent Properties Using Molecular Representations*, Yehyeon Shin [yehyeon23@yonsei.ac.kr], Jong-souk Yeo, Chae-won Lee, Jong-Seok Lee,* Yonsei University, Korea

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

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

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

CM-ThP-13 Structural and Morphological Assessment of a Si/SiO_2/Cr/Au Thin-Film Electrode Stack via Correlative AFM with SEM & EDX*, Satyam Ladva [Satyam@qdusa.com],* Quantum Design, USA

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

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

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

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

Surface Engineering - Applied Research and Industrial Applications
Room Town & Country A - Session IA-ThP
Surface Engineering – Applied Research and Industrial Applications Poster Session

IA-ThP-2 Interface-Engineered Grain Boundary Diffusion for Enhanced Coercivity, Corrosion Resistance, and Thermal Stability in Thick NdFeB Magnets with Efficient Rare-Earth Utilization*, Ching-Chien Huang [huangcc@nkust.edu.tw],* National Kaohsiung University of Science and Technology, Taiwan

Grain boundary diffusion (GBD) has emerged as a powerful interface engineering strategy to enhance the magnetic performance and environmental durability of sintered NdFeB magnets. This study presents a single-stage GBD process utilizing dysprosium (Dy) vapor adsorption, followed by subsequent aging treatment, to overcome coercivity degradation and thermal instability in thick-section magnets. By precisely controlling the diffusion temperature between 940 and 950 °C and the duration from 8 to 16 hours, significant improvements in intrinsic coercivity ($_iH_c$) were achieved. For samples with thicknesses of 5.5 mm and 6.5 mm, $_iH_c$ increased to 25.78 kOe and 25.06 kOe, corresponding to enhancements of 34.06 % and 30.32 %, respectively. These improvements enabled a magnetic grade transition from N44H to G42UH without compromising remanence (B_r) or maximum energy product ($(BH)_{max}$). Microstructural analysis using glow discharge optical emission spectroscopy (GDOES) and field-emission electron probe microanalysis (EPMA) confirmed uniform Dy enrichment at grain boundaries and the formation of thermally stable $(Nd, Dy)_2Fe_{14}B$ intergranular phases, supporting deep and homogeneous diffusion. Electrochemical evaluation via Tafel polarization revealed substantial reductions in corrosion current density and increased polarization resistance, indicating enhanced grain boundary chemical stability. The proposed method enables simultaneous enhancement of coercivity, thermal stability, and corrosion resistance. This interface-focused strategy provides a scalable and resource-efficient solution for fabricating high-performance NdFeB magnets for electric vehicles, offshore wind turbines, and aerospace applications.

IA-ThP-3 Advanced Coating Solutions for High-Pressure Injectors under Bioethanol Fuel Conditions*, Sung Chul Cha,* Hyundai Motor Group- Hyundai Kefico, Republic of Korea*; Jongkuk Kim,* KIMS, Republic of Korea*; Kyoung Il Moon, Hae Won Yoon,* KITECH, Republic of Korea*; Chang Ha Park, Dong Sik Kim,* ATF, Republic of Korea*; **Gi-Hoon Kwon [kgh9900a@kitech.re.kr]**,* KITECH, Republic of Korea

This work presents the results of a ta-C coating developed by Co. ATF for injector balls, offering high hardness and superior corrosion resistance in bioethanol fuel environments. In the 2035 automotive trend, the use of biofuels is expected to continue expanding. Therefore, ensuring the durability of next-generation powertrain components for biofuel applications is essential. Conventional SiO-doped diamond-like carbon (DLC) coatings, 1.8-2.2 µm thick with 22-25 GPa hardness and 300 °C heat resistance, fail under bioethanol exposure due to delamination and severe corrosion of counterpart components. To overcome these limitations, a tetrahedral amorphous carbon (ta-C) coating was developed in collaboration with a domestic research institute and an industry partner. The ta-C coating, with a total thickness of 1.5-1.6 µm, features a two-layer structure consisting of a Ti bonding layer and a ta-C functional layer deposited using filtered cathodic vacuum arc (FCVA). It exhibits a hardness of 64-68 GPa, bonding strength rated HF1, and heat resistance up to 400 °C. Corrosion resistance was validated under aggressive conditions, including exposure to hydrochloric acid and ethanol, demonstrating superior performance compared to SiO-DLC. Additionally, both coatings were compared in a complex severe test sequence involving high-temperature exposure at 400 °C, subsequent corrosion, and friction/wear testing. The ta-C coating consistently outperformed SiO-DLC across all evaluations. These results indicate that ta-C coating offers strong potential for application in biofuel-compatible injector systems.

IA-ThP-4 The Influence of Long-Term Aging in Air Atmosphere on the Precipitation Process of Inconel 740H Alloy*, **Adam Zielinski [adam.zielinski@git.lukasiewicz.gov.pl]**, Hanna Purzynska, Radoslaw Swadzba,* SIEC BADAWCZA LUKASIEWICZ - GORNOSLASKI INSTYTUT TECHNOLOGICZNY, Poland

This paper presents the authors' knowledge of the assessment of the precipitation process in Inconel 740H alloy during long-term aging in an air atmosphere at temperatures of 700°C and 750°C for up to 50,000 hours. This enabled the development of material characteristics for use in assessing the service life of the tested alloy, taking into account the type and size distribution of precipitates across the sample cross-section. The introductory section analyzes the current state of knowledge regarding the development of high-temperature alloys, presents their basic performance characteristics, and presents the research methods used in assessing service life. The research section discusses and defines the degradation process of Inconel 740H alloy under long-term temperature exposure. The scope of the research included microstructural studies (SEM, TEM), identification and analysis of the precipitation process, and mechanical properties. The paper focused in particular on analyzing the changes occurring in the microstructure of the tested alloy. Precipitation processes were characterized quantitatively and qualitatively depending on temperature and aging time. These results were compared to mechanical property tests for individual material states. A relationship between the precipitation process and changes in mechanical properties was demonstrated. Comparative analysis of test results, documented in the form of comprehensive material characteristics, is a key element in determining the safe operating time of components operating under creep conditions without knowing the previous operating parameters. This provides a practical database of reference materials for the actual loss of service life of austenitic matrix alloys.

IA-ThP-5 Nanolayers Based on Ti/TiN, Zr/ZrN, and Cr/CrN in Multilayer PVD Systems: Tribological and Micro-impact Response*, **Daniel Toboła [daniel.tobola@kit.lukasiewicz.gov.pl]**,* Łukasiewicz Research Network – Krakow Institute of Technology, Poland*; Ben D. Beake,* Micro Materials Ltd., UK*; Łukasz Maj,* Institute of Metallurgy and Materials Science of Polish Academy of Sciences, Poland*; Tomasz Liskiewicz,* Manchester Metropolitan University, UK*; Cezary Drenda,* AGH University of Krakow, Poland

Advanced transition–metal nitride coatings are widely employed to enhance the durability and functional performance of components operating under severe contact conditions, particularly in machining and forming. Among these, Ti/TiN, Zr/ZrN, and Cr/CrN multilayer architectures have gained significant attention due to their favorable combination of hardness, wear resistance and good adhesion. Despite extensive studies on their mechanical properties, a comprehensive comparison of their tribological and micro–impact responses – especially under dynamic loading remains limited.

This work investigates the wear mechanisms, frictional behavior, and micro–impact durability of $(Ti/TiN)_{25}$, $(Zr/ZrN)_{25}$, and $(Cr/CrN)_{25}$ coatings deposited by arc-evaporation on hardened M2 steel substrate. Reciprocating tests were performed under 2N load and sliding frequency of 5 Hz to evaluate friction coefficient evolution, wear scars morphology, and counterbody interactions. Micro–impact experiments, conducted using a cyclic loading, enabled the assessment of crack initiation and propagation pathways, and coating deformation modes.

The lowest CoF values were recorded for the $(Zr/ZrN)_{25}$ system, which was over 2.2 times and 43% lower, respectively for $(Cr/CrN)_{25}$ and $(Ti/TiN)_{25}$ coatings. These results directly correlated with the lowest values of the volume of removed material.The wear scars for the Zr/ZrN-based variant were dominated by the abrasive wear mechanism.

Acknowledgments

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IA-ThP-6 Cathodic-Driven Alkalization and Interfacial Reaction Competition in Cathodic-Excess MAO of AZ31B Magnesium Alloy*, **Shih-Yen Huang [f08525129@g.ntu.edu.tw]**, Yueh-Lien Lee,* National Taiwan University, Taiwan

Micro-arc oxidation (MAO) with cathodic bias has been shown to modify discharge behavior and improve corrosion performance of magnesium alloys. However, under cathodic-excess operation (cathodic input exceeding anodic input), the coating/substrate interfacial growth coatings would be different, indicating that interfacial reactions are shifted compared with balanced bipolar conditions. In aluminum MAO, cathodic-excess bipolar conditions have often been associated with discharge softening and improved coating compactness, and the underlying interfacial chemistry has been discussed in detail in terms of phase evolution and reaction pathways. In contrast, for magnesium MAO, excessively high cathodic input is frequently reported to cause coating delamination or peeling, and the explanation is commonly limited to intensified hydrogen evolution and associated mechanical disruption at the interface.

In this research, AZ31B magnesium alloy was treated by bipolar MAO under cathodic-excess conditions with balanced total charge ($Q_c:Q_a$ = 1:1) but higher cathodic current density ($|J_c|:J_a$ = 4:3).The voltage–time response and surface roughness exhibited a soft-sparking-like trend compared with aluminum MAO; however, the corrosion resistance decreased under these cathodic-excess conditions. Cross-sectional observations revealed a non-uniform coating/substrate interface with locally uneven microstructure, suggesting that the interfacial growth pathway changes when excess cathodic current density is introduced. These results indicate that hydrogen evolution alone cannot fully explain the interfacial instability under cathodic-excess MAO on magnesium. The observations are consistent with cathodic-driven changes in local alkalization and OH^--involved interfacial reactions, which alter coating growth and lead to reduced corrosion resistance despite the moderated voltage behavior. To further evaluate this hypothesis, the NaF concentration in the electrolyte was increased. The higher fluoride availability stabilized coating formation and increased the low-frequency impedance by approximately one order of magnitude compared with the baseline electrolyte, supporting the importance of competitive interfacial chemistry beyond hydrogen evolution under cathodic-excess operation.

IA-ThP-7 In-Situ Diffusion-Induced Micro-Carburization of SAE 4140 Steel: Tailoring Surface Integrity and Torsional Resistance via Controlled-Atmosphere Heat Treatment, ***Te-Kang Tsao [tktsao@nkust.edu.tw]***, Dep. of Mechanical Engineering, National Kaohsiung University of Science and Technology, Taiwan; *Wen-Hao Chiu,* Department of Mechanical Engineering, National Kaohsiung University of Science and Technology, Taiwan

Surface engineering plays a critical role in enhancing the structural reliability of high-strength steels subjected to severe mechanical loading. In this study, an in-situ diffusion-induced micro-carburization approach was developed by modulating atmospheric carbon potential (Cp) during the austenitization stage of a conventional quench-and-tempering (Q&T) process. SAE 4140 steel was treated at 840 °C for 1 h under controlled carbon potentials (0.3, 0.4, and 0.8 wt.%). Under the 0.8 wt.% Cp condition, a diffusion-controlled carburized martensitic surface layer approximately 40–50 μm thick was formed without requiring an additional carburizing cycle. Microstructural characterization and hardness profiling revealed a graded surface structure with hardness exceeding 800 Hv, while the tempered martensitic core retained bulk toughness. The experimentally measured hardness gradient showed strong agreement with carbon diffusion profiles predicted using Fick's second law, confirming the diffusion-driven formation mechanism. Residual stress analysis indicated a 21% reduction in detrimental surface tensile stress (from 182 to 144 MPa), attributed to differential transformation kinetics between the carbon-enriched layer and the core during quenching. Mechanical validation under torsional loading demonstrated a 22% increase in maximum torque capacity (from 273 to 334 Nm). Finite element simulations employing the Cockcroft–Latham criterion further revealed that the graded layer acts as a high-strength energy barrier, elevating the cumulative strain energy density threshold required for crack initiation. Although a marginal reduction in torsional fatigue life was observed due to increased surface brittleness and torsional fretting fatigue (TFF), the results demonstrate that in-situ micro-carburization provides an effective strategy for diffusion-based surface engineering. The proposed approach integrates surface modification directly into standard heat treatment, offering a scalable and cost-efficient alternative to discrete coating or vacuum-based processes for high-performance, torque-loaded steel components.

IA-ThP-8 Influence of the Parameters of Producing Oxide Coatings on Aluminum Tapes on Their Structure and Insulating Properties, ***Aleksander Iwaniak [aleksander.iwaniak@polsl.pl]***, *Andrzej Posmyk, Łukasz Bąk, Adrian Krysiak,* Silesian University of Technology, Poland

The windings of most electromagnet coils, transformers and electric motors are made of copper wires. Due to the high price and high density of this element, work is underway to replace copper wires with aluminum tapes. The windings of the timing actuators of combustion engines, the windings of linear motors and transformers, and the windings of electric motors for individual drives of electric vehicles could be made of insulated aluminum tapes, which would result in a reduction in their weight and price.

The conducted research determined the possibility of shaping the insulating properties of oxide coatings by selecting the electrolyte chemical composition and oxidation parameters. The microstructure of the produced anodized oxide layers was examined and their breakdown voltage was measured to determine their dielectric strength.

Studies have shown that adding glycerin to an H2SO4 electrolyte allows the formation of an anodic coating with the same breakdown voltage as an electrolyte without glycerin, while using three times less electricity. Continuous oxide layers were obtained. These layers could be used as electrically insulating coatings in windings.

Protective and High-temperature Coatings
Room Town & Country A - Session MA-ThP
Protective and High-temperature Coatings Poster Session

MA-ThP-1 Multienvironment Tribological Assessment of TiB_2:h-BN:a-C Coatings Deposited on 316L Stainless Steel, ***Ihsan Efeoglu [iefeoglu@atauni.edu.tr]***, *Gokhan Gulten, Banu Yaylali, Mustafa Yesilyurt, Ali Emre, Yasar Totik,* Atatürk University, Turkey; *Justyna Kulczyk-Malecka, Peter Kelly,* Manchester Metropolitan University, UK

AISI 316L stainless steel is widely employed in mechanical and aerospace components; however, its tribological performance is often limited under dry and high-temperature sliding conditions. In this study, a solid-lubricating TiB_2:h-BN:a-C nanocomposite coating was deposited on 316L substrates using closed-field unbalanced magnetron sputtering (CFUBMS) with a hybrid HiPIMS + pulsed-DC power configuration. The coating architecture integrates hard TiB_2 domains for load support, h-BN for lamellar lubrication and thermal stability, and amorphous carbon for low shear and transfer-film formation. A Cr interlayer was introduced to improve interfacial bonding and accommodate residual stresses at the film–substrate interface. The tribological response of the coatings was evaluated under three different environments: dry sliding at room temperature, elevated temperature (300 °C), and boundary-lubricated contact with SAE 50 oil. Results demonstrated that the TiB_2:h-BN:a-C coating effectively reduced friction and wear compared with the uncoated steel, maintaining stable performance across varying temperature and lubrication regimes. Scratch testing further indicated strong adhesion and cohesive integrity. These findings confirm the effectiveness of TiB_2:h-BN:a-C nanocomposites as multifunctional protective coatings for extending the durability of stainless steel components operating under diverse tribo-mechanical conditions.

MA-ThP-2 Understanding Solid Particle Erosion in Multicomponent $Ti_{1-x}Al_xN$ Based Coatings Using Synchrotron Nanodiffraction, ***Anna Hirle [anna.hirle@tuwien.ac.at]***, *Rainer Hahn, Philip Kutrowatz, Tomasz Wojcik,* Christian Doppler Laboratory for Surface Engineering of High-performance Components, TU Wien, Vienna, Austria; *Anton Davydok,* Helmholtz-Zentrum Hereon, Institute of Materials Physics, Hamburg, Germany; *Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials GmbH, Lechbruck am See, Germany; *Anders.O Eriksson, Carmen Jerg, Klaus Boebel,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Balzers, Liechtenstein; *Helmut Riedl,* Christian Doppler Laboratory for Surface Engineering of High-performance Components, TU Wien, Vienna, Austria; Institute of Materials Science and Technology, TU Wien, Vienna, Austria

Protecting components operating in harsh environments, such as in energy production, aviation, and the tooling industry, is essential for ensuring sustainability and long service life. Solid particle erosion (SPE) occurs when high-velocity solid particles impact a material surface, leading to repeated mechanical damage and material loss. This phenomenon critically affects components such as turbine blades, compressor parts, and piping systems. A thorough understanding of SPE is therefore key to improving material durability and performance under erosive conditions. $Ti_{1-x}Al_xN$ protective coatings are widely applied due to their excellent oxidation, corrosion, and erosion resistance. However, increasing operational temperatures demand the development of new coating materials. Alloying $Ti_{1-x}Al_xN$ with Ta and Si has shown promising improvements in oxidation and corrosion resistance [1,2], yet their behavior under SPE conditions remains insufficiently understood.

The objective of the present study is to investigate the solid particle erosion resistance of $Ti_{1-x}Al_xN$ and $Ti_{1-x-y-z}Al_xTa_ySi_zN$ thin films. Accordingly, the coatings were deposited via cathodic arc evaporation using an industrial-scale Oerlikon Balzers INNOVA 1.0 system. SPE tests were performed employing a Jet Erosion Tester with corundum (Al_2O_3) particles at 70 m/s and impingement angles of 30° and 90°. Crater analysis by synchrotron nano-diffraction was employed to assess stress evolution induced by SPE, complemented by profilometry, scanning electron microscopy and transmission electron microscopy characterization. Both coatings demonstrate a significant reduction in mass erosion rates, with approximately 90% decrease compared to uncoated substrates. Synchrotron measurements reveal a clear influence of the as-deposited residual stress state on the stresses induced during erosion.

These results provide new insights into the interplay between residual stress and erosion-induced deformation in multicomponent $Ti_{1-x}Al_xN$ based coatings, contributing to the development of next-generation protective materials for high-temperature and erosive environments.

[1] X. Sun et al., Surf. Coat. Technol. 461 (2023) 129428.
[2] A.R. Shugurov et al., Vacuum. 216 (2023) 112422.

MA-ThP-3 Applicability of Mos2-Asic Heterostructure for Durable Supercapacitance and No2 Gas Sensing in Harsh Environment, ***Habeebur Rahman [habeeb.physics10@gmail.com]***, *Davinder Kaur,* Indian Institute of Technology Roorkee, India

In the present work, the heterostructure of molybdenum disulfide (MoS_2)with amorphous silicon carbide (aSiC) on stainless steel (SS) and Si substrates was fabricated using a DC magnetron sputtering system. This unique heterostructure was examined for energy storage and NO_2 gas sensing applications suitable for harsh environmental conditions. The 2D MoS_2 nanostructured with dissolution resistive aSiC supercapacitor electrode delivers 1.5-fold enhancement in the gravimetric capacitance, a voltage window enlargement from 0.8V to 1.8 V, and an excellent stability of more than 4,000 charge-discharge cycles. Further, the high concentration NO_2 gas sensing performance of the MoS_2-aSiC on Si substrate revealed the stable and recoverable response at high operating temperatures. Therefore, loading aSiC with 2D MoS_2 enables durable electrode material for energy storage and NO_2 gas sensing applications in adverse conditions. The as-fabricated heterostructure was systematically studied by various material and electrochemical characterizations.

MA-ThP-4 Comparative Analysis of the Mechanical Properties of Layers Obtained in Three Different Steels by Atomic Diffusion of Boron., *Enrique Hernández Sánchez,* ***Luz Alejandra Linares Duarte [alejandra.linarespr@gmail.com]****, Diego Hernández Domínguez, Yesenia Sánchez Fuentes,* Instituto Politécnico Nacional, Mexico*; Raúl Tadeo Rosas,* Universidad Autónoma de Coahuila, Mexico*; José Guadalupe Miranda Hernández,* Centro Universitario UAEM Valle de México*; Rafael Carrera Espinoza, Melvyn Alvarez Vera,* Universidad de las Américas Puebla, Mexico*; Jonathan Jorge Ruíz Domínguez,* Instituto Méxicano de la Propiedad Industrial, Mexico

The boriding process was applied to generate hard layers on three different steels —AISI 1018, AISI 316L stainless steel, and AISI 4340 crankshaft steel —with varying treatment times and temperatures (2, 4 and 6h, and 900, 950, and 1000 °C). X-ray diffraction analyses were performed to characterize the phases formed in the coatings. Microscopy techniques were used to evaluate the morphology and thickness of the layers. In addition, micro- and nano-scale mechanical tests were performed to determine the change in the structural and functional properties of the steel. These steels, due to their nature, are subject to wear processes under operating conditions. Therefore, coating these steels with a hard layer that exhibits better properties could help them withstand the working conditions. The boride layers formed on the different steels exhibited varying morphologies. On the one hand, layers with a strong sawtoothed morphology formed on AISI 1018 steel. On the other hand, extremely flat layers were observed on AISI 316L stainless steel, and, finally, layers with a moderate front of growth were obtained on AISI 4340 crankshaft steel. The results indicated that not only were the layers' morphologies different, but also their chemical composition and mechanical properties changed. The layers obtained on AISI 1018 and the 4340 crankshaft steel were of monophasic Fe_2B nature with an 8.83% wt. of boron content, while the nature of those obtained on AISI 316L stainless steel was biphasic FeB/Fe_2B, with a 16.23% wt. of boron content. That difference in composition gives the layers different properties. The higher content of boron gives the biphasic layers the highest hardness, but also makes them more brittle than the monophasic layers. Therefore, it is essential to assess the characteristics of the resulting layers in relation to a specific application.

MA-ThP-5 Reactively Sputtered High-Entropy Metal-Sublattice Carbide Thin Films Based on Al-Cr-Nb-Ta-Ti, ***Thomas Astecker [thomas.astecker@tuwien.ac.at]****,* TU Wien, Austria*; Peter Polcik,* Plansee SE, Austria*; Alexander Kirnbauer, Paul Heinz Mayrhofer,* TU Wien, Austria

High-entropy metal-sublattice carbide thin films based on the equimolar Al-Cr-Nb-Ta-Ti system were synthesized by reactive magnetron sputtering in an acetylene-argon (C_2H_2-Ar) atmosphere. Films were deposited at varying reactive gas flow ratios and substrate temperatures between 450 and 650 °C, yielding single-phase rock-salt structured (fcc) solid solutions. Compositional analysis revealed the presence of an amorphous carbon phase and/or metallic sublattice vacancies. To explore the effect of silicon alloying, additional coatings containing 2.6, 6, and 8.8 at.% Si were prepared, which retained the single-phase crystal structure. The Si-free film exhibited an indentation hardness of 32.8 ± 0.4 GPa, decreasing slightly to 29.5 ± 1.1 GPa for the 8.8 at.% Si film, accompanied by a reduction in the average columnar grain width from 113 nm to 18 nm. No secondary phases formed during vacuum annealing up to 1000 °C for 15 min. While the unalloyed film softened significantly after the thermal treatment starting at 900 °C, the Si-containing coatings maintained their structural stability. Oxidation behavior in ambient air strongly depended on the Si content: at 800 °C, the Si-free film developed a thick (~7.8 µm) rutile-type oxide scale after 1 h, whereas the film with the highest Si-content formed only a dense, thin “passive” oxide layer, even after prolonged exposure at 1000 °C. These results highlight the pronounced beneficial effect of Si alloying on the thermal and oxidative stability of high-entropy carbide coatings, without compromising phase stability or mechanical properties.

MA-ThP-7 Synergistic Alloying Effects of Si and Y in Cr-Mn-Mo-N Thin Films: A Combined Experimental and DFT Study, ***Christian Gutschka [christian.gutschka@tuwien.ac.at]****,* TU Wien, Austria*; Lukáš Vrána, Matej Fekete,* Masaryk University, Czechia*; Zsolt Czigány,* Hungarian Academy of Sciences, Hungary*; Tatiana Pitoňáková,* Masaryk University, Czechia*; Katalin Balázsi,* Hungarian Academy of Sciences, Hungary*; Pavel Souček,* Masaryk University, Czechia*; Helmut Riedl-Tragenreif,* TU Wien, Austria

This study investigates the impact of Si and Y alloying on the microstructure and mechanical properties of Cr–Mn–Mo-based high- and medium-entropy nitride thin films. These films are fabricated by reactive DC magnetron sputtering, employing a combination of both ab initio calculations and experimental analysis. While the Cr–Mn–Mo–N system, in its pure form, displays a stable face-centred cubic (fcc) structure with a negative formation energy (E_f), the latter is known to decrease further with alloying with Si, Y, or both, thus enhancing thermodynamic stability. However, the process of alloying is accompanied by an increase in unit cell distortion, which in turn leads to the destabilization of the crystal structure – manifesting itself in amorphization of experimental thin films, with increasing alloying contents.

Chemical analysis of the grown films revealed that silicon and yttrium promoted nitrogen incorporation. However, complete stoichiometric metal-to-nitrogen ratios were not achieved, and systems with a considerable amount of nitrogen vacancies are formed. Similarly, simulations elucidated a prominent trend of nitrogen vacancies to relax alloy related cell distortions. Structural analyses confirmed the formation of a single-phase fcc solid solution presented here, with lattice expansion and crystallite size refinement being induced by increasing alloying concentrations. Furthermore, the simulations determined both nitrogen vacancy concentration and chemical composition to have a significant impact on ductility, with the highest levels of this property being observed at low nitrogen vacancy levels and when alloying with either Si or Y individually. These predictions showed a fair match with ductility estimates from experiment. More prominently, predictions of elastic properties from experiment and simulation agreed within error range, demonstrating that alloying has a beneficial effect on hardness without compromising the material's elasticity, with Si alloying alone achieving the highest hardness values of 20.5 GPa. An analysis of chemical bonding in the compounds found a synergistic sharing of nitrogen atoms between tetrahedral coordinated silicon species and yttrium atoms, mediated through N-vacancy introduction, as possible explanation for the good mechanical performance of the thin films.

MA-ThP-9 Thermal Stability and Mechanical Performance of Si-Modified High-Entropy (Al,Mo,Ta,V,W)C Coatings, *Muhammad Awais Altaf,* ***Balint Istvan Hajas [balint.hajas@tuwien.ac.at]****,* TU Wien, Institute of Materials Science and Technology, Austria*; Szilard Kolozsvari,* Plansee Composite Materials GmbH, Germany*; Tomasz Wojcik, Alexander Kirnbauer, Paul Heinz Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria

High-entropy carbide (HEC) thin films (Al,Mo,Ta,V,W)C were reactively deposited on sapphire substrates with varying Si content to investigate its influence on microstructure, mechanical performance, thermal stability, and oxidation behavior. All coatings exhibit a single-phase face-centered cubic structure, with lattice parameters decreasing from ~4.34 Å for Si-free HEC to ~4.24 Å for the 7-at%-Si containing HEC-Si7, indicating preferential substitution of Si into the metallic sublattice, because fcc-SiC would have a lattice parameter of 4.35 Å. Si addition transformed the microstructure from coarse, columnar grains to smooth, dense, and near-amorphous surfaces, and shifted the preferred growth orientation from random to (200).

Nanoindentation revealed that as-deposited coatings exhibit hardness and elastic modulus of 30.7 GPa and 506 GPa for HEC, which decrease with increasing Si content to 28.0 GPa and 383 GPa for HEC-Si7. Upon vacuum annealing at different temperatures T_a, HEC degraded significantly, with hardness and modulus dropping to 14.4 GPa and 168 GPa for T_a = 1000 °C, whereas HEC-Si7 retained high mechanical stability, maintaining 26.3 GPa hardness and 381 GPa elastic modulus for T_a = 1000 °C and 24.2 GPa and 389 GPa for T_a = 1200 °C. Isothermal oxidation experiments at 600 and 800 °C for 1 h showed no protective oxide scale formation with or without Si, as already at 600 °C all coatings are oxidized through. However, the stability during vacuum annealing treatment demonstrate that controlled Si incorporation enhances microstructural integrity and mechanical robustness of these high-entropy carbide coatings, offering a promising route for high-temperature protective applications.

MA-ThP-10 Influence of the Ti/Al Ratio on the Performance of Ti-Al-N Coated Tools in the Machining of Stainless Steel 304, ***Felipe Batista dos Anjos [batista.anjos@pucpr.edu.br]***, *Carlos Bernardo Gouvêa Pereira, Carlos Augusto Henning Laurindo, Fred Lacerda Amorim, Michelle Sostag Meruvia, Paulo Cesar Soares Junior, Ricardo Diego Torres,* Pontificia Universidade Católica do Paraná, Brazil

Machining austenitic stainless steel presents significant challenges due to various factors. One key issue is the material's low thermal conductivity, which can lead to thermal overload on the cutting tool. Additionally, these materials tend to adhere to the tool's cutting edge, resulting in adhesive wear and the formation of a built-up edge. To enhance tool performance, ceramic coatings can be applied, as they improve hot hardness and provide thermal and chemical insulation.

This study focused on evaluating the effect of the Ti/Al ratio in titanium, aluminum, and nitrogen-based coatings during the turning process of AISI 304 stainless steel. The coatings investigated were Ti0.56Al0.44N (TiAlN – Futura Nano®) and Ti0.37Al0.63N (AlTiN – Latuma®), both produced by Oerlikon Balzers Revestimentos Metálicos LTDA. Characterization of the coatings through Energy Dispersive X-ray Spectroscopy (EDS) revealed that the atomic ratio of Ti to Al in the Ti0.56Al0.44N coating is 1.27, while for the Ti0.37Al0.63N coating, the ratio is 0.59.

Machining tests were conducted on a CNC lathe equipped for cutting force acquisition, which was monitored over time until the end of the tool's life. To assess tool wear, the surface roughness of the workpiece was measured using a profilometer after each force test, and the tool geometry was analyzed using a scanning electron microscope (SEM). Preliminary results suggest that the tool coated with Ti0.37Al0.63N may exhibit lower cutting forces and a longer tool life compared to the Ti0.56Al0.44N coating. Additionally, nanoindentation tests indicated that the Ti0.37Al0.63N coating has a higher hardness than the Ti0.56Al0.44N coating, resulting in greater wear resistance.

Keywords: PVD Coatings, Tool Wear, Cutting Forces.

MA-ThP-13 Nitrogen-Dependent Structural and Mechanical Properties Evolution of AlCrNbSiTiN$_x$ High Entropy Alloy Nitride Coatings Deposited by HiPIMS, *Sheng-Jui Tseng,* National Taipei University of Technology, Taiwan; ***Jyh-Wei Lee [jefflee@mail.mcut.edu.tw],*** Ming Chi University of Science and Technology, Taiwan; *Yung-Chin Yung,* National Taipei University of Technology, Taiwan; *Bih-Show Lou,* Chang Gung University, Taiwan; *Chia-Lin Li,* Ming Chi University of Science and Technology, Taiwan

High entropy alloy (HEA) nitride coatings have drawn significant attention owing to their excellent mechanical strength, corrosion resistance, and superior thermal stability. In this study, AlCrNbSiTiNx HEA nitride coatings were deposited on Si wafers, AISI 420, and 304 stainless steel substrates using high power impulse magnetron sputtering (HiPIMS). The effect of nitrogen content on the target poisoning behavior of the equimolar AlCrNbSiTi target was monitored and controlled through a plasma emission monitoring (PEM) feedback control system. Target poisoning ratios ranging from 10% to 90% were systematically examined to evaluate their influence on the microstructure and properties of the coatings. The nitrogen-free AlCrNbSiTi coating exhibited an amorphous structure, while the introduction of nitrogen promoted the formation of a face-centered cubic (FCC) nitride phase. Both the hardness and elastic modulus increased with nitrogen addition due to solid-solution strengthening and the formation of metal nitrides. Thermogravimetric analysis (TGA) conducted at 950 °C in air demonstrated that the AlCrNbSiTiNx coatings possessed excellent oxidation resistance. The relationship between nitrogen content, target poisoning ratio, mechanical properties, and oxidation behavior at 950 °C of the AlCrNbSiTiNx coatings was comprehensively studied in this work.

Functional Thin Films and Surfaces
Room Town & Country A - Session MB-ThP
Functional Thin Films and Surfaces Poster Session

MB-ThP-2 Scalable Surface Engineering of PDMS for Uniform Inkjet-Printed Silver Patterns, ***Hsuan-Ling Kao [snoopy@mail.cgu.edu.tw],*** Chang Gung University, Taiwan; *Li-Chun Chang,* Ming Chi University of Technology, Taiwan; *Min-Hsuan Lu,* Chang Gung University, Taiwan

The advancement of flexible and wearable electronics has increased the demand for materials compatible with the human body. Polydimethylsiloxane (PDMS) stands out due to its biocompatibility, transparency, chemical stability, and skin-like mechanical properties, making it suitable for bio-integrated devices. Its elastomeric nature also allows conformal contact with curved surfaces, making it suitable for epidermal and implantable electronics. Despite these advantages, achieving reliable inkjet printing of conductive traces on PDMS remains challenging due to poor ink adhesion and inconsistent droplet behavior. This study introduces a scalable surface modification approach using dielectric barrier discharge (DBD) plasma to improve PDMS wettability for inkjet printing of silver nanoparticle films. The DBD plasma treatment was performed under ambient conditions, and the discharge parameters were tuned to ensure uniform activation across the entire surface. The optimized argon flow rate and electrode gap facilitated consistent plasma exposure, resulting in reproducible surface energy enhancement. By optimizing argon flow and electrode-substrate distance, the treated area was expanded to 5 × 5 cm^2. Water contact angle (WCA) measurements across nine points confirmed uniformity, averaging 50° ± 1.8°, and white-light interferometry verified the surface remained undamaged. Substrate temperature was also found to play a role comparable to WCA in determining film quality, particularly in relation to printed pattern dimensions. At 50 °C, 200 μm-wide lines printed with three layers exhibited slight wrinkling or cracking, while 300 μm-wide lines showed minor edge spreading. Four-layer prints at this temperature led to bulging. At 60 °C, three- and four-layer 200 μm-wide lines suffered from severe wrinkling and cracking, while 300 μm-wide lines showed edge drying or bulging in three layers, and slight bulging in four layers. An appropriate substrate temperature was identified as essential, enabling both 200 μm and 300 μm-wide silver lines to maintain structural integrity and electrical performance across three to four printed layers. Under these optimized conditions, 300 μm-wide, 4 cm-long silver transmission lines exhibited excellent conductivity with low insertion loss. These results demonstrate the effectiveness of the proposed surface engineering and printing strategy for enabling high-quality, large-area conductive patterns on PDMS, supporting the development of next-generation bio-integrated electronic systems.

MB-ThP-4 Spatially Resolved Molecular Arrangement on the Surface of PEDOT:PSS Film via Laser Scanning, *Chanwoo Kim,* ***Habeom Lee [hblee@pusan.ac.kr],*** Pusan National University, Republic of Korea

Conjugated polymers, particularly poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS), are extensively studied for their intriguing electronic and optical properties, making them promising candidates for various functional applications. Precise and spatially resolved control over their molecular organization and morphology is one of challenging things for the tailored innovations. Here, we present a comprehensive investigation into the localized and spatially precise surface structural reorganization of PEDOT:PSS films, achieved through Laser-induced photo thermal effect without any chemical agents. Our focus is on delineating the intricate morphological and molecular changes and understanding the underlying mechanism that enables this spatial control.

Our study delineates the morphological evolution on surface of PEDOT:PSS films (~ 10 μm thickness) under varying laser doses (wavelength: 532 nm, spot size: 7 μm, continuous wave). Notably, a moderate laser dose induces significant morphological transformations, including undulating and dome-like micro-scale surface features with color change. Critically, the moving continuous laser induces a localized thermal distribution. This consistent thermal propagation, coupled with the kinetic state of the laser, induces a rearrangement within the PEDOT:PSS molecular system. The evidenced AFM phase images exhibit a distinct geometry, providing direct visual evidence of spatially controlled molecular reorganization on the surface. These observations promise a powerful approach for achieving spatially resolved control over molecular arrangement, enabling precise patterning and local property tuning.

Further characterization using XPS, UV-Vis, AFM, XRD, Raman, and FT-IR spectroscopy provides insights into the mechanisms driving these changes. This comprehensive study not only significantly elucidates fundamental understanding of laser-PEDOT:PSS interactions for functional film design but also suggests the intricate potential of this technique for creating advanced functional surfaces with tailored properties through precisely engineered molecular architectures.

MB-ThP-5 Influence of the Si Alloying on the Growth Stability and Electrical Properties of Aln Thin Films, ***Norma Salvadores Farran* *[norma.salvadores@tuwien.ac.at]***, *Tomasz Wojcik,* TU Wien, Austria*; Astrid Gies, Jürgen Ramm, Klaus Böbel,* Oerlikon Balzers, Liechtenstein*; Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials, Austria*; Tobias Huber, Jürgen Fleig, Helmut Riedl,* TU Wien, Austria

Aluminum nitride-based ceramics are well known for their insulating properties combined with high thermal conductivity. Their range of applications is wide, in both structural components and thin films. However, the electrical conductivity of these materials is highly temperature-dependent. As the temperature increases, the mobility of charge carriers also rises, which poses significant challenges to their insulating performance.

This study investigates the growth of insulating AlSiN thin films using physical vapor deposition (PVD) and evaluates their electrical insulation at temperatures up to 750 °C. Various reactive PVD techniques were explored, including high-power impulse magnetron sputtering (HiPIMS) and bipolar pulsed sputtering. All depositions utilized a 3-inch aluminum target with varying silicon concentrations in an Argon/Nitrogen (Ar/N_2) atmosphere. Depending on the silicon content, either hexagonal AlN films containing an amorphous Si_3N_4 phase or fully amorphous AlSiN films were produced. The target's alloying concept was designed to enhance deposition stability during sputtering. Within this framework, we also investigated the formation of a fully nitride film at lower reactive gas ratios while maintaining excellent electrical insulating properties.

Phase formation has been examined using X-ray diffraction (XRD), while the deposition rate and film morphology were characterized by scanning electron microscopy (SEM). The insulating behavior of the coatings was evaluated via in-situ impedance spectroscopy across a temperature range from 300°C to 750°C, using Ti/Pt lithography pads as electrodes.

The electrical properties are related to the morphology of the films, particularly whether the films were crystalline or amorphous. Additionally, the influence of impurities, such as O_2, plays a significant role in reducing the insulating properties of the films.

MB-ThP-8 Different Morphologies of Gallium Oxide Thin Films Fabricated by Liquid-Target Reactive DC-Pulsed Magnetron Sputtering, ***Jan Koloros [koloros@ntis.zcu.cz]***, *Petr Novák, Sayed Alireza Ataie, Jiří Rezek, Radomír Čerstvý, Pavel Baroch,* University of West Bohemia in Pilsen, Czechia

Gallium oxide (Ga_2O_3) remains a focus of research due to its outstanding optoelectronic properties, including an ultra-wide bandgap of approximately 4.8 eV, a high electron saturation velocity, and its ability to withstand a high breakdown electric field of about 8 MV/cm. Although Ga_2O_3 is typically prepared using methods such as MBE, MOCVD, or ALD, it would be advantageous to find a viable method for preparing this material using magnetron sputtering as well. This is because this method is known for its high deposition and ease of up-scaling the process. Despite some published work in this area, it has not yet been possible to find conditions that lead to layers with satisfactory electrical properties.

In this work, we focus on reactive magnetron sputtering of Ga_2O_3 films using a liquid gallium metal target on different substrates and under various conditions (oxygen and argon partial pressures, substrate temperature, and pulse-averaged target power density). The resulting films exhibit a broad range of morphologies, from compact solid thin films to wire-like microstructures. We present the optical, electrical, and microstructural properties of the films and suggest their correlations with the discharge parameters as well as the substrate used. We found that the crystalline quality of Ga_2O_3 films and their preferential orientation play a crucial role in achieving improved electrical properties. The optimal crystal structure can be obtained primarily by selecting an appropriate temperature and substrate that promotes the crystalline growth of the film.

MB-ThP-10 3-Layer Polymer Film Composites Based on PE Recyclates, ***Marcin Bilewicz [marcin.bilewicz@polsl.pl]***, *Tomasz Tanski,* SILESIAN UNIVERSITY OF TECHNOLOGY, Poland*; Tomasz Glinski,* Sinoma, Poland

Keywords: n-layer films; blow molding; polymer composites; recycling; hot-tack

Multilayered films are used recently for many applications like packaging, materials with special barrier properties or with resistance for specific liquids or radiation, e.g. UV. The investigation aimed to obtain the composite in form of 3-layer polymer film and nextly to perform the analysis of the structure and properties of newly developed composite produced using 20 meter high blow moulding technology supported by a precision gravimetric dispensing system. To keep better control, the process was supported by advanced, rotating basket and precise sensors. The film samples were prepared, including a reference film labelled as PE pure and made from standard material, and films with a modified middle layer B, containing regranulate and calcium carbonate in specified proportions. The mechanical strength tests of the sealed films were conducted to verify strength of films in aim to be used for FFS (Form-Fill-Seal) packaging lines and are very promising comparing to single layer films. 3-layer packaging films based on PE recyclates and calcium carbonate in the middle layer, retain their required mechanical properties.

MB-ThP-11 Plasma-Polymer Fluorocarbon Based High Sensitivity Surface Enhanced Raman Spectroscopy Application, ***Jimin Han [jimin7479@chungbuk.ac.kr]***, *Sang-Jin Lee,* Chungbuk National University, Republic of Korea

Surface-enhanced Raman spectroscopy (SERS) provides a powerful analytical tool for molecular identification through the amplification of Raman scattering signals from target analytes on plasmonic nanostructures. In this study, we present a plasma–polymer–fluorocarbon (PPFC)-based nanocomposite thin-film platform designed to achieve high SERS sensitivity via controlled nanoparticle formation. By tuning the sputtering power density during mid-frequency magnetron sputtering, the distribution and ratio of Ag and Cu nanoparticles embedded in the PPFC matrix were precisely modulated, as confirmed by X-ray photoelectron spectroscopy (XPS) and ultraviolet–visible–near infrared (UV–Vis–NIR) spectroscopy. The optimized Ag–Cu PPFC (CAP) thin films exhibited distinct localized surface plasmon resonance (LSPR) absorption peaks and demonstrated an enhancement factor (EF) of up to 10^8 for rhodamine 6G, supported by finite-difference time-domain (FDTD) simulations showing strong electromagnetic localization at the metal–metal nanogaps. Furthermore, a simplified fabrication approach employing a single composite target of Cu, carbon nanotube (CNT), and PTFE powders (5:60–80:35–15 wt.%) was developed to produce Cu–PPFC nanocomposite films with moderate SERS sensitivity (EF $\approx 2.18 \times 10^4$). The prepared CAP and Cu–PPFC nanocomposite films successfully detected rhodamine 6G on flexible polyethylene terephthalate substrates, maintaining distinguishable Raman signals even with reduced optical transmittance. These results demonstrate that plasma–polymer fluorocarbon nanocomposites incorporating Cu and Ag nanoparticles offer a scalable, flexible, and cost-effective route toward high-performance SERS-active substrates suitable for on-site and point-of-care molecular detection applications.

MB-ThP-12 Radio Frequency Magnetron Sputtered CdS-Plasma Polymerized Fluorocarbon Nanocomposite Thin Films : Structural Properties and Electrochemical Performance for Lithium-Ion Battery Anodes, ***Joowon Lee [ljw0821@chungbuk.ac.kr]***, *Sang-Jin Lee,* Chungbuk National University School of Semiconductor Engineering, Republic of Korea

Radio Frequency (RF) magnetron sputtering was employed to synthesize CdS–plasma polymerized fluorocarbon (PPFC) nanocomposite thin films. This work presents a comprehensive analysis of the structural, chemical, and morphological characteristics of these films, followed by an evaluation of their potential as anode materials for lithium-ion batteries.

Advanced characterization techniques, including Transmission electron microscopy (TEM), X-ray diffraction (XRD), grazing incidence small-angle X-ray scattering (GISAXS), and X-ray photoelectron spectroscopy (XPS), were utilized to elucidate the film properties. These analyses confirmed the successful incorporation of CdS nanoparticles within the polymeric matrix as shown in **Figure 1**.

Electrochemical testing demonstrated that the CdS–PPFC nanocomposite thin films exhibit stable performance as battery anodes. Notably, thinner films displayed superior battery performance compared to thicker electrodes. This enhancement is attributed to the evolution of surface morphology; specifically, a reduction in film thickness leads to increased surface roughness, which in turn provides a larger surface area for electrochemical reactions.

Acknowledgments

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MB-ThP-13 Synthesis of Bismuth Molybdate Photocatalytic Films by Reactive Magnetron Sputtering for the Photo-Discoloration of Carmine Indigo Dye, *Ricardo González-Campuzano,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*; David E. Martínez-Lara,* Escuela Nacional Preparatoria No.7 "Ezequiel A. Chávez", Universidad Nacional Autónoma de México*; Agileo Hernández-Gordillo,* ***Monserrat Bizarro-Sordo [monserrat@materiales.unam.mx]****, Sandra E. Rodil-Posada,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México

Water pollution has increased significantly due to rapid industrial growth. A significant issue arises from dyes produced by various industries, including the chemical, medical, leather, and other sectors, which pose significant environmental impacts due to their difficult disposal. Photocatalysis has recently attracted considerable attention and demonstrates significant promise for the degradation of diverse organic and inorganic contaminants. It is considered one of the most sophisticated advanced oxidation methods for removing an extensive variety of organic and inorganic pollutants. Bismuth molybdates (BMO) are photocatalytic semiconductors employed in potential applications including water pollutant degradation, air purification, and carbon dioxide reduction, among others.In this work, we report on the synthesis, morphological, structural, compositional, and optical characterization, as well as the evaluation of the photocatalytic response of BMO in thin-film form. The films were produced through co-deposition by sputtering from two independent targets: bismuth oxide (α-Bi_2O_3) and molybdenum (Mo). This approach allows precise control over composition and the attainment of various phases without the need to fabricate targets with different compositions. The deposits were produced by maintaining a constant power of 30 W on the α-Bi_2O_3 target while varying the power on the Mo target from 20 to 100 W. The substrates were heated to 150 °C during deposition, followed by a 1-hour heat treatment at 500 °C in air to induce crystallization. The phases observed were determined by X-ray diffraction and Raman spectroscopy, while their optical properties, specifically the band gap, were estimated using UV-Vis reflectance spectroscopy.The photocatalytic response of the films was evaluated by photodecolorization of indigo carmine (IC) dye solutions at five ppm and pH 3.5 under irradiation from a 385 nm light source. The results showed a decrease in the intensity of the 610 nm absorption band of the IC solution with increasing irradiation time, achieving almost 100% photodecolorization in approximately 2 hours. Subsequent tests for reuse and stabilization were performed for practical applications, repeating the IC blue photodegradation experiments ten times using the sample that showed the best photocatalytic performance. No significant reduction in photocatalytic activity was observed after 10 cycles of testing.

MB-ThP-14 Microstructure and Electrochemical Behavior of Aps Coatings Deposited on Agricultural Plows, *Corneliu Munteanu,* ***Bogdan Istrate [bogdan.istrate@academic.tuiasi.ro]****,* "Gheorghe Asachi" Technical University of Iasi, Romania*; Boris Nazar,* Technical University of Moldova*; Fabian Cezar Lupu, Ramona Cimpoesu, Gelu Ianus,* "Gheorghe Asachi" Technical University of Iasi, Romania*; Teodor Marian,* Technical University of Moldova

This research focuses on the application of thermal spray technologies aimed at optimizing the functional properties of agricultural components intended for soil tillage. The investigation is based on thermal coatings obtained through Atmospheric Plasma Spray (APS) technology applied to the constructive elements of agricultural ploughs, which are subjected to aggressive operating conditions. The specific properties of these components—microstructural analysis and corrosion resistance—constitute determining parameters for ensuring enhanced durability of agricultural equipment (mainshare and foreshare).

Within the experimental investigation, protective coatings were deposited through thermal spray technology using metallic powders based on WC12%Co (commercial designation WOKA 3101). Characterization of the microstructural properties and electrochemical behavior of the deposited layers was evaluated on laboratory specimens in specific corrosion environments. The obtained results demonstrated that thermal spray coatings presents an optimal method for enhancement and potential reconditioning of components.

The deposited layers exhibited satisfactory adhesion and characteristic microstructure, composed of successive splats with reduced porosity. Analysis of electrochemical behavior revealed superior corrosion resistance compared to the base material, an aspect indicating significant improvement of functional properties and enhanced functional capacity of the coated components.

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MB-ThP-15 Influence of Microstructure on Dealloying Kinetics of Nanoporous Thin Films, *Ezgi Hatipoğlu,* Max Planck Institute for Sustainable Materials, Germany*; Ayman El-Zoka,* Imperial College London, UK, Germany*; Yujun Zhao,* Max Planck Institute for Sustainable Materials, Germany*; Stanislav Mraz, Jochen Schneider,* RWTH Aachen University, Germany*; Baptiste Gault,* ***Aparna Saksena [a.saksena@mpi-susmat.de]****,* Max Planck Institute for Sustainable Materials, Germany

Nanoporous metals offer an important platform for tailoring composition and surface-to-volume ratio, both aspects critical for applications in catalysis where nanoporous thin films can offer further ease of handling. These films are however prone to intergranular cracking during dealloying, limiting their stability and potential applications. Here, we set out to systematically investigate the grain boundaries (GBs) in Au28Ag72 (± 2 at.%) thin films. We observe that sample synthesized at 400 °C is at least 2.5 times less prone to cracking compared to sample synthesized at RT. This correlates with a higher density of coincident site lattice (CSL) GBs, especially the density of Σ3, increased, which appear resistant against cracking. Atom probe tomography (APT) of random high-angle GBs reveals prominent Ag enrichment of up to 77at.%, whereas Σ3 coherent twin boundaries show Au enrichment of up to 30at.%. APT also reveals a strong texture dependence on the dealloying kinetics where the (111)-textured film retains a higher Ag concentration within the nano-ligaments and the untextured film already exhibits coarsening, indicating a faster reaction kinetics, and a lower Ag content. Our study highlights the potential of microstructure engineering in tailoring the properties of nanoporous metals for possible future catalytic and electrochemical applications.

MB-ThP-17 Effect of UHTC Nanoparticle-Reinforced Micro Arc Oxidation Composite Coatings on the Surface Performance of Al 2024 Alloy, *Suleyman Sukuroglu,* ***Ebru Emine Sukuroglu [eesukuroglu@gumushane.edu.tr]****,* Gumushane University, Turkey

Aluminum (Al) and its alloys are widely used as structural materials in various engineering applications, particularly in the automotive, aerospace, and space industries, due to their high strength-to-weight ratio, corrosion resistance, high machinability, and superior specific strength. Despite these advantages, their relatively low surface hardness, high friction coefficient, limited wear resistance, and poor corrosion performance in aggressive environments restrict their application range. To overcome these drawbacks and expand the usability of Al and its alloys, surface modification processes have been extensively applied.

Micro Arc Oxidation (MAO) is an environmentally friendly coating technique that enables the formation of hard, strongly adherent ceramic oxide coatings on aluminum and its alloys. The aluminum oxide (Al_2O_3)-based ceramic coatings produced by this method significantly enhance the mechanical, tribological, and corrosion resistance of the substrate material. However, prolonged exposure of Al_2O_3-coated substrates to aggressive service environments may lead to coating degradation and deformation.

To mitigate these limitations and to tailor the mechanical, adhesive, and corrosion-resistant properties of the coatings, the incorporation of nanoparticles into the MAO electrolyte has emerged as an effective approach. Among these additives, ultra-high-temperature ceramic (UHTC) materials exhibit exceptional hardness, wear and corrosion resistance, and outstanding stability under extremely high-temperature conditions, making them highly promising for advanced aerospace and space applications. Artificially synthesized ceramics such as hafnium carbide (HfC) and zirconium carbide (ZrC) are among the materials with the highest known melting temperatures and are extensively utilized in extreme environments, including hypersonic systems, missile and rocket components, and thermal protection structures.

In this study, composite coatings reinforced with two different ultra-high-temperature ceramic nanoparticles, HfC and ZrC, were fabricated on Al 2024 alloy using the MAO method. The effects of these composite coatings on the structural, mechanical, tribological, and corrosion properties of the alloy were systematically investigated.

MB-ThP-18 Ion-Beam Assisted Deposition of Oxide Semiconductor Thin Films for Optical Devices, ***Pin Yao Hsiang [hsiangpy@gmail.com]****,* Chang Gung University, Taiwan*; Tsung Yu Huang,* Ming Chi University of Technology, Taiwan, Republic of China

This study investigated the use of a tin-based oxide (SnOx) semiconductor layer as the active layer for a light-addressable potentiometric sensor

(LAPS) on a commercial indium tin oxide (ITO)/glass substrate. We characterized the optical absorption properties of the SnOx layer, as well as changes in Hall mobility and Raman spectroscopy, using ion beam assisted discharge (IBAD) and varying argon/oxygen flow ratios. The experimental results demonstrate the potential of SnOx as an active layer for LAPS, but the stability and lifetime performance of SnOx LAPS require further process optimization.

MB-ThP-19 Insulation Coatings for Temperature Sensors in Molding Tools*, **Martin Welters [welters@kcs-europe.com]**, Rainer Cremer,* KCS Europe GmbH, Germany

The mobility sector is one of the largest emitters of greenhouse gases. Consequently, providers of mobility services and systems are facing a profound transformation towards climate neutrality. A key lever on the path to emission-free production is circular value creation, which significantly reduces the use of primary raw materials and thus lowers environmental impact. The overarching goal of the project is to improve the CO_2 and environmental performance of structural and hybrid components by consistently increasing efficiency, using recyclates, and implementing an ecologically optimized component design.

One sub-project focuses on the development and design of sensor-equipped tool inserts for **in-situ temperature measurement**during the production of automotive components made from recycled materials. The sensor layer system consists of multiple layers - sensor layers and an electrical insulation and a wear-protection layer - applied on top of each other to form a layer stack. A key requirement is that the coatings must meet not only the sensory specifications but also the durability criteria necessary for their application - particularly when used with polymer melts containing recyclate components. For the development of the insulating layer, special sensor dummies as well as fixturing for PVD processes were developed to enable the investigation of local differences in the properties of the insulating layer. In this way, the aluminum-based insulation layers used could be iteratively improved with regard to the application, eliminating the need to coat numerous elaborately manufactured sensors.

MB-ThP-20 Corrosion-Inhibiting, Antibacterial Coatings for Soft Tissue Anchors*, **Simon Cremer [simon.cremer@kcs-europe.com]**, Rainer Cremer,* KCS Europe GmbH, Germany

Conventional biodegradable soft tissue anchors are exposed to severe corrosion due to their contact with blood, causing them to lose their integrity after only 8-12 weeks. PVD coatings are aimed at specifically influencing this corrosion. PVD coatings have long been studied for their corrosion protection properties. Although layers deposited by magnetron sputtering or arc evaporation nowadays have a dense microstructure. However, contact with corrosive media such as blood usually leads to pitting corrosion very quickly, which severely attacks the substrate materials underlying the coating. Such attacks occur primarily at layer growth defects.

In order to prevent controlled degradation of the implants and the negative effects of pitting corrosion, which manifests itself in excessively rapid corrosion, round samples of an Fe-Mn alloy were polished and coated with a thin titanium layer by KCS Europe using a sputtering process. To obtain an antibacterial surface, the samples were coated with a silver layer of 3, 10, and 30 nm in a second coating process. The thickness of the silver layer is decisive for the antibacterial effect of the surface. If the silver layer is too thin, the antibacterial properties of the surface can be lost because individual areas of the surface are not coated. A continuous silver layer, on the other hand, prevents the desired controlled degradation of the implants. A surface on which individual silver cells were deposited locally in island-like formations, but did not completely cover the substrate, proved to be optimal for controlled decomposition and the antibacterial effect of the coatings.

MB-ThP-21 Partial Laser Ablation in PVD Multilayers for Multicolored and Nanostructured Surfaces*, Raphael André,* Berner Fach Hochschule, Switzerland*; Christian Petitot,* Université Marie et Louis Pasteur, UTBM, CNRS, Institut FEMTO-ST (UMR 6174), France*; Rainer Kling, Sylvain Le coultre,* Berner Fach Hochschule (BFH), Switzerland*; **Pascal briois [pascal.briois@utbm.fr]**,* Université Marie et Louis Pasteur, UTBM, CNRS, Institut FEMTO-ST (UMR 6174), France

The APLM (*Ablation Partielle par Laser dans des Multicouches PVD pour des surfaces Multicolores et nanostructurées in french*) project is supported by the INTERREG VI France–Switzerland 2021–2027 program. The project consortium consists of two universities, namely the Bern University of Applied Sciences (BFH) and the University of Technology of Belfort-Montbéliard (UTBM), as well as four industrial partners (Plasmadiam and Gravity for Switzerland, and SILSEF and SAIREM for France).

The objective of APLM is to develop all the technical expertise required to industrialize a process invented and patented by BFH and Plasmadiam in May 2024. The invention combines vacuum deposition technologies for ultrathin coatings using PVD and PECVD, together with partial ablation by means of nanosecond, picosecond, and femtosecond pulsed lasers, enabling the generation of cavities within multilayers with nanometric control and precision. Prototypes of multicolored watch dials, as well as molds for nanoimprint lithography (NIL), embossing, and plastic injection molding, will be produced. These prototypes will help promote the technology and enhance the value of the invention, generating economic benefits for all industrial partners of the consortium within the regions and beyond.

The main actions of the project consist in developing various robust processes for depositing brightly colored layers or layers with specific optical properties by combinatorial PVD sputtering, with or without the use of MW-PECVD plasma, while meeting the mechanical specifications required for the targeted applications. Subsequently, a database of laser ablation thresholds (in J/cm^2) will be established for the different colored or functional PVD layers produced (20–500 nm thickness range) at different wavelengths. A predictive model will also be designed to estimate the ablation threshold of a material based on its physical properties. Finally, flagship prototypes demonstrating the patented technology will be developed in the fields of multicolored watch dials and nanostructured molds for NIL, embossing, and plastic injection, through the ablation of nanometric cavities structured on three or four levels.

During this poster presentation, a general overview of the project will be provided, along with a presentation of the first colored coatings obtained by BFH and UTBM. These coatings were produced by reactive magnetron sputtering.

MB-ThP-23 Numerical Modelling for Optimized Experimental Design in Vernier Ellipsometry Sensing*, Kawshik Shikder, Zhang Yun, Md Rashedul Huqe, Yishu Foo, May Thawda Phoo, Yee Man Kwong, **Juan Antonio Zapien [apjazs@cityu.edu.hk]**,* City University of Hong Kong

In Vernier Ellipsometry Sensing (VES) two zero-reflection points (ZRPs) in p-pol and s-act in synergy to enable a refinement optical measuring scale akin to a Vernier scale. These new class of sensors are enabled by: i) strong coupling between p-pol surface plasmon polariton and p-pol photonic waveguide leading to Rabi splitting with phase singularities of the resulting hybrid resonances; ii) spectrally overlap between the s-pol photonic modes and the hybrid p-pol resonances; and, importantly, iii) the ellipsometric sensing strategy where the s-pol ZRPs provide a stable reference to boost the sensor performance in terms of the amplitude ratio and phase difference of both ZRPs.

In VES fine angle of incidence (AoI) tuning enables resetting the sensor to its optimal sensing point.We will present new numerical simulations that are able to track the performance of this VES with high efficiency to determine the optimum operation conditions in terms of (AoI) and spectral overlap resonance for la large dynamic range in changes of refractive index unit (RIU) in the sensing media. We discuss the implications of these results for the design of a dedicated AoI- and wavelength- resolved ellipsometer system capable to instantaneously track the best-point sensitivity and achieve lowest limit of detection (LoD) and large dynamic range.

MB-ThP-24 Selective Etching of Boron Doped Si1-XGeX Epitaxial Layers for Vertically Stacked Memory Device*, **Joosung Kang [jws1204@yonsei.ac.kr]**, Dongmin Yoon, Seonwoong Jung, Dae-hong Ko,* Yonsei University, Republic of Korea

Dynamic random access memory (DRAM) devices have continuously increased their integration density through aggressive device scaling and have progressively evolved toward three-dimensional (3D) architectures to overcome the limitations of planar designs. Among various approaches, 3D DRAM structures employing highly stacked Si channels and SiGe sacrificial layers are regarded as promising candidates for cell designs beyond the $4F^2$ node. In such vertically stacked channel architectures, the selective removal of SiGe sacrificial layers from epitaxial Si/SiGe multilayers represents a critical process requirement.

In this study, the selective etching behavior of boron-doped SiGe epitaxial layers—introduced to compensate for strain arising from lattice mismatch between Si and SiGe—was systematically examined as a function of boron concentration. Dopant-dependent variations in etching behavior were observed in both blanket films and Si/SiGe multi-stack structures. To gain insight into the underlying mechanisms, the chemical bonding states of etched SiGe surfaces were analyzed using X-ray photoelectron spectroscopy (XPS), with a focus on dopant-induced modifications of oxide-related surface chemistry. The results reveal that boron incorporation significantly alters the etching response of SiGe layers through changes in surface oxide chemistry, leading to distinct dopant-dependent trends. These findings provide fundamental insight into dopant-mediated surface reactions during selective etching and offer useful considerations for process optimization in vertically stacked semiconductor device fabrication.

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Tribology and Mechanics of Coatings and Surfaces
Room Town & Country A - Session MC-ThP

Tribology and Mechanics of Coatings and Surfaces Poster Session

MC-ThP-1 Evaluation of Stress Field in a Borided Inconel 718 Superalloy Under Dry Sliding Wear*, Alan Daniel Contla Pacheco, Iván Campos Silva,* Instituto Politécnico Nacional, Mexico*; Arturo Ocampo Ramírez,* Universidad Veracruzana, Mexico*; Daybelis Fernández Valdés,* Tecnológico Nacional de México*; GERMAN ANIBAL RODRIGUEZ CASTRO,* ***Felipe Nava Leana [felnaval@gmail.com]****, ALFONSO MENESES AMADOR,* Instituto Politécnico Nacional, Mexico

In this work, the wear resistance of Inconel 718 superalloy hardened by the boriding process was evaluated by means of dry sliding. A powder-pack boriding process was used to modify the alloy surface in which nickel borides were obtained in the sample due to the boron diffusion into the substrate material. The thermochemical treatment was carried out at a temperature of 950 °C for 2 and 6 h of exposure time. The Ni2B, Ni4B3 and Ni3B intermetallic compounds formed on the surface of the Inconel 718 superalloy were confirmed by XRD analysis. Berkovich nanoindentation tests were conducted to determine both hardness and Young's modulus of the borided samples. The dry sliding wear tests were performed on the surface of the borided sample using an alumina ball with diameter of 6 mm, a constant load of 20 N and distances of 50, 100, 150 and 200 m. Wear coefficient was obtained by the Archard's model. The finite element method using mesh nonlinear adaptivity was used to obtain the stress field during the wear test. Results of the failure mechanisms over the worn tracks showed that the sample with thicker thickness had better wear resistance.

MC-ThP-3 Tribological and Corrosion Performance of Alloy 718 coated with WC/Co Applied by HVOF*,* ***Nathalia Kappaun Vieira [nathaliakapp@hotmail.com]****,* PUCPR, Brazil*; Steffen Aicholz,* Oerlikon Balzers, Brazil*; Michelle Sostag Meruvia, Paulo Soares, Ricardo Diego Torres,* PUCPR, Brazil

Nickel-based superalloys, such as Inconel 718 and Inconel 625, are widely used in oil and gas industry due to their mechanical and Chemical properties. The extraction and processing environments involve high temperatures, high pressures, and corrosive environments. Nickel alloys offer high mechanical strength at elevated temperatures, and excellent resistance to corrosion and oxidation, ensuring safety and a longer service life for components that use them. Inconel 718 has high corrosion resistance, but its application is limited due to low hardness and wear resistance. One method of solving this problem is to combine heat treatment with application of coatings. The present work carried out a comparative study of the tribological and tribocorrosive properties of nitride Inconel 718 and Inconel 718 with a WC/Co coating, applied by the HVOF method, which was chosen due to the obtention of a dense layer with low porosity, improving the wear resistance of the material. The surfaces were characterized using X-ray diffractometry (XRD), microhardness, and scanning electron microscopy (SEM) techniques. The tribological, tribocorrosive, and corrosive properties were evaluated in five environments: (a) Distilled water saturated with CO2; (b) distilled water with sodium chloride; (c) distilled water saturated with H2S; (d) distilled water with sodium chloride and saturated with CO2; (e) distilled water with sodium chloride, CO2and H2S. Where in the end the surfaces will be compared across three requirements: i) corrosion current and potential, ii) wear rate, iii) wear rate considering the synergistic effect of tribocorrosion.

MC-ThP-4 Influence of Coating Thickness and Bias Voltage on Cracking Behavior of TiAlCrN PVD Coating*, Kirsten Bobzin,* ***Christian Kalscheuer [kalscheuer@iot.rwth-aachen.de]****, Wenting Xu,* Surface Engineering Institute - RWTH Aachen University, Germany

Physical Vapor Deposition (PVD) TiAlCrN coatings show outstanding mechanical properties, thermal stability and oxidation resistance. Therefore, TiAlCrN coatings exhibit great potential to be deposited on cutting tools in order to minimize wear during cutting operations. Both the coating thickness and the bias voltage applied during the PVD process can influence the cracking behavior of the coating, which in turn affects the machining capacity and lifetime of the cutting tools. In this study, TiAlCrN coatings with thicknesses of s = ~ 2.2 µm, ~ 2.8 µm and ~ 3.8 µm were deposited on cemented carbide WC-Co substrates under a constant applied bias voltage of U_B = -80 V. In addition, TiAlCrN coatings were deposited with different applied bias voltages of U_B = -60 V, -80 V and -100 V at a constant thickness of s = ~ 2.8 µm. The cracking resistance was evaluated using nanoscratch tests with constant forces of F = 250 mN, 500 mN and 750 mN. A conical diamond indenter was used for the nanoscratch tests. Nanoscratches were analyzed for cracks on the surface and in cross-section for coating deformation using scanning electron microscopy (SEM). Additionally, the depth of the nanoscratches were measured with confocal laser scanning microscopy (CLSM). In this study, thicker coatings exhibit better cracking resistance. With increasing thickness, the permanent deformation is reduced. In addition, the coating deposited with a bias voltage of U_B = -100 V exhibits the lowest deformation. The results reveal valuable insights in the cracking behavior of TiAlCrN coatings. These findings can contribute to enhancing the machining performance and the lifetime of cemented carbide tools through targeted coating design.

MC-ThP-5 Enhancing Corrosion Resistance and Tribological Performance of Inconel 718 through Plasma Nitriding and CrAlN/DLC Coatings for Oilfield Applications*,* ***Heloísa Scalabrin [heloisa.scalabrin@pucpr.edu.br]****, Michelle Sostag Meruvia, Paulo Soares, Ricardo Diego Torres,* Pontifícia Universidade Católica do Paraná (PUC-PR), Brazil

Oil and gas environments are highly corrosive due to the presence of H_2S, CO_2, and chloride ions, which accelerate material degradation through both chemical and mechanical mechanisms. This study investigates the impact of plasma nitriding on the tribological performance, adhesion, and corrosion resistance of CrAlN/DLC coatings deposited on Inconel 718 substrates. The goal is to develop an alternative surface treatment suitable for extreme oilfield conditions.

The Inconel 718 specimens were aged at 760 °C for 6 hours. Three groups were analyzed: (i) nitrided Inconel 718, (ii) nitrided Inconel 718 with CrAlN/DLC coating, and (iii) Inconel 718 with CrAlN/DLC coating without nitriding. Characterization was conducted using nanoindentation to assess mechanical properties, pin-on-disk testing for wear evaluation, and scratch testing for adhesion. The tribocorrosion performance was evaluated in a simulated oilfield environment. Structural and phase integrity of the coatings were analyzed using Raman spectroscopy and X-ray diffraction (XRD), while surface morphology and failure mechanisms were examined via scanning electron microscopy (SEM).

Plasma nitriding enhances surface hardness and promotes the formation of a diffusion layer, which improves coating adhesion and compatibility with the substrate. This combination reduces friction and wear under tribocorrosive conditions. Additionally, DLC deposition lowers friction coefficients and wear rates, further enhancing resistance to tribocorrosion. Preliminary results indicate that nitriding significantly increases surface hardness and coating adhesion. XRD analysis confirms the structural integrity of CrAlN/DLC coatings after exposure, supporting the proposed surface treatment as a multifunctional solution for harsh oilfield environments.

MC-ThP-6 High Temperature Stability of Different Diamond-Like Carbon Thin Films*,* ***Daniel Pölzlberger [daniel.poelzlberger@tuwien.ac.at]****,* Institute of Materials Science and Technology, TU Wien, Austria*; Julien Keraudy, Klaus Böbel,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; Tomasz Wojcik, Philip Kutrowatz,* Christian Doppler Laboratory for Surface Engineering of High-performance Components, TU Wien, Austria*; Carsten Gachot,* Institute of Design Engineering and Product Development, Research Unit Tribology, TU Wien, Austria*; Helmut Riedl,* Institute of Materials Science and Technology, TU Wien, Austria

The transition to a more energy-efficient world requires innovative solutions, with materials science and tribology playing critical roles. Improving lubrication and reducing wear are essential for lowering the carbon footprint, conserving energy, and meeting climate targets. While conventional liquid lubricants perform well under many conditions, extreme environments, such as high or cryogenic temperatures, high contact pressures, vacuum, or radiation, demand the use of solid lubricants combined with advanced materials. However, many solid lubricants, including MoS_2, MXenes, and graphite, oxidize rapidly above approximately 400 °C, limiting their applicability. Developing self-lubricating materials that also provide excellent corrosion and wear resistance is, therefore, crucial. Among solid lubricating coatings, diamond-like carbon (DLC) is one of the most established. Yet, its performance at high temperatures above 400 °C remains questioned, as DLC coatings are suspected to degrade under such conditions. A systematic comparison and extreme condition testing that links tribological performance to coating properties is still missing.

This study investigates different DLC-based thin film materials, classifying them by dominant mechanisms, application ranges, and performance. Several DLC coatings are compared, including non-hydrogenated DLC (a-C), hydrogenated DLC (a-C:H), hydrogenated DLC with an oxide former (a-C:H:Si:O), and tetrahedral amorphous carbon (ta-C). These coatings, which vary in mechanical properties and sp_2/sp_3 ratios, were tribologically tested at different temperatures and loads. Subsequent surface characterization included nanoindentation, Raman spectroscopy to analyze the effects of graphitization after thermal exposure, and X-ray photoelectron spectroscopy. Further insights into the limits of carbon as a solid lubricant are provided through high-resolution characterization techniques such as high-resolution transmission electron microscopy.

In summary, this work highlights the potential of advanced DLC coatings for solid lubrication. It highlights the need for a deeper understanding of their mechanisms and the design of innovative coatings to enable future high-performance applications.

MC-ThP-7 The Impact of Nitriding Parameters on the Tribological and Corrosion Behavior of Inconel 718*, Gabriel Queiroz Carara, Heloisa Scalabrin, Cesar Neitzke, Michelle Meruvia, Paulo Soares,* ***Ricardo Torres [ricardo.torres@pucpr.br]****,* PUCPR, Brazil

The mechanical and tribological properties, along with the corrosion resistance of plasma-nitrided Inconel 718, were evaluated at nitrided treatment temperatures of 400°C and 500°C. The treatments varied in duration, lasting 1 hour, 2 hours, or 4 hours, and utilized gas compositions of 5% N_2 / 95% H_2 and 25% N_2 / 75% H_2 at a pressure of 530 Pa. Microstructural characterization was conducted using X-ray diffraction. For mechanical characterization, Vickers hardness measurements were performed using a force of 245.2 mN. The tribological properties were assessed through a reciprocating wear test involving an Inconel 718 and cemented ball pair, from which the wear rate was determined. Corrosion resistance was evaluated through potentiodynamic polarization testing. The results indicated that treatment at 400°C led to the formation of the expanded austenite phase, while the samples nitrided at 500°C formed the CrN phase. As anticipated, increasing the nitriding parameters resulted in a progressive increase in sample hardness—from 4.5 GPa for untreated samples to 9.75 GPa for those treated at 500°C with 25% N_2 for 4 hours. A notable reduction in the coefficient of friction was observed in all nitrided samples compared to the non-nitrided sepecimen, with the samples treated at 500°C exhibiting the lowest friction coefficient values. Additionally, the wear rate saw a significant decrease when comparing nitrided samples to non-nitrided ones.

MC-ThP-9 Effect of Sodium Tungstate on the Wear and Corrosion Behavior of Micro-Arc Oxidation Coatings on AZ31 Magnesium Alloy*,* ***Yueh-Lien Lee [yuehlien@ntu.edu.tw]****,* National Taiwan University, Taiwan

Magnesium alloys offer advantages such as low density and high specific strength, but their practical application is often limited by insufficient wear and corrosion resistance. Micro-arc oxidation (MAO) is a promising surface treatment for modifying surface characteristics of magnesium alloys. In this study, MAO coatings were formed on AZ31B magnesium alloy using a silicate-based electrolyte, with and without the addition of boric acid.

Coatings were prepared in a boric-acid-free electrolyte and in electrolytes containing 2 g/L and 5 g/L boric acid, respectively. The influence of boric acid addition on coating morphology, discharge behavior, and wear- and corrosion-related characteristics was examined. The results indicate that the presence of boric acid alters the MAO discharge behavior and coating formation, leading to observable differences in coating compactness and surface features. Variations in wear response and electrochemical impedance behavior were observed among the coatings prepared under different electrolyte conditions.

At higher boric acid concentrations, changes in discharge intensity were associated with increased coating porosity, which influenced wear and corrosion behavior. Additional electrolyte modification was explored to assess the effect of conductivity on coating characteristics. These results provide preliminary insight into the role of boric acid in controlling MAO coating formation and wear–corrosion behavior on AZ31B magnesium alloy.

MC-ThP-10 Advantages of Ultra–High Vacuum Tribology*,* ***Esteban Broitman [ebroitm@hotmail.com]****, Sven Kelling, Rickmer Kose,* Sentys Inc., USA

Tribological behavior —friction, wear, and adhesion— depends strongly on the local environment. In air, adsorbed water, oxygen, and organics form boundary films that dominate contact mechanics; reducing pressure thins these films and shifts interactions toward intrinsic solid–solid processes. Ultra–high vacuum (UHV, below 10^{-9} mbar) effectively removes physisorbed monolayers on laboratory timescales, exposing atomic–scale adsorption, chemisorption, cold–welding, and intrinsic wear mechanisms otherwise masked at higher pressures. UHV tribology is therefore critical for vacuum–service industries (space mechanisms, semiconductor tools, accelerators, vacuum MEMS), yet remains rare because of specialized chambers, rigorous bakeout, vacuum–compatible instrumentation, and long pumpdown cycles. Commercial UHV tribometry options are limited; **PREVAC** currently offers a commercial UHV tribometer reaching ~10^{-9} mbar. This review synthesizes UHV studies, compares UHV, HV, and atmospheric results for common materials and coatings, and issues practical recommendations to improve industrial uptake and reproducibility.

MC-ThP-11 Influence of Boriding Time on the Wear Behavior and Structural Stability of Ti6Al4V Under Simulated Physiological Conditions*,* ***J. A. Nieto-Sosa [jnietos2100@alumno.ipn.mx]****, M. A. Melo-Pérez, I. Arzate-Vázquez, L. A. Moreno-Ruíz,* Instituto Politécnico Nacional, Mexico*; E.E. Vera-Cárdenas,* Tenológico Nacional de México/Instituto Tecnológico de Pachuca, Mexico*; G. A. Rodríguez-Castro, J.A. Andraca-Adame, Josué Escobar-Hernández,* Instituto Politécnico Nacional, Mexico

This work evaluates the tribological performance of Ti6Al4V alloy modified via powder pack boriding for potential use in high-load biomedical implants. The study investigates the mechanical response and structural stability of biphasic TiB_2/TiB layers exposed to two distinct simulated physiological environments: Hanks' solution and Simulated Body Fluid (SBF), providing a comprehensive insight into the performance of these surfaces in ionic media. Mechanical characterization revealed that the boriding process at 1100 °C for 5 and 20h significantly increases surface hardness, reaching a range of 1900 to 3600 HV for the titanium boride phases. Interfacial integrity was assessed via Rockwell C adhesion tests (VDI 3198), showing a transition from HF3 to HF4 as treatment time increased to 20 h. This shift reflects a highly compressed and hardened surface state that maintains structural integrity without coarse delamination during mechanical contact. The reciprocating sliding results highlighted a reduction in the steady-state Coefficient of Friction (CoF), dropping from 0.40 for the untreated alloy to 0.22 (5 h) and 0.12 (20 h). A significant contrast was observed between the biological fluids: SBF proved to be more aggressive than Hanks' solution, inducing a 15% increase in the specific wear rate (k) and higher signal tortuosity due to increased ionic activity and chloride-mediated interaction. Despite this, the 20 h condition (28.2 µm thickness) achieved a 97.6% reduction in k (1.60 x10^{-6} mm^3/Nm) compared to the untreated reference (61.87 mm^3/Nm). Morphological analysis via optical profilometry confirmed that the boride layers do not fail by traditional material removal. Instead, they exhibit a sinking-in effect, where the hard ceramic layer is pressed into the thermally softened substrate. This mechanism was quantified through the Plastic Deformation Ratio (PDR), which decreased from 0.33 in the untreated alloy to 0.05 in the 20 h condition. These findings demonstrate that a 20 h boriding treatment is critical to providing the necessary load-bearing capacity and dimensional stability required for orthopedic applications in iogenic environments.

MC-ThP-12 Vapor Deposition Coatings for Hard Chrome Replacement in Advanced Mechanical Components*,* ***Giacomo Bernardelli [256293@studenti.unimore.it]****, Luca Lusvarghi, Giovanni Bolelli,* Universita degli Studi di Modena e Reggio Emilia, Italy*; Alessio Bassano,* Leonardo S.p.A., Italy

Metallic chromium coatings produced by electrochemical deposition starting from hexavalent chromium oxide (CrO3) are widely employed due to their excellent mechanical and tribological properties. However, Cr6+ substances have been classified cancerogenic for many years. Therefore, according to European Union REACH regulation, they cannot be used in Europe without a temporary authorization. Chrome platers must apply for reauthorization before the old one expires. In this context, in collaboration with Leonardo S.p.A. alternative deposition technologies are being investigated to replace Cr6+ plating for mechanical components currently treated with this process. A further challenge in this path towards safety and sustainability is imposed by the European Union through a list of Critical Raw Materials (CRMs), which combine raw materials of high importance to the EU economy and of high risk associated with their supply. Therefore, the alternative coatings materials used with hexavalent Cr-free deposition processes should also exclude CRMs.

The selected technology is PVD in a MS configuration, using Cr targets to obtain Cr-based films. The substrate is a quenched and tempered alloy steel comparable to that used in the final application. The primary goal of the work was to get reasonably thick coatings (>10 µm) on planar samples and then refining the coating architecture to improve mechanical and tribological performance. Specifically, a comparison is made between two sample sets fabricated using the same deposition technique, with variations in the process parameters.

Nanoindentation and scratch testing were used to analyse mechanical characteristics and adhesion and ball-on-disc tests were used to examine tribological behaviour. A rather dense coating structure was identified by morphological investigations, obtaining high hardness values (about 1300 HV), surpassing those of ordinary hard chromium. Excellent adherence was shown in scratch testing, and no coating delamination was seen within the applied load range (20 mN–30 N). Ball-on-disc tests against Al_2O_3 balls showed relatively low wear rates in the range of 10^{-6} to 10^{-7} mm/N·m and a relatively low friction coefficient (~0.4).

These results are encouraging toward the improvement of the coating architecture and the development of a deposition technology which could be applied by the company to achieve a complete replacement of hexavalent chromium in their applications.

MC-ThP-14 Temperature–Driven Tribofilm Evolution in Oscillating Sliding Contacts Revealed by Advanced Surface Characterization, *Florian Pape,* Bruker Inc., USA*; Alexander Dulebo, Udo Volz,* ***Ude D. Hangen [ude.hangen@bruker.com],*** Bruker Nano GmbH, Germany

Tribofilms are essential for reducing friction and wear in mechanical systems, directly influencing efficiency and component lifetime. To investigate additive–driven tribofilm formation, oscillating sliding tests were conducted on a Bruker UMT TriboLab using a 6 mm 100Cr6 steel ball against silicon and steel substrates. A base oil with 5% ZDDP, known for promoting phosphate–based tribolayers, and 1 wt% graphene platelets was used to study friction behavior and film growth.

Experiments were run on pristine silicon under a 2 N normal load, 2 mm stroke, 2 Hz frequency, for 15 minutes at temperatures of 25–30°C, 70°C, and 100°C. The resulting wear tracks were examined using complementary Bruker instruments. A stylus profiler quantified topographical changes and tribofilm height variations. Mechanical properties of the resulting layers and its friction were characterized with high spatial resolution using the Bruker Hysitron TI–990 TriboIndenter. Nanoscale mapping of surface structures and mechanical contrast was performed on a Bruker Dimension Icon AFM operating in PeakForce QNM mode, enabling visualization of additive–derived features inside and outside the wear scars.

This combined characterization approach provides detailed insights into how ZDDP and graphene additives influence tribofilm formation under oscillating contact, supporting the development of more effective lubricant systems for advanced tribological applications.

Surface Engineering of Biomaterials, Devices and Regenerative Materials: Health, Food, and Agriculture Applications
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Surface Engineering of Biomaterials, Devices and Regenerative Materials: Health Food, and Agriculture Applications Poster Session

MD-ThP-1 Eco-Friendly Synthesis of Graphene Intercalation Material for Highly Sensitive Maldi-Ms Bioanalysis, *Yao-Tsung Hsu,* Graduate Institute of Medical Sciences, College of Medicine, Taipei Medical University, Taiwan*; Shih-Min Wang,* National Atomic Research Institute, Taiwan*;* ***Fu-Der Mai [fordmai@tmu.edu.tw],*** Department of Biochemistry and Molecular Cell Biology, School of Medicine, College of Medicine, Taipei Medical University, Taiwan

Introduction: Developing highly sensitive and environmentally benign materials for biomolecular analysis remains a critical challenge. Matrix-Assisted Laser Desorption/Ionization-Mass Spectrometry (MALDI-MS) is a powerful tool in proteomics, but its sensitivity is often limited by the co-crystallization matrix. We propose a novel, eco-friendly synthesized intercalation material designed to function as an "amphiphile attractor" to significantly boost analytical performance.Methods: Our methodology begins with the sonication-induced scission of few-layer precursory graphene, leading to the asymmetric cleavage and production of nanoscale Asymmetrically Cleaved Graphene (ACG), with an average dimension of 41.58 nm. The ACG exhibits high surface energy, making it intrinsically "amphiphile-attractive." Subsequently, ACG is self-assembled and wrapped by amphiphiles into a hemimicelle structure, allowing it to intercalate into bulk graphite to form the final Asymmetrically Cleaved Graphene Intercalated Material (ACGIM).Results and Discussion: The unique structure of ACGIM is highly promising for bioanalysis. The attracted amphiphiles within the ACGIM effectively stabilize biomolecules, which is crucial for signal integrity. To validate its analytical potential, we conducted a signal enhancement experiment using ACGIM as a novel matrix substitute for peptide detection via MALDI-MS. The results demonstrated a remarkable 22-fold enhancement in the detection signal for the target peptide compared to conventional methods.Conclusion: The ACGIM represents a new class of amphiphile-attractive intercalation materials synthesized under green conditions. Its superior ability to stabilize biomolecules and significantly enhance signal intensity in MALDI-MS offers a robust platform for highly sensitive bioanalysis, particularly in peptide and protein research. Further exploration into its application for diverse biomolecule types is warranted.

MD-ThP-2 Study of the Antimicrobial and Osteoinductive Properties of Polymeric Nanocomposite Membranes, ***Lucia Sofia Flores-Hidalgo [floreshidalgol@pceim.unam.mx],*** Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México*; Phaedra S. Silva-Bermúdez,* Unidad de Ingeniería de Tejidos, Terapia Celular y Medicina Regenerativa; Instituto Nacional de Rehabilitación Luis Guillermo Ibarra Ibarra, Mexico*; Gina Prado-Prone,* Laboratorio de Biointerfases, DEPeI, Facultad de Odontología, Universidad Nacional Autonoma de Mexico, Mexico*; Monserrat Ramirez-Arellano,* Facultad de Medicina, Universidad Nacional Autonoma de Mexico, Mexico*; Sandra. E Rodil,* Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México

Nanofibers have garnered considerable attention in recent years due to their wide-ranging applicability in various fields, including tissue engineering, biotechnology, medicine, sensing, and bioremediation. Among the different fabrication methods for composite membranes, electrospinning stands out for its ability to utilize a wide range of polymers and copolymers. Several configurations of the electrospinning process exist; among them, co-electrospinning is noteworthy, as it allows the simultaneous spinning of two independent polymer solutions while preserving their individual properties.

Polycaprolactone (PCL) and gelatin are two polymers widely studied for biomedical applications due to their good biocompatibility and biodegradability. In parallel, nanoparticles of various metal oxides, such as zinc oxide (ZnO) and magnesium oxide (MgO), have been investigated for their antibacterial and osteoinductive properties, respectively.

For this reason, the present work reports the porous microfibrous structure of PCL/gelatin nanocomposite membranes obtained via electrospinning by combining fibers containing ZnO nanoparticles and fibers containing MgO nanoparticles. These membranes were characterized morphologically and compositionally using SEM, FTIR, TGA, EDS, DSC, and ICP analyses. Finally, biological assays were performed to evaluate their antibacterial efficacy and their potential to promote an osteoinductive environment, assessing their possible use as an adjuvant in the treatment of open fractures.

MD-ThP-3 Understanding the Influence of Sn and Nb on Morphology, Sustainable Synthesis of Calcium Phosphate 1d Nanostructures via Electrospinning for Advanced Functional Applications*, Yao Mawuena Tsekpo, Weronika Smok,* Faculty of Mechanical Engineering, Silesian University of Technology, Poland*; Adrian Adrian Radon,* Łukasiewicz Research Network – Institute of Non-Ferrous Metals, Poland*; Pawel Jarka, **Tomasz Tanski [tomasz.tanski@polsl.pl]**,* Faculty of Mechanical Engineering, Silesian University of Technology, Poland

Calcium phosphate compounds are a sustainable material with applications in biomedicine and environmental remediation. The influence of dopants on the morphology of one-dimensional (1D) structures prepared by the electrospinning technique with biogenic calcium as a starting material remains understudied. This work presents a novel method for synthesising calcium phosphate nanowires doped with Sn and Nb using Galatea paradoxa clamshells as a calcium source. The process integrates electrospinning and sol-gel techniques to achieve 1D nano calcium pyrophosphate and aims to elucidate the influence of temperature on the process. Thermogravimetric analysis (TGA), Scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR) were employed to characterise the nanostructures. Calcination at 600 ºC and 700 ºC reveals the formation of wire-like structures at the nanoscale with diameters ranging from 68 – 403 nm. The Sn-doped wires were observed to be more thermally stable at higher temperatures (700 ºC) whilst having narrower wire diameters as compared to the Nb-doped wires. XRD analysis confirmed the presence of Sn and Nb, corroborating the presence of their oxide and aligning with the Fast Fourier Transform (FFT) diffraction patterns obtained in TEM. These findings indicate the successful formation of 1D nanostructures of calcium phosphate nanowire doped with Sn and Nb. The observed structure and morphology of the prepared nanostructure exhibit properties suitable for application in bone regeneration and biomedicine, adsorption of harmful heavy metals, and as a sustainable photocatalyst.

MD-ThP-4 Advancing Surface Engineering of Additively Manufactured Dental Implants by HiPIMS β-Ti Coatings*, **Juan Carlos Sanchez-Lopez [jcslopez@icmse.csic.es]**,* Instituto de Ciencia de Materiales de Sevilla (CSIC-US), Spain*; Amanda Robau-Porrua,* Universidad de Concepción-Chile*; Marleny Rodríguez-Albelo,* Universidad de Sevilla, Spain*; Celia Garcia-Hernandez, Cristina Garcia-Cabezon,* Universidad de Valladolid, Spain*; Jesús Eduardo Gonzalez-Ruiz,* Universidad de la Habana, Cuba*; Yadir Torres,* Universidad de Sevilla, Spain

Improving the mechanical compatibility and corrosion resistance of metallic implants is essential for long-term clinical success. Titanium and its alloys are widely used for dental and orthopedic devices, yet surface reactivity and elastic modulus mismatch with bone can limit their performance. Surface modification by magnetron sputtering offers an effective strategy to tailor surface properties at the nanoscale while preserving bulk integrity.The β-phase Ti alloys show a significant reduction of the elastic modulus compared with bulk titanium, improving biomechanical compatibility and mitigating stress-shielding effects.

Building upon our previous studies on flat titanium substrates, the present work represents a significant step forward by applying high-power impulse magnetron sputtering (HiPIMS) coatings to real 3D titanium implant geometries. This transition allows us to assess the feasibility of conformal deposition on complex surfaces while maintaining the advantageous features of HiPIMS. Ti-35Nb-7Zr-5Ta (wt. %) β-type coatings were deposited onto dental implants fabricated by Laser Bed Fusion (LBF), producing dense, adherent layers with controlled nanoroughness and uniform coverage, even within threaded regions.

Microstructural and chemical analyses (SEM, XRD, XPS) confirmed homogeneous β-phase formation and the presence of a protective TiO_2 surface layer. Nanoindentation revealed a reduction in elastic modulus of up to 30% compared with uncoated titanium, mitigating stress-shielding effects. Electrochemical tests in simulated physiological media demonstrated enhanced corrosion resistance and surface stability.

These results highlight the versatility of HiPIMS as a scalable tool for the conformal coating of complex 3D implants, enabling the development of next-generation dental and orthopedic biomaterials with optimized mechanical and corrosion performance.

MD-ThP-5 Electrochemical Characterization of Copper-Coated Commercial Ti6Al4V Alloy for Advanced Biomedical Applications*, **Bryan Angel Zárate Verduzco [1629251c@umich.mx]**,* Universidad Michoacana de San Nicolás de Hidalgo, Mexico*; Victor Manuel Solorio García, Miguel Ivan Dávila Perez,* Tecnologico Nacional de México/ Instituto Tecnológico de Morelia, Mexico*; Roberto Guerra González,* Universidad Michoacana de San Nicolás de Hidalgo, Mexico*; Héctor Javier Vergara Hernández,* Tecnológico Nacional de México/ Instituto Tecnológico de Morelia, Mexico*; Julio César Villalobos Brito,* Tecnologico Nacional de México/ Instituto Tecnológico de Morelia, Mexico

Electrodeposited copper (Cu) coatings on titanium alloys are promising candidates for multifunctional biomaterials combining antibacterial and conductive properties. This study evaluates the electrochemical performance and corrosion resistance of Cu coatings applied to commercial Ti6Al4V. Open-circuit potential (OCP), linear polarization resistance (Rp), electrochemical impedance spectroscopy (EIS), and potentiodynamic polarization tests were performed in Hank's solution at 37 °C, with pH measurements during the tests. Results showed that Cu deposition modifies the passive behavior of Ti6Al4V, shifting the corrosion potential toward more active values while maintaining acceptable polarization resistance. Among the tested conditions, deposition exhibited the lowest corrosion rate compared to the base material. Equivalent circuit modeling of EIS data revealed two time constants associated with the outer Cu layer and the Ti oxide interface, evidencing a dual protective mechanism. The combined analysis indicates that optimized deposition time can balance ion-release kinetics and surface passivation, contributing to long-term functional stability. These insights lay the groundwork for predictive corrosion models and the rational design of antibacterial, corrosion-resistant coatings for next-generation biomedical implants.

MD-ThP-6 TiO_x Nanocoating as Antimicrobial for Personal Protective Equipment*, **Lorena Reyes-Carmona [lorena.unam753@gmail.com]**, Sandra Rodil,* UNAM, Mexico*; Omar Sepúlveda-Robles,* IMSS, Mexico*; Gina Prado-Prone, Argelia Almaguer-Flores,* UNAM, Mexico

Introduction: Pathogenic bacteria and viruses could be transmitted by aerosols formed from saliva droplets. These bioaerosols are becoming the main airborne transmission source for respiratory microorganisms. It has been reported that health professionals are highly exposed to bioaerosols generated during medical or dental procedures since rotary instruments are used, which produce pathogenic bioaerosols. The development of nanomaterials with antimicrobial activity to cover personal protective equipment (PPE), such as facemasks, could be an option to avoid the transmission of these pathogens.

Objective: The aim of this study was to evaluate the antibacterial and antiviral capacities of titanium oxide nanocoating (TiO_x) deposited on polypropylene (PP) fabrics used to produce medical and dental protective equipment.

Methods: TiOx nanocoating was deposited on PP fabric by magnetron sputtering. They were characterized using optical microscopy, XPS, WCA, optical profilometry, and ICP-MS. For antimicrobial evaluation, pathogenic bacteria and surrogates virus (RNA and DNA bacteriophages) were used. Two methodologies were used: short (2 min) and long (24 h) term interaction of nanocoatings with bacterial and viral aerosols.

Results: ZnO nanocoating was homogeneously deposited on the PP. The antimicrobial results showed a reduction of the bacteria between 18-95 %, depending of the bacterial strain tested. With respect to viral assays with RNA bacteriophages, a total reduction of the viral replication was achieved after 24 h. However, the DNA phage was not completely inactivated.

Conclusions: TiO_x nanocoating showed antimicrobial potential against bacteria and surrogate viruses. This nanocoating has the potential to be used to cover medical PPE, to reduce and prevent the transmission of pathogens in medical and dental environments.

Keywords: Nanocoating, titanium oxide, antibacterial.

Acknowledgments: UNAM-PAPIIT project# IN207824.

MD-ThP-10 Investigating the Corrosion Behavior of Sol Gel and PEO Coatings on Magnesium for Biomedical Applications*, Vinod Prabhakar, **Avirup Sinha [asinha38@uic.edu]**, Sujoy Ghosh,* University of Illinois at Chicago, USA*; Hamdy Ibrahim,* Kennesaw State University, USA*; Mathew T. Mathew,* University of Illinois College of Medicine at Rockford and Rush University Medical Center, USA

Magnesium (Mg) alloys have been applied to orthopedics as its elastic modulus resembles bone, and its stress-strain behavior resembles ductile metals. Mg alloys exhibit high corrosion rates including high degradation and H_2 release. Existing coatings, such as titanium, sol-gel, and plasma electrolytic oxidation (PEO) have improved corrosion properties of Mg alloys. This study evaluates corrosion in bovine calf serum (BCS), a fluid that simulates lubricating human synovial joints. The goal of this study was to test the corrosion behavior of magnesium alloys with sol-gel and PEO coatings in BCS, and the hypothesis was that under BCS, the different coatings will increase the corrosion resistance of the Mg alloy. The experiments were conducted under a three-electrode setup, with the SCE reference electrode, graphite counter electrode, and Mg working electrode. Microstructures were analyzed through scanning electron microscopy (SEM) and profilometry to confirm corrosion sites, oxide damage, wear, and surface roughness. Corrosion current decreased, corrosion potential increased and the system's resistance and capacitance increased and decreased as the coating increased. These trends were expected as the coated alloys corrode slower and have less tendency for corrosion. Overall, this study effectively simulated Mg alloy corrosion in BCS.

MD-ThP-11 Antimicrobial Potential of Silver-Copper Nanocoatings Deposited on Medical and Dental Polymeric Materials, ***Argelia Almaguer-Flores [aalmaguer@comunidad.unam.mx]***, *Lorena Reyes-Carmona, David E. Martínez-Lara, Gina Prado-Prone, Sandra E. Rodil,* UNAM, Mexico

Introduction: During medical and dental procedures, infection prevention is vital because patients are often more vulnerable, and an infection could be life-threatening. Additionally, maintaining a microbial-free clinical environment—including instruments and surfaces—is essential to prevent contamination by microorganisms such as bacteria, fungi, and viruses that could be transmitted to patients.

Objective: To evaluate the antibacterial potential of a silver-copper nanocoating (SakCu®) deposited on medical-grade polyurethane (flat substrates and medical hoses) to reduce the adhesion of opportunistic pathogens associated with medical and dental devices.

Methods: The silver-copper nanocoating was deposited by magnetron sputtering in an inert argon (Ar) atmosphere, using a DC power source at 200 W. The characterization included scanning electron microscopy (SEM), Transmission electron microscopy (TEM), X-ray energy dispersive spectroscopy (EDS). The antibacterial assays included analysis of the effect of the SakCu® nanocoating on Gram-positive and Gram-negative bacterial strains, including *Escherichia coli* (ATCC 33780), *Pseudomonas aeruginosa* (ATCC 43536),*Staphylococcus aureus* (ATCC 25923), and *Staphylococcus epidermidis* (ATCC 14990).

Results: The nanocoating thicknesses obtained were 15, 30, and 50 nm. Surface morphology, analyzed by scanning electron microscopy (SEM), revealed a homogeneous coating in all cases. Transmission electron microscopy (TEM), elemental mapping, and electron diffraction (EDS) analyses confirmed an average composition of 42% Ag and 58% Cu, uniformly distributed, indicating the formation of an alloy. The antibacterial results showed a reduction in bacterial viability of more than 90% across all species tested.

Conclusions: The results showed the antibacterial potential of the silver-copper nanocoating (SakCu®) to prevent the adhesion of important opportunistic pathogens to medical-grade polyurethane surfaces on devices such as dialysis fluid bags and medical and dental hoses.

MD-ThP-12 Effects of the Temperature and Target Power on Microstructure and Electrochemical Properties of Fe-Mn-C-Zn Coatings via Magnetron Sputtering Co-Deposition, *Xinna Zhu,* Department of Engineering "Enzo Ferrari" University of Modena and Reggio Emilia, Modena, Italy; *Carlo Paternoster,* Laboratory for Biomaterials and Bioengineering, (CRC-Tier I), Dept Min-Met-Materials Eng., & Regenerative Medicine, CHU de Quebec, Laval University, Québec, QC, Canada; *Andrea Gatto,* Department of Engineering "Enzo Ferrari" University of Modena and Reggio Emilia, Modena, Italy; *Carlos Henrique Michelin Beraldo,* Laboratory for Biomaterials and Bioengineering, (CRC-Tier I), Dept Min-Met-Materials Eng., & Regenerative Medicine, CHU de Quebec, Laval University, Québec, QC, Canada; *Silvio Defanti,* Department of Engineering "Enzo Ferrari" University of Modena and Reggio Emilia, Modena, Italy; *Paolo Mengucci, Gianni Barucca,* Department SIMAU, Università Politecnica delle Marche, Ancona, Italy; *Helton José Wigger,* Laboratory for Biomaterials and Bioengineering (LBB-BPK), Associação de Ensino, Pesquisa e Extensão BIOPARK, Toledo, Brazil; *Andranik Sarkissian,* Plasmionique Inc., Varennes, QC, Canada; ***Diego Mantovani [Diego.Mantovani@gmn.ulaval.ca]***, Laboratory for Biomaterials and Bioengineering, (CRC-Tier I), Dept Min-Met-Materials Eng., & Regenerative Medicine, CHU de Quebec, Laval University, Québec, QC, Canada

Iron–manganese (Fe–Mn) alloys recently gained attention as promising materials for biodegradable metallic implants due to their excellent mechanical properties, comparable to stainless steel. However, their clinical translation is limited by two key issues: a high risk of post-surgical bacterial infections and a slow degradation rate. *Staphylococcus* species are among the main causes of implant-associated infections, forming resilient biofilms highly resistant to antibiotics and disinfectants. To overcome these limitations, this study develops Fe–Mn–Zn composite coatings with improved antibacterial and corrosion properties. Zinc was selected for its antibacterial and electrochemical properties: the higher electronegativity compared to iron (–1.2 vs –0.89 V) and lower solubility in a Fe-Mn-C matrix is expected to promote galvanic effects and controlled ion release.

Coatings were produced by dual magnetron sputtering using commercial zinc and Hadfield steel targets. The Fe–Mn target was kept at 300W, while the zinc target varied between 0–150 W to modulate composition. Depositions were carried out on silicon wafers at room temperature and 150 °C. The coatings were characterized by scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), transmission electron microscopy (TEM), contact angle measurements, potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), scratch testing, and nanoindentation.

Zinc incorporation produced coatings with low surface roughness (1–10 nm) and no visible defects, maintaining a homogeneous surface at all deposition powers, with a columnar structure and intercolumnar spaces observed. Coating thickness ranged from ~500 to 700 nm. EDS showed zinc content increasing with Zn target power, reaching about 35 wt%, while iron and manganese decreased proportionally. XPS revealed strong zinc enrichment at the surface compared to bulk concentration. Mechanical testing indicated a slight reduction in hardness with increasing zinc, though values remained comparable to stainless steel and titanium alloys made by similar techniques.

Overall, dual magnetron sputtering enabled fabrication of high-purity Fe–Mn–Zn coatings with uniform morphology and modulable composition. Temperature was identified as a key factor influencing microstructure and elemental distribution. Further studies are needed to validate antibacterial properties and elucidate their effect on different classes of bacteria, responsible for infections and pathologies in biomedical applications of degradable materials.

MD-ThP-17 On the Adhesion of a-C:H Coatings Deposited by PECVD on PDMS for Biomedical Applications, *Lidi Astrid Yáñez-Hernández, Linda Victoria Bonilla-Gameros,* ***Pascale Chevallier [pascale.chevallier@crchudequebec.ulaval.ca]***, Université Laval, Canada; *Laurent Houssiau,* University of Namur, Belgium; *Andranik Sarkissian,* Plasmionique Inc., Canada; *Diego Mantovani,* Université Laval, Canada

Polydimethylsiloxane (PDMS) is widely used in biomedical devices. Despite its favorable properties, such as hemocompatibility, elasticity, and stability, it remains prone to bacterial colonization, which can lead to severe infections and device failure. Hydrogenated amorphous carbon (a-C:H) coatings have emerged as a versatile route to enhance biomaterial surfaces, and can serve as platforms for the controlled release of antibacterial agents. However, adhesion of a-C:H coatings to soft polymers such as PDMS remains a critical bottleneck for clinical success. This study investigates how substrate bias and hydrogen incorporation during plasma-enhanced chemical vapor deposition (PECVD) affect adhesion, morphology, and interface integrity of a-C:H coatings on PDMS. Coatings deposited without bias were termed polymer-like carbon (PLC), and those deposited at −300 V as diamond-like carbon (DLC). The incorporation of hydrogen during deposition produced the hydrogenated counterparts, PLCH and DLCH. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) depth profiling revealed greater coating thickness and sharper interfaces for non-biased coatings. In contrast, biased coatings showed thinner films with evidence of intermixing with substrate components. Regarding hydrogen incorporation, a decrease in coating thickness and surface roughness was observed, as well as a reduction in crack density after tensile deformation. Furthermore, immersion tests under pseudo-physiological conditions demonstrated that the PLCH remained stable for 21 days, with only localized cracks and no significant delamination under static and dynamic conditions. These results suggest that this coating can withstand physiological stresses while maintaining mechanical integrity. Therefore, among the variants studied, PLCH (non-biased + H_2) emerges as the most promising coating for flexible PDMS biomedical devices, offering an optimal balance of thickness, adhesion, flexibility, and chemical durability.

Keywords: Polydimethylsiloxane, Hydrogenated amorphous carbon, coatings, diamond-like carbon, polymer-like carbon, plasma-enhanced chemical vapor deposition, adhesion.

MD-ThP-18 An Asymmetric Capillary-Driven Microtiter Platform Enabling Centrifuge-Free Point-of-Care Diagnostics*, **KangKug Lee [klee3@wilberforce.edu]**, Yasmine Jones, Anastesia Smith,* Wilberforce University, USA

We present an innovative microtiter platform that leverages asymmetric capillary action to enable rapid plasma separation and colorimetric analysis from ultra-low volumes of whole blood. In contrast to conventional workflows that rely on large sample volumes (>10 mL) and centrifugation, our simplified approach requires <10 µL of whole blood and no instrumentation. The platform is polymer-based and features spray-coated superhydrophilic nanoporous surfaces combined with hydrophobic screw-shaped sidewalls. Plasma separation is initiated through simple manual shaking using two fingers, which provides sufficient centrifugal force to displace blood cells toward the hydrophobic sidewalls, while asymmetric capillary-driven lateral flow retains the plasma in the bottom nanoporous zone. This streamlined process substantially reduces sample volume, cost, and processing time, offering a portable and user-friendly solution for point-of-care (PoC) diagnostics.

MD-ThP-20 Effect of Current Density Variation on Cu-Incorporated Mao Coatings on Ti-30nb-5mo Alloy*, Giovana Collombaro Cardoso,* Universidade Estadual Paulista, UNESP, Bauru, Brazil*; Gustavo da Silva Diniz,* Universitdade Estadual Paulista, UNESP, Bauru, Brazil*; **Carlos Roberto Grandini [carlos.r.grandini@unesp.br]**,* Universidade Estadual Paulista, UNESP, Bauru, Brazil

Titanium and its alloys are widely used as biomaterials due to their excellent mechanical performance and corrosion resistance [1]. However, their inert surfaces limit biological interactions after implantation [2]. Surface modification by Micro-Arc Oxidation (MAO) is a versatile and cost-effective approach to produce porous TiO_2 coatings that can incorporate bioactive elements, enhancing osseointegration and antibacterial behavior [3]. This study investigates the effect of current density on the properties of MAO coatings formed on Ti-30Nb-5Mo alloy substrates. The process was carried out at 300 V for 3 minutes in an electrolyte containing calcium acetate, sodium glycerophosphate, and copper chloride, with current densities ranging from 1.0 to 2.5 A/cm^2. X-ray diffraction (XRD) revealed that higher current densities promoted the formation of rutile TiO_2 and increased surface roughness. Consequently, the water contact angle decreased, indicating improved hydrophilicity and potential for better cell adhesion. X-ray photoelectron spectroscopy (XPS) confirmed copper incorporation into the coatings, suggesting that the modified surfaces may provide antibacterial functionality. These results demonstrate that tuning the current density during MAO treatment is an effective strategy for tailoring the surface morphology, chemistry, and biological performance of Ti-based alloys for biomedical applications. (Financial Support: CNPq and FAPESP).

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MD-ThP-21 Influence of Microstructure and Processing Voltage on the Formation and Properties of Coatings Obtained by Micro-Arc Oxidation (MAO) in Ti-25Ta-xNb Alloys*, **Fernanda de Freitas Quadros [ff.quadros@unesp.br]**,* Sao Paulo State University (UNESP), Brazil*; Katia Barbaro,* Istituto Zooprofilattico Sperimentale del Lazio e della Toscana, Italy*; Diego Rafael Nespeque Corrêa,* Sao Paulo State University (UNESP), Brazil*; Julietta V. Rau,* Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Italy*; Carlos Roberto Grandini,* Sao Paulo State University (UNESP), Brazil

The Micro-Arc Oxidation (MAO) technique has emerged as one of the most effective methods for improving the surface properties of metallic materials, particularly in titanium (Ti) alloys used for biomedical applications[1]. Although Ti exhibits good mechanical performance, high corrosion resistance, and excellent biocompatibility, issues such as corrosion, infection, and implant rejection may still occur[2]. Ti is an allotropic element, displaying a hexagonal close-packed (α) structure below 882 °C and a body-centered cubic (β) structure above this temperature[2]. The addition of β-stabilizing elements, such as tantalum (Ta) and niobium (Nb), lowers the β-transus temperature and can enhance the material's corrosion resistance and biocompatibility due to the intrinsic properties of Ta and Nb [3]. This study aimed to investigate the influence of microstructure, particularly through variations in Nb content, on coatings obtained by MAO in Ti-25Ta-xNb alloys (x = 10, 20, and 30 wt.% Nb) under different applied voltages (200, 250, and 300 V). X-ray diffraction (XRD) analyses revealed the predominance of Ti oxides in the anatase and rutile phases, with rutile being more pronounced in samples processed at higher voltages [3]. Scanning electron micrographs showed that both the alloy microstructure and the applied voltage significantly influenced coating formation and morphology, with variations in pore size, shape, and interconnectivity [3]. Rockwell C microhardness tests demonstrated good film adhesion to the substrate under all conditions analyzed [3]. In biological assays, Ti-25Ta-xNb substrates (200–300 V) exhibited non-cytotoxic behavior toward stem cells and effective antibacterial activity against Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Enterococcus faecalis, with the Ti-25Ta-30Nb alloy treated at 300 V showing the most promising performance. These findings indicate that surface modification via MAO, combined with controlled Nb addition, produces coatings with excellent adhesion, biocompatibility, and antimicrobial properties. The authors acknowledge the financial support from the funding agencies FAPESP, CAPES, and CNPq.

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MD-ThP-22 Using X-Ray Photoelectron Spectroscopy to Probe Lateral and Depth Distribution of Copper Based Photocatalytic Biocidal Film*, **David Surman [dsurman@kratos.com]**,* Kratos Analytical Inc, USA*; Jonathan Counsell,* Kratos Analytical Limited, UK*; Heather Yates,* University of Salford, UK

Copper based antimicrobial coatings are of increasing interest for reducing surface mediated transmission of pathogens, particularly in healthcare environments. In this study, X-ray photoelectron spectroscopy (XPS) was used to characterise the surface chemistry, lateral homogeneity, and depth distribution of copper within a copper oxide-titania composite thin film. The film was deposited on glass by open environment chemical vapour deposition (CVD), mimicking an industrial online process.

Large area XPS survey spectra confirmed the presence of copper at the outermost surface despite sequential deposition of titania over the copper oxide layer. This suggests either a non-continuous copper layer or a copper layer thinner than the ca. 10 nm sampling depth of XPS. Lateral compositional variation was assessed using XPS group array analysis over several millimetres, revealing a non-uniform surface distribution of copper across the sample.

High resolution Cu 2p spectra acquired from copper rich regions showed characteristic shake–up satellite features consistent with Cu(II), with no evidence of X–ray induced reduction during extended analysis. Destructive sputter depth profiling using Ar^+ ions revealed a high initial copper concentration at the surface (*ca.* 35 at.%), decreasing through the titania layer to *ca.*5 at.% and falling to background levels at the titania-silica interface. No copper diffusion into the glass substrate was observed.

These results demonstrate the capability of XPS to resolve both lateral and depth dependent copper distributions in complex antimicrobial coatings. They also provide critical insight into surface chemistry and elemental migration relevant to biocidal performance and coating optimisation.

MD-ThP-23 Surface-Engineered Graphene/PDMS Coatings Reduce Multispecies Uropathogenic Biofilms Under Urine-like Conditions*, ***Francisca Sousa-Cardoso [francisca.sousa.cardoso@outlook.pt]****,** *Rita Teixeira-Santos, Luciana C. Gomes, Rita Vieira,* University of Porto, Portugal*; Brian A. Korgel,* University of Texas at Austin, USA*; Olívia S. G. P. Soares, Filipe J. Mergulhão,* University of Porto, Portugal

Silicone elastomers such as polydimethylsiloxane (PDMS) are widely used in indwelling urological medical devices, yet their hydrophobic surfaces provide a favorable substrate for polymicrobial biofilm development under urine-like conditions. This work reports a thin, surface-engineered graphene/PDMS composite coating designed to reduce mixed uropathogenic biofilms through intrinsic, contact-active surface properties rather than soluble antimicrobials.

Graphene nanoplatelets were functionalized via melamine-assisted mechanochemical processing, followed by thermal treatment and incorporated at 1 wt.% into PDMS to obtain spin-coated films onto glass slides. Surface morphology and topography were assessed through Scanning Electron Microscopy (SEM), which showed a uniform elastomeric coating decorated with graphene-associated micro/nano-asperities and protrusions, and white-light optical profilometry (OP), which confirmed increased roughness and topographic complexity compared with unmodified PDMS. To confirm the surface chemistry of the functionalized graphene material used to fabricate the coating, additional characterization was performed by Scanning Transmission Electron Microscopy (STEM) imaging with Energy-Dispersive X-ray Spectroscopy (EDX) elemental mapping and X-ray Photoelectron Spectroscopy (XPS), which corroborated nitrogen incorporation at the graphene surface.

Antibiofilm performance was evaluated after 24 h in artificial urine medium using a 1:1:1 tri-species community of *Staphylococcus aureus*, *Pseudomonas aeruginosa* and *Klebsiella pneumoniae*. Total biofilm cells were quantified by flow cytometry, and confocal laser scanning microscopy enabled 3D reconstruction of biofilm architecture and spatial organization within the mixed community. Relative to PDMS controls, the graphene/PDMS coating reduced total cells by ~41% in tri-species biofilms. Confocal reconstructions further indicated substantial architectural attenuation on the composite surface, with ~30% lower biovolume and ~70% lower thickness, and the most pronounced suppression associated with *S. aureus* within the mixed biofilm.

Overall, the engineered graphene/PDMS surface reduced tri-species biofilm cells and thickness compared to bare PDMS. This material and coating strategy can thus be promising for silicone indwelling medical devices, including catheters and ureteral stents.

MD-ThP-24 Flexible Negative Pyramid Microarrays Coated with Ag NanoParticles for Raman Enhancing Detection*, ***Ting-Yu Liu [tyliu0322@gmail.com]****,** Ming Chi University of Technology, Taiwan

Light-capturing flexible PDMS substrates with negative pyramid microarrays are fabricated through a sequential replication process using silicon master stamps. These stamps, containing negative pyramid structures, are produced via photolithography followed by wet chemical etching. Silver (Ag) is then thermally deposited onto the flexible PDMS surface, forming densely packed nano-islands. These nano-islands generate localized surface plasmon resonance (LSPR), which produces strong surface-enhanced Raman scattering (SERS) “hot spots.” In addition, the negative pyramid structures enhance the SERS signal by approximately four times due to multiple reflections of the incident laser within the microarrays. The PDMS-NP-Ag substrates demonstrate a detection limit below 10^{-8} M for rhodamine 6G (R6G) and malachite green, indicating high sensitivity. They also show excellent reproducibility, with a variation of only 7.6% across 20 randomly selected measurement points. Furthermore, the flexible nature of these substrates allows them to conform to irregular surfaces, such as apples, enabling practical applications in detecting pesticides and microorganisms. Overall, the substrates exhibit efficient and reproducible detection of environmental pollutants (e.g., R6G, malachite green, and paraquat) as well as bacteria (E. coli) at ultra-low concentrations.

Plasma and Vapor Deposition Processes
Room Town & Country A - Session PP-ThP
Plasma and Vapor Deposition Processes Poster Session

PP-ThP-3 Predictive Modelling of Magnetron Sputtering: Bridging Computational and Experimental Approaches for Metallic Glass Thin Films*, Jaroslav Zenisek, Tereza Schmidtova,* Masaryk University, Czechia*; Antonin Kubicek, Vjaceslav Sochora,* SHM, Czechia*; **Pavel Soucek [soucek@physics.muni.cz]**,* Masaryk University, Czechia

Computational simulations are rapidly transforming the way magnetron sputtering processes are designed, understood, and optimized. They offer a powerful means of increasing experimental efficiency, accelerating process development, and improving reproducibility—particularly when transitioning from laboratory-scale research to industrial-scale coating production. Despite major advances in plasma-assisted deposition, one fundamental challenge remains: precise control of particle sputtering from the target and their subsequent transport toward the substrate. These parameters govern the particle abundance and energy while arriving at the substrate, ultimately determining coating stoichiometry, phase structure, microstructure, and performance.

While compositional gradients and local variations can be highly beneficial for combinatorial thin-film research, they are detrimental in industrial environments, where uniformity in thickness, composition, and phase structure are essential for high-throughput and large-area coating.

In this contribution, we demonstrate the combined use of SDTrimSP and SiMTra simulation tools to predict industrial magnetron sputtering of metallic glasses based on Zr–Cu(–Ni/Al) systems and on W–Ni–B and W–Zr–B systems, representing examples with comparable and strongly contrasting atomic masses. The simulations provide detailed predictions of relative thickness profiles, elemental composition distributions, and the energy spectra of the arriving species under varying process conditions.

The calculated results are compared with experimental data obtained from thin films deposited under controlled conditions, enabling a quantitative assessment of model accuracy and applicability. Furthermore, the functional properties of the deposited metallic glass coatings are correlated with the predicted parameters, establishing a clear link between process simulation and coating performance. This integrated computational–experimental approach provides a valuable framework for scaling magnetron sputtering from laboratory research to robust industrial production of chemically relatively complex coatings.

PP-ThP-4 How to Predict the Deposition Rate During Reactive Sputtering Using an One-Volume Reference Resource?*, ***Diederik Depla [Diederik.Depla@ugent.be]****,** 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) 113546D. Depla, J. Van Bever, Calculation of oxide sputter yields Vacuum 222 (2024) 112994

PP-ThP-5 Properties and Behavior of Infrared Materials : Towards High Efficiency and High Durability Antireflection Coating*, **Manon Dewynter [manon.dewynter@orange.fr]**,* *Fabien Paumier, Éric Le-Bourhis, Cyril Dupeyrat,* Institut Pprime - CNRS - ENSMA - Université de Poitiers, France

This PhD research focuses on developing advanced thin-film coatings for substrates with complex geometries, aiming to achieve uniform properties and enhanced resistance under demanding operational environments. The study emphasizes optimizing deposition parameters to ensure consistent film characteristics—critical for the performance and durability of optical components in optronic systems. These systems incorporate diverse optical elements, including windows, lenses, filters, and dichroic plates, all requiring precise functionalization through thin-film treatments to meet stringent optical, mechanical, and chemical specifications.

Front optics in optronic devices play a key role in detection, observation, and identification. Operating under harsh and variable conditions—such as corrosive, erosive, and chemically aggressive environments—these components require coatings that maintain high optical transmission while exhibiting robust mechanical and chemical stability.

Typically, coatings are deposited by vapor-phase techniques such as Electron Beam Physical Vapor Deposition (EB-PVD) and Ion Beam Assisted Deposition (IBAD), enabling the formation of dense, uniform multilayer interference stacks. However, substrates with complex geometries—characterized by large diameters or high curvatures—pose significant challenges for achieving uniform coating deposition. Variations in thickness, density, and mechanical properties across the surface can lead to performance degradation, including chemical attack, delamination, and loss of optical quality, particularly under critical conditions such as saline fog exposure.

This project aims to elucidate the underlying growth mechanisms and physical phenomena at the material scale, focusing initially on single-layer coatings to establish a solid foundation of knowledge. Comprehensive characterizations—including nanoindentation, ellipsometry, and strain measurements—are employed to assess mechanical and optical properties and to study the influence of deposition parameters. The insights gained will guide the design of novel multilayer architectures incorporating new materials and interfaces to enhance thermomechanical performance.

Ultimately, this research supports the evolving specifications of optronic devices by delivering coatings with improved robustness and consistent functional properties, thereby advancing the performance and reliability of front optics in demanding operational environments.

PP-ThP-6 Plasma Research Reactor to Validate Nanocalorimetry as a Prospective Plasma Diagnostics Technique*, **Carles Corbella [carles.corbellaroca@nist.gov]**,* National Institute of Standards and Technology (NIST)/ University of Maryland, College Park, USA*; Feng Yi, Andrei Kolmakov,* National Institute of Standards and Technology (NIST), USA

Recent advances in microelectronics require techniques for faster, more accurate, and comprehensive characterization of plasma-based nanofabrication processes, such as film deposition and surface etching or cleaning. Our recent demonstration of using membrane-based differential nanocalorimetry to measure atomic radicals in reactive plasmas sensitively [Diulus et al, J. Vac. Sci. Technol. B 43, 020601 (2025)] has inspired the further development of this new plasma probe. This probe aims to analyze plasma parameters and fundamental plasma-surface interactions through heat exchange measurements.The present work describes a research plasma reactor equipped with adjustable ICP and CCP sources and standard plasma diagnostics tools to benchmark the nanocalorimeter output: (1) single and double Langmuir probes to provide plasma parameters and electron energy probability function (EEPF); (2) retarding field energy analyzer (RFEA) with a built-in quartz microbalance to evaluate ion energy distributions and mass variation rates, and (3) optical emission spectroscopy (OES) together with (4) quadrupole mass spectrometer for plasma/wall chemistry monitoring. Key nanocalorimeter characteristics, such as sensitivity, response time, lifetime, and stability, as well as parasitic signal interference, will be discussed. This new sensor is well-suited for monitoring surface modification processes in multiple plasma treatment applications.

PP-ThP-8 Ion Acceleration on Insulating Substrates: Synchronized Floating Potential HiPIMS for AlN and AlScN Thin Film Growth*, **Oleksandr Pshyk [oleksandr.pshyk@empa.ch]**,* *Jyotish Patidar, Kerstin Thorwarth, Lars Sommerhäuser, Sebastain Siol,* Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Ion acceleration is one of the main process tools in the field of ionized physical vapor deposition (IPVD) for thin-film microstructure manipulation. However, the acceleration of film-forming ions onto insulating substrates has been limited, if not impossible, using conventional approaches. Recently, the demonstration of synchronized floating potential HiPIMS (SFP-HiPIMS) has opened new avenues for controlled metal-ion acceleration on insulating substrates [1].

In this presentation, we report on systematic studies of two industrially relevant materials – AlN and AlScN thin films – grown on a range of insulating substrates using SFP-HiPIMS. The substrates include single-crystalline silicon (001), Z-cut quartz, c-cut sapphire, and amorphous borosilicate glass. The concept of SFP-HiPIMS is based on synchronizing the arrival of film-forming ions at the substrate surface with the build-up of the negative floating potential. Since the sputtered species in HiPIMS are time-separated and the build-up of the negative floating potential is transient, achieving this requires precise synchronization between the HiPIMS pulse-on time and the floating potential-on time (defined as the time offset). Such synchronization allows the attraction of film-forming ions to the substrate while avoiding Ar^+ process gas ion bombardment and incorporation into the growing film. Although the SFP-HiPIMS can be implemented using at least two HiPIMS pulses, we demonstrate its feasibility not only for a multiple-magnetron configuration but also for a single-magnetron setup. We evaluate the microstructural quality of AlN and AlScN thin films grown by conventional HiPIMS and SFP-HiPIMS under different magnetron configurations and time offsets in terms of rocking-curve full-width at a half maximum (FWHM), Ar content, and surface roughness.

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PP-ThP-9 Effect of Si and B Incorporation in TiCN-based Thin Film on Physical Properties by Direct Current Plasma Chemical Vapor Deposition*, **Rizu Kurogi [ss25435t@st.omu.ac.jp]**,* *Takeyasu Saito, Noki Okamoto, Mika Kawamoto,* Osaka Metropolitan University, Japan

Ti-based carbonitride thin films such as TiN, TiC, and TiCN have been used to enhance wear resistance and lifetime of cutting tool. Recent studies employed additional elements such as Si or B to form multi component thin films like TiSiCN and TiBCN to improve oxidation resistance and thermal stability. These films are considered to consist of Ti(C,N) nanocrystals dispersed in amorphous TSiCN or TiBCN, which effectively suppresses grain coarsening and also enhances oxidation resistance.

However, most of the TiSiCN and TiBCN thin films have been synthesized to date by physical vapor deposition methods such as magnetron sputtering or arc evaporation, which often result in poor step coverage and interfacial adhesion strength on complex-shaped substrates. Most of previous studies employed physical vapor deposition methods such as magnetron sputtering or arc evaporation, while plasma enhanced chemical vapor deposition (CVD) provides potential advantage on higher conformality, stronger interfacial adhesion and low temperature fabrication for complex-shaped tools and components.

In this study, TiSiCN and TiBCN thin films were deposited on Si and cemented carbide (WC–Co) substrates using direct current plasma CVD at around 600 ℃ where WC–Co substrates were pretreated with aqua regia to improve interfacial adhesion.

The precursor gases were $TiCl_4$, CH_4, N_2, tetramethyl silane (TMS), and BBr_3. The effects of deposition parameters on the film structure and physical properties were systematically investigated using X-ray diffraction, X-ray photoelectron spectroscopy, and nanoindentation.

Si content in the TiSiCN thin films increased with increasing TMS flow rate, while the B content in the TiBCN thin films also increased with increasing BBr_3 flow rate. TiSiCN thin films exhibited higher hardness as maximum value of HV 2585 than that of TiCN thin film. However, the hardness of TiSiCN film decreased according to increase of Si content in the film. The effects of addition of Si and B on grain refinement and structural densification will be discussed.

PP-ThP-11 Magnetron Discharge Modelling using SAPIC, a 2D PIC-MCC AMR Code, *Adrien REVEL, **Tiberiu MINEA [tiberiu.minea@universite-paris-saclay.fr]***, University of Paris-Saclay, LPGP, France

Magnetron sputtering is a widely used Physical Vapor Deposition technique for thin film growth. A target (or cathode) is bombarded by ions from the plasma resulting in the sputtering of the former and emission of secondary electrons. Electrons are confined near the target by a magnetic field created by permanent magnets placed under the cathode. This confinement enhances the ionization efficiency of the working gas allowing to operate at relatively low pressure (0.4 – 4 Pa).

The understanding of the plasma behavior is key to fully control the sputtered material and, therefore, the thin film growth. It involves complex phenomena such as ExB gradient, curvature and drift coupled with kinetic reactions and plasma-surface interactions. Hence, the motion of individual particles and the whole plasma is subject to intricate phenomena difficult to apprehend.

Recently the TMP-D&S (Theory and modelling of Plasma – Discharge & Surface) team of LPGP (Laboratoire de Physique des Gaz et des Plasmas) has developed a 2D Particle-In-Cell – Monte Carlo Collision exploiting the power of AMR (Adaptive Mesh Refinement). Because magnetron plasmas are highly inhomogeneous, using the smallest Debye length as the upper limit of the mesh size for the entire domain results in a waste of computational resources although it is a mandatory criterion to avoid numerical issues. Instead, AMR refines the mesh only where it is required.

The principle of the ARM approach will be presented with the advantages and its implementation. Further, the first results of the SAPIC (Saclay simple AMR Particle-in-Cell) code applied to a conventional magnetron show the effectiveness of the method and pave the way towards further numerical optimizations.

PP-ThP-12 Calorimetric and Electrostatic Probe Diagnostics of a Gas Aggregation Source Plasma, ***Caroline Adam [c.adam@physik.uni-kiel.de]**, Viktor Schneider, Jessica Niemann,* Kiel University, Germany*; Daniil Nikitin, Jan Hanuš, Ronaldo Katuta, Iqra Whid, Veronika Červenková, Andrey Shukurov, Hynek Biederman,* Charles University, Czech Republic*; Holger Kersten,* Kiel University, Germany

Gas aggregation cluster sources (GAS) have been emerging as a key technology for the production of clusters and nanoparticles (NPs) of precise size and composition. The resulting NP properties are significantly affected by the thermal balance during their growth in the aggregation zone. In this study, the characteristics of a novel controllable GAS setup are investigated, using a post (cylindrical) magnetron with a rotating magnetic circuit [1] equipped with a copper target in Ar and/or N_2 atmosphere, respectively. Energy fluxes are quantified by calorimetric measurements using passive thermal probes (PTP) [2], while the plasma parameters are assessed by Langmuir probes. These quantities are critical to develop a comprehensive understanding of the correlation between (external) process parameters (e.g., current, voltage, continuous or pulsing, gas pressure) and (internal) plasma parameters and their correlation with NP growth, transport and microstructure.

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PP-ThP-13 Comparative Study of High-Order Silanes for Low-Temperature SiGe Epitaxy in Ultra-High Vacuum Chemical Vapor Deposition, ***Dongmin Yoon [ehdals360127@yonsei.ac.kr]***, 50, Yonsei-ro, Seodaemun-gu, Republic of Korea*; Hyerin Shin, Seokmin Oh, Seonwoong Jung, Dae-Hong Ko,* Yonsei University, Korea

In recent semiconductor device fabrication processes, the epitaxial growth of Si and SiGe has become a critical technology. Beyond conventional selective epitaxial growth for source/drain formation, SiGe/Si superlattices are now employed as backbone structures in nanosheet-based transistors, extending the application of epitaxy to channel formation. Furthermore, the rapid adoption of 3D integration technologies—including vertically stacked device architectures and hybrid bonding—has significantly increased the demand for epitaxial processes that can be performed within a constrained thermal budget. These requirements have driven interest in high-order silanes (Si_nH_{2n+2}, n ≥ 2) as potential alternatives to conventional Si precursors, including $SiHCl_3$, SiH_2Cl_2, and SiH_4. High-order silanes contain Si–Si bonds with lower bond dissociation energies, enabling decomposition at lower temperatures and potentially achieving higher growth rates compared with conventional precursors.

In this study, we investigate the epitaxial growth of SiGe films using Si_2H_6, Si_3H_8, and Si_4H_{10} under ultra-high vacuum chemical vapor deposition conditions. The effects of varying the flow rates of each Si precursor on growth characteristics were systematically examined. The Ge concentration and growth rate were analyzed under different growth conditions, and the crystallinity and surface morphology of the resulting films were evaluated. Our results demonstrate the feasibility of employing high-order silanes for low-temperature SiGe epitaxy, providing insight into their potential application in next-generation semiconductor device fabrication.

PP-ThP-14 Reaction Characteristics of Germanium Tetrabromide on Si1-XGeX(:B) and Si(:P) Films Using Ultra-High Vacuum Chemical Vapor Deposition System, ***Hyerin Shin [hyerinshin@yonsei.ac.kr]**, Dongmin Yoon, Seokmin Oh, Dae-hong Ko,* Yonsei University, Korea

As semiconductor devices evolve toward vertically stacked architectures, selective epitaxial growth (SEG) of Si and SiGe for source/drain regions has become increasingly challenging due to strict thermal budget requirements. To overcome these limitations, new precursors capable of enabling efficient low-temperature reactions are needed. Although Cl_2 has recently been proposed as a potential alternative to traditional SEG etchant, its insufficient etch rate at extremely low temperatures (≤500℃) underscores the need for novel etchant gases. In this study, we report the first systematic investigation of $GeBr_4$ as a precursor for low-temperature SEG applications. The reaction characteristics of $GeBr_4$ were investigated on $Si_{1-x}Ge_x$ (:B) films and Si (:P) films using a UHV-CVD system.

Crystalline and amorphous undoped $Si_{1-x}Ge_x$ films (0≤x≤0.3) were prepared to evaluate etch selectivity, defined as the etch-rate ratio between amorphous and crystalline films. Experiments were conducted using H_2 and N_2 as the carrier gases within the temperature range of 375 to 500℃. The behavior of B-doped SiGe and P-doped Si films was compared with those of undoped films. Scanning electron microscopy and spectroscopic ellipsometry were employed to measure film thickness. Atomic force microscopy and high resolution-transmission electron microscopy were utilized to examine the surface morphology and microstructure of etched films, respectively. We performed surface analysis after the reaction with $GeBr_4$ using time-of-flight secondary ion mass spectrometry (ToF-SIMS). Additional density functional theory simulations were performed to elucidate the origin of the observed behavior of $GeBr_4$.

$GeBr_4$ exhibited a substantially higher etch rate than pure Cl_2, particularly at low Ge contents. B-doped films showed reduced etch rates compared with undoped films, whereas P-doped Si demonstrated a significantly enhanced etch rate. These findings provide insight into the SEG behavior of dopant-incorporated Si films and offer a foundation for predicting growth characteristics under low-temperature conditions.

PP-ThP-15 Thickness-Dependent Electrical Properties of MoN Films Grown by Thermal ALD Using MoO_2Cl_2, ***So Young Kim [skim544@yonsei.ac.kr]***, Yonsei University, Republic of Korea*; Tai-su Park,* Justem Corporation Ltd., Republic of Korea*; Dae-Hong Ko,* Yonsei University, Republic of Korea

Molybdenum (Mo) has emerged as a promising candidate for next-generation contact and interconnect applications due to its favorable electrical properties and scalability. Similarly, molybdenum nitride (MoN), which can function as a seed layer, diffusion barrier, or electrode material, has attracted significant attention for advanced microelectronic applications owing to its high electrical conductivity and chemical stability. Although MoN deposition by atomic layer deposition (ALD) has been widely explored using halide and organometallic precursors, MoO_2Cl_2 has not been reported for MoN thin-film growth, and its ALD growth characteristics for MoN remain unexplored.

In this work, MoN thin films were deposited by thermal ALD at 600 ℃ using MoO_2Cl_2 as the metal precursor and NH_3 as the co-reactant. Film thickness was systematically varied by adjusting the number of ALD cycles to investigate the evolution of structural, chemical, and electrical properties as a function of thickness. The deposited films were characterized by X-ray diffraction, X-ray photoelectron spectroscopy, and transmission electron microscopy to analyze phase formation, bonding states, and microstructural development, along with electrical resistivity and surface roughness measurements. The thickness dependence of the electrical properties and microstructural evolution of the MoN films were systematically analyzed. This study establishes MoO_2Cl_2 as a viable precursor for thermal ALD of MoN, providing quantitative insights into thickness-dependent electrical properties governed by microstructural evolution and a fundamental baseline for future process optimization, including plasma-assisted or hybrid ALD approaches, to improve early-stage electrical performance.

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PP-ThP-16 Plasma-enhanced Atomic Layer Deposition of Smooth Layers of Tungsten Nitride and Boron Nitride for Optical Application*, Alan Uy* ***[alanuy@hotmail.com],*** University of Maryland College Park, USA*; Maxim Markevitch,* NASA, USA

Metal nitrides have been studied extensively as they have properties useful in applications such as barrier coatings against Cu interdiffusion in electronics as well as hydrogen catalysis [1]. Tungsten nitride (WN) is an attractive material for these applications when deposited as a thin layer. Likewise, boron nitride (BN) thin films have found use in electronics as an insulative coating with high thermal stability and oxidative resistance. Thin films of WN and BN have been generated in multiple ways including sputtering, physical vapor deposition, chemical vapor deposition, and atomic layer deposition [1,2].

We are investigating WN and BN as novel thin film materials for potential use in X-ray mirrors. Thin layers of WN and BN could be tuned for Bragg reflections in the X-ray spectrum, which would prove useful in astronomical devices. Such a Bragg reflector would require hundreds of conformal layer pairs, with each layer under a nanometer thick and very smooth, with rms roughness ~1 Å and no interlayer diffusion [3].

Plasma-enhanced atomic layer deposition (PEALD) is attractive for this application as the use of plasma allows for lower temperature depositions, which are typically associated with amorphous structuring and lower generated roughness. An experimental PEALD reactor was used for deposition onto 1" Si wafers. Precursors bis(tert-butylimino)bis(dimethylamino)tungsten (BTBMW) and a nitrogen/hydrogen mixture for were studied for WN deposition, while tris(ethylmethylamino) borane (TEMAB) and the nitrogen/hydrogen mixture were studied for BN growth.

The PEALD reactor demonstrated WN growth rates of ~0.55 Å/PEALD cycle and BN growth rates of ~0.4 Å/PEALD cycle at relatively low temperatures of 200 °C. Very low rms roughness of 1 Å was observed for ultrathin (< 5 nm) deposited films. Varying PEALD process parameters such as the deposition temperature, plasma exposure times, and plasma power were found to have interesting effects on the film growth rate. Composition, roughness, and other optical properties for deposited films will also be presented.

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[2] Park, H., Kim, T., Cho, S. et al.Sci Rep 7, 40091 (2017)

[3] B. Salmaso, D. Spiga. et al. Proceedings Vol. 8147, Optics for EUV, X-Ray, and Gamma-Ray Astronomy V, 814710 (2011)

PP-ThP-17 Electrocatalytic Performance of AlCrCoNiFeX (X = C, O)HighEntropy Alloy Films for Oxygen and Hydrogen Evolution Reactions*, Amna Waheed,* Ming Chi University of Technology, Taiwan*; Bih-Show Lou,* Chang Gung University, Taiwan*; Jyh-Wei Lee,* ***Krishnan Tiwari [KRISHHH0901@GMAIL.COM],*** Ming Chi University of Technology, Taiwan

The growing demand for sustainable and efficient energy conversion technologies has intensified interest in developing advanced electrocatalysts for water splitting. Highentropy alloys (HEAs), composed of multiple principal elements in near-equiatomic ratios, offer a promising platform due to their unique compositional flexibility, tunable electronic structure, and synergistic catalytic effects. In this work, AlCrCoNiFeX (X = carbon and oxygen) HEA films were synthesized via reactive HiPIMS to assess their bifunctional electrocatalytic activity for the oxygen and hydrogen evolution reactions (OER and HER) in alkaline media. The carbon and oxygen contents were systematically varied to study their combined effects on the structural, morphological, and electrochemical properties of the deposited HEA films. The enhanced catalytic behavior can be ascribed to the synergistic interactions among multiple metallic constituents and the optimized surface structure resulting from carbon–oxygen–carboxylic incorporation. Electrochemical evaluations, including linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), and double-layer capacitance (C_{dl}) measurements, confirmed the superior charge transfer kinetics, larger electrochemically active surface area, and improved catalytic efficiency of the optimized composition. Furthermore, long-term stability and durability tests demonstrated excellent sustainability of the catalyst under continuous operation, validating its structural robustness and electrochemical reliability. This study highlights the potential of AlCrCoNiFeXHEA films as a new generation of efficient and durable bifunctional electrocatalysts for practical water-splitting applications.

Topical Symposium on Sustainable Surface Engineering
Room Town & Country A - Session TS1-ThP

Coatings for Batteries and Hydrogen Applications Poster Session

TS1-ThP-1 Hydrogen Permeation Testing: Electrochemical vs. Pressurized Methods*, Phillip Rückeshäuser* ***[phillip.rueckeshaeuser@tuwien.ac.at],*** TU Wien, Austria*; Szilard Kolozsvari, Peter Polcik,* Plansee Composite Materials GmbH, Germany*; Timea Stelzig,* Oerlikon AM Europe GmbH, Germany*; Konrad Fadenberger,* Oerlikon Balzers Coating Germany GmbH, Germany*; Klaus Boebel,* Oerlikon Balzers, Liechtenstein*; Tomasz Wojcik, Helmut Riedl,* TU Wien, Austria

The interactions between hydrogen and materials are subjects of significant interest in both research and industry. Consequently, the hydrogen charging of samples and following detection are crucial aspects of this field. Currently, there are two primary methods for hydrogen charging: electrochemical charging and pressurized hydrogen charging.

In electrochemical charging, atomic hydrogen is produced through the dissociation of water, while in pressurized charging, hydrogen is introduced in gaseous form and subsequently thermally dissociated. Although these two methods are based on fundamentally different principles, they ultimately achieve the same goal: the absorption and permeation of atomic hydrogen in the sample. However, most studies tend to focus on either one method or the other. Thus, it becomes essential to explore the correlation between these methods and identify equivalent charging conditions for specific hydrogen permeation characteristics.

In this study, we conducted hydrogen permeation tests using both electrochemical and pressurized setups. We applied nitride coatings such as TiN and CrN to steel substrates using physical vapor deposition (PVD) techniques and compared the permeation performance of the two charging methods. This comparison involved determining key parameters such as diffusion coefficients and permeation reduction factors. Additionally, we characterized the coating properties using secondary electron microscopy, X-ray diffraction, and linear sweep voltammetry.

TS1-ThP-2 Towards Defect-Free Laser-Induced Graphene Coating on Copper and Aluminum Foils for Anode-Free Li and Na Metal Batteries*,* ***Aarti Gunjal [aartitambe22@gmail.com],*** IISER PUNE, India*; Suparna Saha,* TCG-CREST Kolkata, India*; Swati Jadhav,* IISER PUNE, India*; Satishchandra Ogale,* TCG-CREST Kolkatta, India

Laser-induced graphene (LIG) is a very well-established process for realizing functional carbon coatings on different substrates. Depending on the laser processing parameters it yields structurally, morphologically and chemically interesting forms which are also adherent because of the thermal energy input. In most cases, however, a defect band (D band) is invariably observed in the Raman spectrum of such coatings, in addition to the so-called G-band corresponding to desired graphitic carbon. In this work we have applied CO2 laser processing to carbonize the coatings of the dried powder of aromatic eucalyptus (EU) leaves on metals. The effects of laser power density, scanning speed, substrate choice, and precursor coating thickness on the quality of carbon are carefully examined and optimized to obtain a unique almost defect-free few layers graphene coating, as reflected by a miniscule D-band and a significant 2D signature in the Raman spectra of few-layer graphene. Comparative studies on other aromatic leaves sample (e.g. lemon grass) and non-aromatic leaves suggest that aromaticity is important for realizing an enhanced 2D band, which could be due to internal turbulent cavitation upon laser-induced transient heating. In situ nitrogen doping is also achieved by applying the LIG process to a mixture of EU powder loaded with urea. Remarkably, the nitrogen incorporated coatings on copper and aluminum current collectors render far superior performance in anode-free Li and Na metal batteries, respectively, as against the defect-free few layers graphene coating. In fact, half cells with alkali metals show an impressive cycling stability of over 450 cycles for both Li and Na. Through thorough characterizations employing multiple techniques, an attempt is made to develop a mechanistic understanding of the issues involved.

TS1-ThP-3 HiPIMS Mo_xN and Cu-Mo_xN Thin Films for the Hydrogen Evolution Reaction, *Hung-I Wu,* Department of Electronic Engineering, National Yunlin University of Science and Technology, Taiwan*; Ying-Hsiang Lin,* Department of Materials Science and Engineering, National United University, Taiwan*; Shih-Hung Lin,* Department of Electronic Engineering, National Yunlin University of Science and Technology, Taiwan*; Fan-Bean Wu, Chi-Yueh Chang,* Department of Materials Science and Engineering, National United University, Taiwan*; Thi Xuyen Nguyen, Ruei-Chi Lin, Jyh-Ming Ting,* Department of Materials Science and Engineering, National Cheng Kung University, Taiwan*; **Wan-Yu Wu [wywu@nuu.edu.tw]**,* Department of Materials Science and Engineering, National United University, Taiwan

Hydrogen produced by water electrolysis is a promising clean energy carrier, yet large-scale deployment is hindered by the high cost and limited durability of noble-metal catalysts. Transition-metal nitrides, particularly molybdenum nitride (Mo_xN), offer attractive corrosion resistance and electrical conductivity, enabling hydrogen evolution reaction (HER) catalysis in both acidic and alkaline media.

In this work, Mo_xN thin films were deposited and benchmarked using RF sputtering and high-power impulse magnetron sputtering (HiPIMS). In 0.5 M H_2SO_4, the HiPIMS-Mo_xN catalyst achieved an overpotential of 292 mV, corresponding to a ~61.2% improvement compared with pristine carbon paper (CP). The performance gain is attributed to the superior film adhesion achieved by HiPIMS, leading to a 9.7% reduction in charge-transfer resistance (R_{ct}) and the absence of large-area catalyst delamination after HER testing. Process optimization identified Cu addition is suggested to tune the Mo d-band center and improve overall conductivity, reducing the overpotential to 254 mV (~13.0% improvement vs. HiPIMS-Mo_xN) and decreasing the Tafel slope from 75.9 to 55.0 $mVdec^{-1}$, indicating accelerated HER kinetics via a synergistic effect. In 1.0 M KOH, HiPIMS-Mo_xN achieved the lowest overpotential (199 mV), while Cu addition deteriorated activity, suggesting Mo as the dominant active center in alkaline media and that secondary metals reduce accessible Mo sites.

TS1-ThP-4 Hydrogen Barrier Properties of Thin Oxide Films Prepared by Different Methods: Correlations of Thin Film Properties with Hydrogen Permeation Rates, *Dmitry Kalanov, Juergen W. Gerlach, Patrick C. With, **Yeliz Unutulmazsoy [yeliz.unutulmazsoy@iom-leipzig.de]**, Ulrike Helmstedt,* Leibniz Inst. of Surface Eng. (IOM), Germany

Efficient hydrogen barriers are essential for the hydrogen economy, where minimizing hydrogen loss and ensuring material safety are critical. In the present study, we investigate thin oxide films, using TiO_2 as a model oxide system, deposited on PET substrates by UV photochemical conversion of metalorganic precursors under ambient conditions and by High-Power Impulse Magnetron Sputtering (HiPIMS) deposition without substrate heating. Using a dedicated gas-permeation measurement system, hydrogen permeation through the oxide films on PET was studied as a function of film thickness. Results demonstrate a strong thickness dependence of the barrier properties: 50 nm TiO_2 films exhibit a fivefold improvement, while increasing the thickness to 70 nm for HiPIMS grown thin films reduces permeation below the detection limit, highlighting the high barrier performance of dense, amorphous TiO_2 films. These findings are discussed in the context of current challenges in measuring hydrogen permeation in thin films on various substrates, compared to other oxide systems such as SiO_x [1], and in relation to differences in structural properties of the films arising from the distinct deposition methods.

[1] P.C. With, T. Pröhl, J.W. Gerlach, A. Prager, A. Konrad, F. Arena, U. Helmstedt, Hydrogen permeation through uniaxially strained SiO_x barrier thin films photochemically prepared on PET foil substrates,
Int. J. Hydrog. Energy 81 (2024) 405-410

Topical Symposium on Sustainable Surface Engineering
Room Town & Country A - Session TS2-ThP

Coatings and Surfaces for Renewable Energy Technology Poster Session

TS2-ThP-2 Comparative Electrochemical Performance of α-MnO_2 and δ-MnO_2 Coatings for High-Performance Supercapacitor Electrodes, ***Eduardo Estrada Movilla [eduardo.estrada.movilla@uabc.edu.mx]**, Álvaro Ortiz Pérez, Jhonathan Castillo Saenz,* Instituto de Ingeniería, Universidad Autónoma de Baja California, Colombia

Transition-metal-oxide functional coatings have emerged as promising candidates for next-generation electrochemical energy storage systems due to their high theoretical capacitance, chemical stability, and tunable ion-transport pathways. In this work, a comparative evaluation of α-MnO_2 and δ-MnO_2 phases is reported, focusing on their performance as active electrode coatings. Four MnO_2 variants were synthesized via hydrothermal processing, yielding two α-type and two δ-type compositions with distinct structural and morphological characteristics. The coatings were deposited onto stainless-steel mesh substrates and characterized by XRD, FT-IR, and SEM, confirming phase purity and the formation of hierarchical nanostructures that directly influence electrolyte accessibility.

Electrochemical testing cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy, revealed that δ-MnO_2 exhibited superior behavior, achieving specific capacitances above 300 F g^{-1} at 0.1 A g^{-1} and enhanced cycling stability (>90% capacitance retention after 2000 cycles). Nyquist analysis confirmed reduced charge-transfer resistance for δ-MnO_2, attributed to improved interlayer ion diffusion and increased electroactive surface area.

These findings highlight δ-MnO_2 as a high-performance material for supercapacitor applications, and demonstrate its potential integration in scalable metal-mesh-based electrode architectures for energy storage systems.

Keywords: MnO_2 coatings, energy-storage electrodes, hydrothermal synthesis, supercapacitors.

Surface Engineering - Applied Research and Industrial Applications
Room Town & Country D - Session IA1-FrM
Advances in Application Driven Research and Hybrid Systems, Processes, and Coatings

Moderators: Hana Barankova, Uppsala University, Sweden, **Ladislav Bardos**, Uppsala University, Sweden

8:00am **IA1-FrM-1 Effect of Alumina Coating and Testing Condition on Tribological Behaviors and the Oxidative Potential of Brake Wear Particles***, Minh Khoi Phan, Ran Cai,* ***Xueyuan Nie [xnie@uwindsor.ca]****, Jimi Tjong,* University of Windsor, Canada*; D.T.A. Matthews,* University of Twente, Netherlands

Brake wear particles (BWPs) are known for contributing to adverse respiratory and cardiovascular health outcomes primarily via their oxidative potential (OP). Plasma electrolytic aluminating (PEA) coating can reduce wear and corrosion of cast iron brake rotor and thus BWPs. However, the effect of the alumina coating and testing conditions on OP of BWPs has not been characterized yet. In this study, BWPs were generated and collected after pin-on-disc (POD) wear test, brake dynamometer test and vehicle road test, respectively. Besides the study on tribological behavior of uncoated and PEA-coated brake disc, the ascorbic acid (AA) depletion assay was used to investigate the OP behavior of those BWPs. The results showed that BWPs from the uncoated brake system exhibited a higher AA depletion rate (meaning a higher OP), whereas those from PEA-coated brake system showed a lower depletion rate after both POD test and dyno test cases. This difference was consistent with the metallic content in BWPs. The AA depletion rate was higher for BWPs from the dyno test than from POD test, suggesting significance in negative impact of high dyno braking temperature. Effect of road environment during the vehicle driving test was even more profound. Given a similar tribological behavior and considerable reduction in wear of the coated brake system, this indicates that PEA coating technique can reduce overall oxidative burden and thus reduce harm to health without compromising the braking performance.

8:20am **IA1-FrM-2 Memristive Effects in PEO Alumina: Mechanisms and Technological Implications***, Aleksey Rogov, Allan Matthews,* ***Aleksey Yerokhin [Aleksey.Yerokhin@manchester.ac.uk]****,* University of Manchester, UK **INVITED**

Modern trends towards sustainable, resource- and energy efficient manufacturing bring surface engineering of light alloys at the forefront of research interest. Plasma Electrolytic Oxidation (PEO) attracts significant attention as an advanced technology platform for high-performance ceramic coatings on light alloys, which enables lightweighting of structural components, improved protection form wear and corrosion as well as development of new functional devices and consumer products. PEO is an electrochemical technique which utilises pulsed bipolar polarisation to grow anodic oxides above the potentials of dielectric breakdown. A large number of experimental variables and significant non-linearity provide major challenges for process optimisation, diagnostics and control, hindering its broader adoption in industry. We attempt to address these challenges by developing a mechanistic understanding of the behaviour of metal-oxide-electrolyte systems using original in-operando process diagnostic techniques. Recent studies of PEO treatments of Al indicate that this behaviour is influenced by dynamic rearrangements in the barrier layer of the anodic alumina grown under alternating cathodic and anodic polarisation. In contrast to common presentation of anodic oxides as dielectric barriers, the revealed dependence on polarisation history implies that such films should be treated as a memristive structures. This new understanding allows explaining unusual discharge behaviour observed during PEO treatments, including soft sparking transition and appearance of scanning waves propagating perpendicular to the direction of electric field. Although the barrier layer occupies a small portion of PEO coating located at the interface with the metal substrate, its evolution appears to influence both structural and morphological transformations in the whole coating. The presentation will therefore discuss the mechanisms underlying structural rearrangements in the barrier layer, their practical significance and implications for process energy efficiency and real-time control over coating characteristics and properties.

9:00am **IA1-FrM-4 Advanced Coating Strategies to Combat Friction and Wear in Low-Viscosity Fuel Systems***,* ***Eun Cairns [Euan.Cairns@woodward.com]****,* University of North Texas, USA*; Satish Dixit, S. Berkebile,* Plasma Technology Inc., USA*; Diana Berman, Samir M. Aouadi, Andrey A. Voevodin,* University of North Texas, USA **INVITED**

Fuel pump components operating with low-viscosity hydrocarbon fuels (< 3 cSt) experience high failure rates due to poor lubricity, leading to scuffing, seizure, and accelerated wear in boundary-lubricated metal contacts. Conventional steel surfaces, both uncoated and coated, are particularly vulnerable under these conditions. This work investigates advanced coating strategies to mitigate friction and wear in multi-fuel pump environments, focusing on hard wear-resistant coatings, soft solid lubricant films, and duplex systems.

A systematic evaluation of state-of-the-art industrial hard coatings was conducted using fuel surrogates (ethanol, decane, dodecane) and F-24 jet fuel. Several coatings demonstrated superior tribological performance, making them strong candidates for multi-fuel applications. In parallel, the potential of solid lubricant coatings, specifically MoS_2 deposited via spray techniques on steel and WC-17Co substrates, was explored. Tribological testing of solid lubricants in low-viscosity hydrocarbons was complemented by surface characterization using X-ray Photoelectron Spectroscopy (XPS), Raman spectroscopy, and Scanning Electron Microscopy (SEM). These analyses reveal how hydrocarbon properties, such as polarity, water affinity, chain length, viscosity, and contact angle affect chemical and structural changes in MoS_2, influencing micro- and nano-scale lubrication mechanisms. Additionally results show how duplex architectures, utilizing a hard, wear resistant underlayer, and a soft lubricious solid lubricant layer, are a step towards developing a more robust coating for low-viscosity fuel pump applications.

9:40am **IA1-FrM-6 Cu Grain Engineering and Plating Process Reliability Study for Heterogeneous Integration***,* ***Shan-Yuan Wu [t113c77009@ntut.org.tw]****, Ying-Chao Hsu, Po-Chun Chen, Sheng-Ru Hsiao,* National Taipei University of Technology, Taiwan

The continuous improvement of integrated circuit (IC) performance is mainly driven by transistor scaling and advanced packaging technologies. In 3D heterogeneous integration with hybrid bonding and 2.5D interposers using through-silicon or through-glass vias (TSV/TGV), advanced packaging plays a vital role. Each application presents distinct reliability challenges: hybrid bonding requires strong adhesion at low temperatures, while TSV/TGV structures demand low stress and void-free filling. Ultra-fine-grained (UFG) copper addresses these issues by enhancing grain boundary diffusion and enabling low-temperature bonding, while its fine-grained structure promotes bottom-up via filling and suppresses seam voids during electroplating.

The formation of Ultra-fine-grained Cu is closely related to organic additives in the electrolyte, particularly polyethylene glycol (PEG) and bis-(sodium-sulfopropyl)-disulfide (SPS). In this study, various additive formulations were investigated under identical plating conditions. Electron backscatter diffraction (EBSD) results revealed that optimized additives reduced the average grain size from above 1 µm to 390 nm, demonstrating a strong correlation between additive control and microstructural refinement.

To elucidate the electrochemical influence of additives, linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS) were performed using an Admiral Squidstat Plus potentiostat. The working electrode was a silicon wafer coated with a 100 nm PVD Cu seed layer.

The presence of PEG introduced a pronounced suppression effect due to the formation of a PEG–Cu–Cl adsorption layer on the cathode surface. In LSV, this suppressor layer increased the overpotential from 0.45V to 0.65V under the $100mA/cm^2$ current density, reducing the critical nucleus radius and promoting finer grain formation. This monolayer structure was further characterized by EIS, where the high-frequency semicircle in the Nyquist plots represented the impedance of the additive-adsorbed layer. Its gradual shrinkage during plating indicated additive depletion and a weakened suppression effect, while recovery after PEG replenishment reflected restored electrolyte stability. These findings provide a practical strategy for monitoring and maintaining plating bath quality through electrochemical analysis.

This study integrates EBSD and EIS to establish a quantitative and time-efficient framework for evaluating electrolyte stability and predicting Ultra-fine-grained Cu formation, offering valuable insights for optimizing copper electroplating reliability and grain size in advanced packaging processes.

10:20am **IA1-FrM-8 Surface Property Enhancement of Al 7075 Alloy via MAO-Based Boron-Reinforced Composite Coatings**, *Erhan Karaca,* Turkish State Railways, Turkey*; **Suleyman Sukuroglu [ssukuroglu@gumushane.edu.tr]**,* Gümüşhane University, Turkey

Al 7075 alloy is a strategic engineering material widely used in the aerospace and defense industries, as well as in the automotive sector, due to its low density, high specific strength, excellent machinability, ductility, high toughness, and superior fatigue resistance. Despite these outstanding mechanical properties, its relatively low fracture toughness, limited damage tolerance, and susceptibility to environment-dependent corrosion restrict its application in certain advanced structural components. These limitations, particularly encountered under long-term service conditions in aircraft structures, increase the demand for effective surface modification techniques.

Ceramic-based coating methods applied to aluminum and its alloys offer a promising solution for improving surface properties by providing high hardness, enhanced wear resistance, and improved corrosion performance. In this context, ceramic coatings produced by the Micro Arc Oxidation (MAO) method have emerged as an effective and widely adopted surface engineering approach.

In this study, composite coatings were fabricated on Al 7075 aluminum alloy using the MAO technique with three different boron-based additives ($B_5H_{10}NaO_{13}$, B_4C, and h-BN) to enhance the surface characteristics of the alloy. The microstructural, mechanical, tribological, and corrosion properties of the resulting coatings were comprehensively investigated. The findings demonstrated that boron-reinforced composite coatings significantly improved the surface performance of the Al 7075 alloy, particularly by providing remarkable enhancements in wear and corrosion resistance.

10:40am **IA1-FrM-9 Advanced HiPIMS Coating Equipment for High-Performance Cutting Tools Amid Tungsten Price Increase**, ***Yafen Chen [chenyafen@hsvacuum.com]**, Wei Zhou,* Guangdong Huasheng Nanotechnology, China

Recent increases in tungsten prices have driven up the cost of tungsten carbide cutting tools, making high-performance coatings—which extend tool lifetime and reduce replacement frequency—more critical than ever for cost-effective precision manufacturing. Cathode arc evaporation (CAE) and direct current magnetron sputtering (DCMS), the most prevalent PVD techniques for cutting tool hard coatings, face critical limitations: CAE generates detrimental droplets that compromise coating integrity, while DCMS produces loose microstructures, both severely restricting cutting tool service lifetime. High-power impulse magnetron sputtering (HiPIMS) overcomes these drawbacks, enabling the deposition of dense, droplet-free hard coatings. Huasheng Nanotechnology's G4Ultra HiPIMS coating system elevates performance further via integrated synchronized bias, reverse bias, and ultra-high pulsed bias technologies. These features yield coatings with superior hardness, ultra-smooth surfaces, and significantly extended cutting tool lifetime. To address HiPIMS' inherent low deposition rate, we additionally integrate HiPIMS with high-power impulse arc, achieving a balance between high coating quality and enhanced production efficiency. Our solutions provide advanced, industry-adaptable PVD equipment for high-performance cutting tool hard coatings, well-aligned with the evolving demands of precision manufacturing.

Tribology and Mechanics of Coatings and Surfaces
Room Palm 3-4 - Session MC1-2-FrM

Friction, Wear, Lubrication Effects, & Modeling II

Moderator: Klaus Boebel, Oerlikon Surface Solution AG, Liechtenstein

8:20am **MC1-2-FrM-2 Active Friction and Wear Control in a-C:Cr Films: Electrical Current and Polarity Effects on Catalytic Graphitization**, ***Newton K. Fukumasu [newton.fukumasu@usp.br]**, Miguel R. Danelon,* University of São Paulo, Brazil*; Abrar Faiyad, Ashlie Martini,* University of California Merced, USA*; Cherlio Scandian,* Federal University of Espirito Santo, Brazil*; Roberto M. Souza,* University of São Paulo, Brazil

Diamond-Like Carbon (DLC) films are established protective coatings for severe contact conditions, yet their tribological response under active electrical currents involves under-explored physical mechanisms. This study investigates the friction and wear behavior of Cr-doped (a-C:Cr) and undoped a-C films under reciprocating sliding with simultaneous electrical current passage. Tests were performed in dry conditions, using AISI 52100 steel balls against coated glass substrates under anodic (positive plane) and cathodic (negative plane) polarizations, applying a 10 N normal load, 4 mm stroke, and a constant current of 100 mA for the electrified cases. While undoped DLC exhibited inert behavior, resulting in a friction coefficient (COF) of 0.15 regardless of electrical conditions, Cr-doped films demonstrated a friction reduction, down to 0.05, and significant responsiveness to the applied current. Although instrumented indentation and microscopy indicated slightly lower hardness and more visible wear marks for a-C:Cr compared to the undoped film, the tribological behavior is attributed to a local shear-induced phase transformation mechanism. Raman spectroscopy of the a-C:Cr wear tracks under cathodic polarization revealed an intense 2D peak, characteristic of ordered, multilayer graphene-like structures. This result provides evidence that Cr catalytically lowers the activation energy for graphitization, activated by local heating and electron flow. Conversely, anodic polarization resulted in clean wear tracks and stable low friction, suggesting a distinct equilibrium between tribofilm formation and oxidative removal. Reactive Molecular Dynamics simulations supported these findings, elucidating atomistic pathways where Cr clusters facilitate bond rehybridization under combined shear and electrochemical stress. These results demonstrate that the tribological performance of a-C:Cr can be actively tuned, enabling "on-demand" low-friction regimes through electrically assisted catalytic graphitization.

8:40am **MC1-2-FrM-3 Tribological Performance of Sputter-Deposited MoS_2 Coatings with Varying Process Gases**, ***Tomas Babuska [tfbabus@sandia.gov]**, Alexander Mings, Steven Larson, John Curry, David Adams,* Sandia National Laboratories, USA

Sputter-deposited molybdenum disulfide (MoS_2) coatings have been used for decades in aerospace applications due to their ultra-low steady-state coefficients of friction ($\mu_{ss} < 0.05$). Developing MoS_2 coatings for demanding applications with predictable and reliable performance over time (i.e., high-quality) requires tuning the coating microstructure through process variations. In this work, we explore process-structure-property-performance relationships of pure MoS_2 solid lubricant coatings where coatings are sputter deposited using different process gases. Helium, kypton, neon, argon and xenon are used to sputter deposit MoS_2 of varying morphologies, and the impact on critical performance traits such as initial friction, run-in, and aging resistance are studied. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

9:00am **MC1-2-FrM-4 Effect of Ta Content in ta-C:Ta Coatings on the Machining Performance of Aluminum Alloy**, ***Kosuke Suzuki [kousukes@mmc.co.jp]**,* Mitsubishi Materials Corporation, Japan*; Takayuki Tokoroyama, Ruixi Zhang, Noritsugu Umehara,* Nagoya University, Japan*; Shun Sato, Kenji Yumoto,* Mitsubishi Materials Corporation, Japan **INVITED**

In recent years, demand for lightweight materials in the automotive and aerospace industries has increased, leading to a growing need for machining aluminum alloys. In aluminum alloy machining, Diamond-Like Carbon (DLC) coatings—especially hydrogen-free tetrahedral amorphous carbon (ta-C) coatings—are widely used due to their excellent wear resistance and low friction, which help suppress material adhesion and tool wear caused by hard Si particles in the alloy.

However, under more severe machining conditions, further improvements in coating performance are required to extend tool life, especially in terms of wear resistance and delamination resistance. One of the representative approaches for such performance enhancement is the addition of transition metal elements to DLC coatings, and numerous studies have been reported in this area. Among these, tantalum (Ta) is known to form strong covalent bonds with carbon and is expected to achieve both mechanical strength and improved adhesion strength through the reduction of residual compressive stress.Nevertheless, studies on its influence on machining performance remain limited.

In this study, tantalum-doped ta-C (ta-C:Ta) coatings with varying Ta contents were fabricated, and the correlation between Ta content and coating properties, as well as its effect on the drilling performance of aluminum alloy (ADC12), was systematically evaluated.

For each coating, microstructural analysis and residual stress measurements were conducted, along with ball-on-disk friction tests and scratch tests. Additionally, aluminum alloy cutting tests were performed to evaluate wear resistance and cutting force. As a result, the friction coefficient and specific wear rate tended to increase with higher Ta content in the friction tests. On the other hand, the scratch tests showed an increase in critical load, and a correlation between critical load and residual compressive stress was confirmed. Observations of the scratch marks revealed that ta-C:Ta coatings exhibited smaller delamination areas compared to undoped ta-C coatings. The dispersed structure of TaC nanocrystals observed in the ta-C:Ta coatings is suggested to suppress delamination propagation and contribute to improved toughness.

In the cutting tests, the coating containing 1.1 at.% Ta demonstrated the best wear resistance and lowest cutting force by significantly suppressing chipping while maintaining resistance to abrasive wear. These results suggest that controlling residual stress through appropriate Ta addition and enhancing toughness via fine TaC structures are effective strategies for improving tool life in aluminum alloy machining.

10:20am **MC1-2-FrM-8 Effects of Silver Nitrate Additives on the Antibacterial and Corrosion Behaviors of Plasma Electrolytic Oxidized AZ31 Magnesium Alloy*, Bo-Xuan Zheng [rick910823@gmail.com]*,** *Chuan-Ming Tseng,* Ming Chi University of Technology, Taiwan, Republic of China

AZ31 magnesium alloy exhibits excellent biodegradability and biocompatibility, making it a promising candidate for temporary biomedical implants. Nevertheless, its rapid degradation and insufficient corrosion resistance severely limit its direct clinical application. In this study, the bioceramic composite coatings on AZ31 magnesium alloy were prepared by using plasma electrolytic oxidation (PEO) under bipolar power mode in alkaline solutions with sodium phosphate, sodium silicate, potassium fluotitanate and silver nitride ($AgNO_3$) additions. The effect of $AgNO_3$ content on antibacterial and corrosion behaviors of PEO coatings on AZ31 magnesium alloy was investigated. The microstructural characterizations of the $AgNO_3$-incorporated PEO coatings were identified by XRD, SEM-EDS and EPMA. The adhesion and wear resistance of PEO coatings were evaluated using scratch testing and pin-on-disk wear tests, respectively. The potentiodynamic polarization measurements were conducted to evaluate the corrosion behaviors of PEO coatings in simulated body fluid (SBF) solutions. The antimicrobial properties of PEO coatings were carried out by measuring the numbers of *Escherichia coli* bacterial colony after various incubation durations. The XRD patterns reveal that the PEO coatings are mainly composed of MgO (inner layer) and Mg_2SiO_4 (outer layer). Cross-sectional SEM–EDS mapping images confirm that Ag elements are well dispersed near surface of PEO coatings. The highest adhesion strength (~36 N) and the lowest wear rate (5.5×10^{-6} mm^3/N m) can be achieved for the PEO coating with 0.2 g/L $AgNO_3$ incorporated. However, the potentiodynamic polarization curves display that the PEO coatings, as compared to AZ31 magnesium alloy, exhibit higher corrosion resistances in SBF solutions. Furthermore, the PEO coating with 0.2 g/L $AgNO_3$ addition shows the optimal corrosion resistance due to its lowest corrosion current density (1.07×10^{-8} A/cm^2). Furthermore, the antibacterial efficiency of the PEO coatings is significantly improved with increasing $AgNO_3$ additives. More interestingly, all the PEO coatings with various $AgNO_3$incorporated exhibit a 100% antibacterial efficiency to *Escherichia coli* after incubation in 45 minutes. In summary, the adhesion, wear resistance, antibacterial efficiency and corrosion resistance of PEO coatings on AZ31 magnesium alloy can be pronouncedly improved by $AgNO_3$ additions, highlighting their potential for biodegradable implant applications.

Keywords: PEO, AZ31, Silver nitrate, Corrosion resistance, SBF.

10:40am **MC1-2-FrM-9 Experimental Investigation of Friction, Wear, and Dielectric Behavior of Hybrid Polymer Nanocomposites for Insulated Bearings with Machine Learning Assisted Optimization*, Unnati Joshi [unnatiajoshi@gmail.com]*,** *Anand Joshi, Vishal Mehta, Jaivik Pathak, Pranav Rathi,* Parul University, India

The present research reports the development and comprehensive investigation of polymer based hybrid nanocomposites composed of Graphene Oxide (GO) and Copper Oxide (CuO) nanoparticles reinforced Polyether ether ketone (PEEK), designed for multifunctional efficacy in advanced high speed electromechanical system applications, including insulated bearings. The objective was to improve the friction-wear characteristics and dielectric properties of the base PEEK polymer. The suitability of the hybrid nanocomposites for insulated bearing applications were evaluated by examining the dielectric constant, dielectric loss, wear rate, and coefficient of friction. Structural and morphological properties were characterized using SEM, EDS, XRD, and FTIR. In this study, the friction, wear and dielectric properties of PEEK based nanocomposites containing 5 wt% Graphene Oxide and varying Copper Oxide nanoparticle contents (1 to 5 wt%) were experimentally investigated. Among all the compositions that were examined, the nanocomposite containing 5 wt.% GO and 5 wt.% CuO nanoparticles demonstrated the highest R^2 value of 88% for wear resistance and 93% for coefficient of friction, thereby validating its optimal performance level and operational stability. The simultaneous enhancements that result from the combination of CuO and GO are indicative of improved surface strength. Furthermore, the machine learning regression models, including Random Forest, XGBoost, and Extra Tree, have exhibited exceptional predictive capabilities for wear and friction forces. The Extra Tree model, in particular, achieved near-perfect accuracy (R^2 = 0.9999) and identified load as the most influential factor. Also, the dielectric constant (ε') and dielectric loss (ε") were predicted and modelled using these machine learning models. The analysis demonstrated that the highest ε' was achieved at 2 wt% Copper Oxide as a result of increased interfacial polarisation, while the most stable dielectric loss (ε") was achieved at 3 and 4 wt% Copper Oxide. The Extra Trees algorithm consistently exhibited superior predictive accuracy and generalisation capability among all the models. This demonstrates that the wear resistance, coefficient of friction, and dielectric behaviour of the composites, were substantially influenced by the synergistic interaction between Graphene Oxide and Copper Oxide nanoparticles. This research advances durable, high performance insulating materials for next-generation electromechanical systems, supporting SDG 9. It also promotes SDG 12 by supporting the design of affordable, durable materials that reduce material waste and enhance industrial component energy efficiency.

Tribology and Mechanics of Coatings and Surfaces
Room Town & Country B - Session MC3-3-FrM

Tribology of Coatings and Surfaces for Industrial Applications III

Moderators: Osman Eryilmaz, Argonne National Laboratory, USA, **Volker Weihnacht**, Fraunhofer IWS, Germany

8:00am **MC3-3-FrM-1 High-performance ta-C-based coatings for tribological applications deposited by laser-arc technique*, Volker Weihnacht [volker.weihnacht@iws.fraunhofer.de]*,** *Frank Kaulfuss, Stefan Makowski, Falko Hofmann, Fabian Härtwig, Martin Zawischa,* Fraunhofer IWS, Germany **INVITED**

Tetrahedral amorphous carbon (ta-C) coatings are increasingly used in tribological contacts and can be found in numerous industrial applications due to their wear resistance caused by super hardness in combination with generally low friction. Fraunhofer IWS has developed a deposition technique for stable industrial coating processes for ta-C using a pulsed, laser-triggered arc discharge on graphite cathodes. The laser-arc technique can be combined with plasma filtering to reduce the density of particle-induced defects in the ta-C coatings. In addition to the further development of plasma filter technology, IWS has currently focused on the development of doped ta-C(:X) coatings by using graphite composite cathodes. In this contribution, it will be shown how doping affects the deposition behavior as well as the structure and properties of the grown ta-C:X coatings. Special emphasis is placed on the tribological properties using various engine oils and alternative, environmentally friendly lubricants.

8:40am **MC3-3-FrM-3 The Development of Amorphous-Based Multi-Component Alloys for the Nanocomposite Coatings and their Properties*, Kyoung Il Moon [kimoon@kitech.re.kr]*,** *Gi hoon Kwon, Hae Won Yoon, Byoungho Choi, Kyong jun An,* Korea Institute of Industrial Technology, Republic of Korea*; Sung Chul Cha,* Hyundai Motor Group-Hyundai Kefico, Republic of Korea

While modern industries are becoming more sophisticated, diversified, and globalized, they requires the development of smart materials have multi-functionality, high mechanical properties, and extreme durability. Also they could be prepared environmentally friendly and energy efficiently. At the same point of view, the smart coating materials capable of simultaneously expressing various mechanical properties or opposite properties such as high hardness with high toughness, high electricity with high corrosion resistance are attracting attentions as an versatile and useful materials in the future. In particular, there is an urgent needs to develop a novel coating materials capable of stably maintaining microstructures and mechanical properties in various external environments, unlike conventional coating materials whose properties and structures are easily changed by the some harsh environments. To get this kinds of objects, the coating material with multi-components are essential. But if the materials should be prepared with one phase with multi components, they could have only one properties. So, nano-composites with various phases should be formed to realize the various properties. So, it is necessary to develop a coating layer composed of various components those could be formed various phases and more complex structures with multifunctional properties.

In this study, various single alloy target materials with various compositions based on the Zr-Cu amorphous materials have been prepared by powder metallurgy methods such as atomization, mechanical alloying, and Spark Plasma Sintering (SPS). The various nanocomposite coatings could be prepared by using single alloying targets. The most important property is the composition of the target material could be transferred to the coating layers. The properties of as-prepared nanocomposite coatings will be summarized in this present including the coating's performance under conditions that simulate EV drivetrain environments.

9:00am **MC3-3-FrM-4 Corrosive Wear Mechanisms and Corrosion Performance of WC-Reinforced Fe–iN625 Coatings Fabricated by Laser Cladding***, Yiqi Wang [suzyiqi@gmail.com],* Northeastern University, China

Marine components are frequently exposed to seawater, where simultaneous mechanical wear and corrosion significantly reduce service life, highlighting the need for coatings with combined wear and corrosion resistance. In this work, WC-reinforced Fe–IN625 composite coatings with 0–10 wt.% WC were fabricated on ductile iron via laser cladding to enhance hardness, wear resistance, and corrosion–wear performance in marine environments. The novelty of this study lies in quantitatively elucidating the dual role of WC particles as heterogeneous nucleation sites that refine dendritic microstructure and as rigid load-bearing reinforcements that stabilize tribofilms under coupled corrosion–wear conditions.Microstructural analysis revealed W-rich dendrites around WC particles, and increasing WC content to 10 wt.% formed a secondary carbide network, raising surface microhardness from 278 HV (0% WC) to 352 HV (10% WC), a 26.6% increase. Under dry sliding, the friction coefficient decreased from 0.63 (S1) to 0.46 (S3), and wear volume decreased from 35,075 $\times10^{-6}$ cm^3 to 24,756 $\times10^{-6}$ cm^3, a 29% reduction. In 3.5 wt.% NaCl solution, corrosion current density dropped from 3.87×10^{-4} A/cm^2 (S1) to 1.15×10^{-6} A/cm^2 (S3), while polarization resistance increased from 19.67 $k\Omega\cdot cm^2$ to 55.25 $k\Omega\cdot cm^2$, reflecting the formation of a dense protective passive film.In combined corrosion–wear tests, the 10 wt.% WC coating (S3) exhibited a wear rate of 4.14×10^{-4} N^{-1}, markedly lower than 8.25×10^{-4} N^{-1} for the substrate and 5.77×10^{-4} N^{-1} for the WC-free coating (S1), while maintaining a stable friction coefficient around 0.13–0.15. WC particles acted as a rigid skeleton to share applied loads, and Ni–Cr-rich tribofilms reduced adhesion and abrasive damage, synergistically improving corrosion-assisted wear resistance.Overall, the 10 wt.% WC-reinforced coating achieved the highest hardness, lowest dry and corrosive wear, minimal friction fluctuation, and maximal corrosion protection. This study provides a quantitative framework linking WC content, microstructural refinement, and coupled corrosion–wear behavior, offering a design strategy for durable Fe–IN625 coatings in marine and harsh corrosive environments.

9:20am **MC3-3-FrM-5 Effect of Boriding on the Surface Hardness and Wear Resistance of Low Carbon Steel Fabricated by Wire Arc Additive Manufacturing (WAAM)***, Abraham Molina-Sanchez [A01363512@tec.mx], Cesar David Resendiz-Calderon, Leonardo Israel Farfan-Cabrera, Christian Ricardo Cuba-Amesquita,* Tecnológico de Monterrey, Mexico

Wire and Arc Additive Manufacturing (WAAM) enables the production of large-scale, geometrically complex components at a significantly lower cost compared to other additive manufacturing (AM) technologies. It offers extensive material availability, including low-carbon steel, which is widely used in mechanical and structural components. However, due to its low hardness and corrosion resistance compared to other steels, its use is limited in high-demand environments. This study evaluates the effect of boriding on the surface hardness and wear resistance of low-carbon steel fabricated using the WAAM technique. WAAM-built low-carbon steel plates were printed layer by layer to complete 60 layers per sample using ER70S-6 steel wire (0.8 mm diameter). The parameters included a welding voltage of 19.7 V, 67 A current, 5 mm/s travel speed, and a shielding gas of 100% CO_2 supplied at 15 L/min. These samples were subjected to a boriding process wherein a sealed container with Ekabor 2 powder as the boron donor was used, heated at 950°C for 3 hours, and cooled at room temperature. A boride layer with an average thickness of 93.5 ± 32.6 µm composed of FeB and Fe_2B phases was formed, as confirmed by X-ray diffraction (XRD). The adhesion of the boride layer on the as-built (AB) samples was evaluated using a progressive scratch test, and nanoindentation revealed an increase in hardness with no significant changes along the material deposition direction. Dry-sliding tests measured the coefficient of friction (CoF) between AB and borided samples, and a considerable wear volume decrease of 20% was observed with the boride layer, as measured by optical profilometry. These results demonstrate no significant changes along the build direction in phase composition, hardness, or tribological behavior, indicating that boriding is an effective surface treatment for enhancing wear resistance in WAAM-fabricated low-carbon steel.

10:20am **MC3-3-FrM-8 Ultralow Wear, Conductive Plasma-Enhanced Atomic Layer Deposited Metal Nitrides***, Brandon Krick [bkrick@eng.famu.fsu.edu],* Florida State University, USA **INVITED**

Plasma and Vapor Deposition Processes
Room Palm 1-2 - Session PP2-3-FrM

HiPIMS, Pulsed Plasmas, and Energetic Deposition III

Moderators: Arutiun P. Ehiasarian, Sheffield Hallam University, UK, **Tetsushide Shimizu**, Tokyo Metropolitan University, Japan

8:00am **PP2-3-FrM-1 Experiments and Modelling of High Power Impulse Magnetron Sputtering Discharges with Metallic Target***, Jon Tomas Gudmundsson [tumi@hi.is], Kateryna Barynova,* University of Iceland*; Martin Rudolph,* Leibniz Institute of Surface Engineering (IOM), Germany*; Joel Fischer,* Linkoping University, Sweden*; Tetsuhide Shimizu,* Tokyo Metropolitan University, Japan*; Daniel Lundin,* Linkoping University, Sweden

High power impulse magnetron sputtering (HiPIMS) discharges with a number of metal targets have been explored experimentally followed by a further study using the ionization region model (IRM). The metal targets studied include, tungsten [1], chromium [2], zirconium [3], titanium [4], and copper [5]. Experimentally, the ionized flux fraction has been found to be in the range 10 - 80 %, and it is found to increase with increased discharge current density, and decreased working gas pressure. However, the deposition rate generally decreases with increased peak discharge current density. There is a trade off between high ionized flux fraction and high deposition rate, sometimes referred to as the HiPIMS compromise. An overview will be given on the experimental results for various target materials and dependence on varying operating parameters such as peak discharge current density and pulse length. The IRM allows for studying the temporal evolution of the discharge current composition, the electron power absorption mechanisms, the ionization and back-attraction probabilities of the sputtered species, the dominant recycling mechanism, and the working gas rarefaction. We discuss how the discharge current composition varies between different target materials, and how the recycled species, and the processes leading to working gas rarefaction, depend on the target sputter yield [4]. In particular we will discuss how the back-attraction probability of the sputtered species depends on the sputter yield of the target material [7].

[1] Swetha Suresh Babu et al., Plasma Sources Science and Technology, 31(6) (2022) 065009

[2] K. Barynova et al. Plasma Sources Science and Technology, submitted 2025

[3] Swetha Suresh Babu et al., Journal of Vacuum Science and Technology A, 42(4) (2024) 043007

[4] T. Shimizu et al. Plasma Sources Science and Technology, 30(4) (2021) 045006

[5] J. Fischer et al., Plasma Sources Science and Technology, 32(12) (2023) 125006

[6] K. Barynova et al., Plasma Sources Science and Technology, 33(6) (2024) 065010

[7] K. Barynova et al., Plasma Sources Science and Technology, 34(6) (2025) 06LT01

8:20am **PP2-3-FrM-2 Knowing and Controlling the Dynamic Plasma Potential and Sheath Voltage as Key Elements in Plasma-Based Deposition***, André Anders [andre.anders@plasmaengineering.com],* Plasma Engineering LLC, USA **INVITED**

It is widely known that a space charge layer exists between plasma and a surface (target, substrate, wall, probe, etc.) which is called the sheath.The sheath voltage is the difference between the surface potential and the potential at the sheath edge, the boundary between plasma and sheath. Space charge is linked via the Poisson equation to an electric field which governs fluxes of charged fluxes and thereby energy delivered to the surface.There is nothing new so far, but in real life, for practical reasons, one uses (earth) ground as the reference, not the plasma potential.This can lead to confusion, especially as the plasma potential is not constant in space and time when using modern approaches to plasma-based deposition that involves magnetic fields and pulsed processing, such as bipolar HiPIMS.In this contribution, the establishment of plasma potential, or better the dynamic plasma potential distribution, will be explored and the consequences for film growth discussed.The local and dynamic plasma potential can be associated with numerous effects such cathode spot and anode spot formation (a.k.a. "arcing" and "fireball" in magnetron systems, respectively), the control of ion and electron flows, which affect a growing film's microstructure, and also with unwanted effects such as sputtering of and arcing on chamber walls and other grounded components.Knowing and controlling the dynamic plasma potential and sheath voltage is therefore important to plasma-based deposition processes.

9:20am **PP2-3-FrM-5 Superposition of HiPIMS with RF on a Single Magnetron: Generation of High Ion Energies***,* ***Caroline Adam [c.adam@physik.uni-kiel.de]****, Luka Hansen, Tobias Hahn, Jessica Niemann, Daniel Zuhayra,* Kiel University, Germany*; Günter Mark, Jonathan Löffler,* MELEC GmbH, Germany*; Jan Benedikt, Holger Kersten,* Kiel University, Germany

High power impulse magnetron sputtering (HiPIMS) has shown significant potential for thin film deposition by providing high ionized flux fractions and ion energies. To optimize the deposition process, HiPIMS can be operated in superposition with an additional discharge on the same magnetron, such as DC or MF (mid-frequency pulses). This increases the deposition rate and enables low-pressure operation by using pre-ionization from the continuous discharge during the off-time between pulses.

In this study, a novel combination of HiPIMS and RF (radio-frequency, 13.56 MHz) is investigated in continuous superposition on the same magnetron, using a planar copper target in argon atmosphere [1]. The discharge is characterized at varied power ratios of HiPIMS and RF with plasma diagnostics employed to analyze the system. This includes measuring the combined HiPIMS/RF voltage signal and conducting optical emission spectroscopy (OES) to gain insights into the plasma composition. Two key factors influencing the microstructure of deposited films are the kinetic energy of particles bombarding the growing film and the substrate temperature. Substrate heating from the plasma is evaluated using a passive thermal probe (PTP) [2], a "non-conventional" calorimetric diagnostic that measures the total energy flux to the substrate surface. The kinetic energy is assessed through energy-selective mass spectrometry, including time-resolved operation. The results regarding the plasma parameters are compared with the morphology of the deposited copper films, analyzed using scanning electron microscopy (SEM).

The addition of an RF plasma provides pre-ionization for the HiPIMS pulses, which allows to reduce the process pressure. Time-resolved OES reveals the transition from the copper-dominated emission during the HiPIMS pulse to an argon plasma in in the HiPIMS off-time. The RF plasma exhibits a pronounced influence on the ion energy distribution, increasing the ion energy by more than 50 eV depending on the applied RF power. This effect is attributed to an increased plasma potential caused by the RF sheath, which accelerates ions in the sheath region toward the substrate, resulting in elevated ion energies. The potential of this process is demonstrated by the deposition of copper thin films, showing significant influence of the deposition mode for their properties [1].

[1] C. Adam *et al. Surf. Coat. Technol.* **520** (2026) 133060.

[2] H. Kersten *et al. Thin Solid Films* **377–378** (2000) 585–591.

9:40am **PP2-3-FrM-6 Low-Temperature Synthesis of Ti_2AC (A = Si or Ge) Max-Based Coatings via Highly Ionized Growth Techniques***,* *Arno Gitschthaler, Philipp Dörflinger, Rainer Hahn,* Christian Doppler Laboratory for Surface Engineering of high-performance Components, TU Wien, Austria*; Jürgen Ramm, Klaus Böbel,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; Szilard Kolozsvári, Peter Polcik,* Plansee Composite Materials GmbH, Germany*; Eleni Ntemou, Daniel Primetzhofer,* Department of Physics and Astronomy, Uppsala University, Sweden*; Dominik Fuchs, Andreas Limbeck,* Institute of Chemical Technologies and Analytics, TU Wien, Austria*; Peter Švec,* Institute of Physics, Slovak Academy of Sciences, Slovakia*; Anton Davydok, Christina Krywka,* Institute of Materials Physics, Helmholtz Zentrum Hereon, Germany*;* ***Helmut Riedl [helmut.riedl@tuwien.ac.at]****,* Institute of Materials Science and Technology, TU Wien, Austria

MAX phases are a unique class of nanolaminated compounds that combine metallic and ceramic properties, offering excellent electrical and thermal conductivity together with remarkable resistance to creep, oxidation, and corrosion. These characteristics make them highly attractive as protective and functional coatings for next-generation hydrogen technologies. However, conventional sputtering techniques struggle to provide suitable growth conditions at reduced synthesis temperatures, often leading to phase instability and the formation of competing phases. Despite more than two decades of research on Ti–A–C (A = Si or Ge) MAX coatings [1,2], it has yet to be achieved to deposit them under less harsh, more practical conditions. To address this issue, Ti_2-A-C (A = Si or Ge) thin films were deposited by cathodic arc evaporation (CAE) and high-power impulse magnetron sputtering (HiPIMS) of metallic TiA (A = Si or Ge) targets in reactive Ar/C_2H_2 plasma atmospheres. To understand the relationship between deposition parameters, chemical composition, and phase formation, the resulting films were comprehensively characterized using high-resolution techniques, including ToF-ERDA-calibrated GD-OES, 2D-BBXRD, and t-CSXRD measurements. Subsequently, these results are correlated with application near electrochemical tests. Overall, these analyses demonstrate, for the first time, that Ti_2-A-C MAX-based coatings can be successfully synthesized by reactive CAE and HIPIMS at temperatures as low as 550 °C and rise their potential for use cases in hydrogen technologies.

[1] Emmerlich J, Palmquist J-P, Högberg H, Molina-Aldareguia JM, Hultman L. Growth of Ti3SiC2 Thin Films by Elemental Target Magnetron Sputtering. J Appl Phys. 2004;96: 4817. doi:10.1063/1.1790571

[2] Högberg H, Eklund P, Emmerlich J, Birch J, Hultman L. Epitaxial Ti2GeC, Ti3GeC2, and Ti4GeC3 MAX-phase thin films grown by magnetron sputtering. J Mater Res. 2005;20: 779–782. doi:10.1557/JMR.2005.0105

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