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≤x≤0.3) were prepared to evaluate etch selectivity, defined as the etch-rate ratio between amorphous and crystalline films. Experiments were conducted using H_2 and N_2 as the carrier gases within the temperature range of 375 to 500℃. The behavior of B-doped SiGe and P-doped Si films was compared with those of undoped films. Scanning electron microscopy and spectroscopic ellipsometry were employed to measure film thickness. Atomic force microscopy and high resolution-transmission electron microscopy were utilized to examine the surface morphology and microstructure of etched films, respectively. We performed surface analysis after the reaction with $GeBr_4$ using time-of-flight secondary ion mass spectrometry (ToF-SIMS). Additional density functional theory simulations were performed to elucidate the origin of the observed behavior of $GeBr_4$.

$GeBr_4$ exhibited a substantially higher etch rate than pure Cl_2, particularly at low Ge contents. B-doped films showed reduced etch rates compared with undoped films, whereas P-doped Si demonstrated a significantly enhanced etch rate. These findings provide insight into the SEG behavior of dopant-incorporated Si films and offer a foundation for predicting growth characteristics under low-temperature conditions.

PP-ThP-15 Thickness-Dependent Electrical Properties of MoN Films Grown by Thermal ALD Using MoO_2Cl_2, ***So Young Kim [skim544@yonsei.ac.kr]***, Yonsei University, Republic of Korea*; Tai-su Park,* Justem Corporation Ltd., Republic of Korea*; Dae-Hong Ko,* Yonsei University, Republic of Korea

Molybdenum (Mo) has emerged as a promising candidate for next-generation contact and interconnect applications due to its favorable electrical properties and scalability. Similarly, molybdenum nitride (MoN), which can function as a seed layer, diffusion barrier, or electrode material, has attracted significant attention for advanced microelectronic applications owing to its high electrical conductivity and chemical stability. Although MoN deposition by atomic layer deposition (ALD) has been widely explored using halide and organometallic precursors, MoO_2Cl_2 has not been reported for MoN thin-film growth, and its ALD growth characteristics for MoN remain unexplored.

In this work, MoN thin films were deposited by thermal ALD at 600 ℃ using MoO_2Cl_2 as the metal precursor and NH_3 as the co-reactant. Film thickness was systematically varied by adjusting the number of ALD cycles to investigate the evolution of structural, chemical, and electrical properties as a function of thickness. The deposited films were characterized by X-ray diffraction, X-ray photoelectron spectroscopy, and transmission electron microscopy to analyze phase formation, bonding states, and microstructural development, along with electrical resistivity and surface roughness measurements. The thickness dependence of the electrical properties and microstructural evolution of the MoN films were systematically analyzed. This study establishes MoO_2Cl_2 as a viable precursor for thermal ALD of MoN, providing quantitative insights into thickness-dependent electrical properties governed by microstructural evolution and a fundamental baseline for future process optimization, including plasma-assisted or hybrid ALD approaches, to improve early-stage electrical performance.

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.

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[2] Park, H., Kim, T., Cho, S. et al.Sci Rep 7, 40091 (2017)

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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.

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