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.

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 $1\text{x}10^{-5}$ 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

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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.

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.

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]

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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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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.

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.

References:

[1] Nature Communications (2025) 16:4719

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.

[1] D. Nikitin et al., Plasma Processes Polym. **18** (2021) 2100068.

[2] H. Kersten et al. Thin Solid Films **377–378** (2000) 585–591.

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}, $n \geq 2$) 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 ($0 \le x \le 0.3$) 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.

Acknowledgment

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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.

[1] M. J. Sowa, Y. Yemane. et al. JVST A 34, 051516 (2016)

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[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.

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

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[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.

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