Topical Symposium on Sustainable Surface Engineering
Room Town & Country B - Session TS1-1-MoM

Coatings for Batteries and Hydrogen Applications I

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

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

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

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

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

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

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

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

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

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

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

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

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[1] **Graduate Student Award Finalist**

findings underscore that hydrogen permeation resistance can be maximized either by coherent interface stabilization or by amorphous/crystalline alternation, highlighting interface engineering and microstructural control as decisive design principles for next-generation energy technologies.

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

Coatings for Batteries and Hydrogen Applications II

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Keywords: High entropy alloy thin films, Hydrogen evolution reaction, FeNi$_x$MoWCu, electrocatalytic property

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

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

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

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

In this contribution, we present a study of the Mg-Co-Ni-Cu-Zn-O system, crystallizing in a rock salt-type (MgCoNiCuZn)O structure, and Cr–Mn–Fe–Ni–Cu–O system, crystallizing in a spinel-type (CrMnFeNiCu)$_3$O$_4$ structure. While the first system represents a “conservative” choice close to current materials used in batteries, the second is entirely free of critical raw materials while offering the potential for improved electrochemical performance and long-term stability, aligning with the vision of sustainable and circular energy storage technologies. The thin films are deposited by reactive DC and High Power Impulse Magnetron Sputtering (HiPIMS), allowing precise control of elemental composition and plasma energy input. The influence of deposition temperature, stoichiometry, and process parameters on the morphology and crystalline structure of the as-deposited coatings is systematically investigated.

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

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

Circular Strategies for Surface Engineering

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Coatings and Surfaces for Renewable Energy Technology I

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

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

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

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

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

[1] E.Dimaggio, A.Masci, A. De Seta, M.Salleras, L.Fonseca, G.Pennelli, *On-chip Thermoelectric Devices Based on Standard Silicon Processing*, **Small** 2405411, 2024

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

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

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

Topical Symposium on Sustainable Surface Engineering
Room Town & Country D - Session TS2-2-ThM

Coatings and Surfaces for Renewable Energy Technology II

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

8:00am **TS2-2-ThM-1 Energy-Efficient Hydrogen Production via Urea-Assisted Electrolysis Enabled by Linker-Engineered NiCo MOFs**, ***Thi Xuyen Nguyen [nguyenxuyen1511@gmail.com]***, *Hui-Chuan Chen, Jyh-Ming Ting,* National Cheng Kung University, Taiwan **INVITED**

Hydrogen (H_2) is widely recognized as a promising sustainable energy carrier for addressing the global energy crisis and achieving the net-zero carbon emission target. Among the various H_2 production strategies, urea-assisted electrochemical water splitting offers an energy-efficient route for H_2 production; however, the inherently sluggish six-electron urea oxidation reaction requires highly active electrocatalysts. Herein, we report a linker-engineering strategy in which the benzene dicarboxylate (BDC) linker of a NiCo-BDC metal-organic framework (MOF) is partially replaced by a redox-active dicarboxylferrocene (DFc) ligand to construct NiCo-MOF-DFc. The strongly coordinated DFc linker effectively modulates the electronic structure, enriching Ni^{3+} species, generating abundant oxygen vacancies, and inducing coordination asymmetry, thereby markedly enhancing urea oxidation activity. The NiCo-MOF-DFc catalyst delivers 100 mA cm^{-2} at a low potential of 1.33 V with excellent durability. Operando characterizations reveal that DFc facilitates rapid electron transfer, accelerates the transformation of the MOF into the catalytically active metal (oxy)hydroxide phase, and stabilizes the active sites. Density functional theory calculations further demonstrate that DFc weakens CO_2 adsorption and lowers the energy barrier of the rate-determining desorption step. An anion exchange membrane electrolyzer employing NiCo-MOF-DFc as the anode achieves 1000 mA cm^{-2} at a low cell voltage of 1.83 V and sustains stable operation for 500 h. Notably, the system requires only 48.6 kWh to produce 1 kg of H_2, representing over 10% lower energy consumption than conventional OER-based electrolysis, highlighting its strong potential for energy-efficient hydrogen production.

9:00am **TS2-2-ThM-4 Optimization of Tunable Interfacial Engineering in WOx/α-Fe_2O_3 Heterostructures via Dc Magnetron Sputtering for Enhanced PEC Activity and Carrier Transport Efficiency**, ***Carlos Gomes [c.e.gomes@ifsp.edu.br]***, *Mariane Murase Murase, Matheus Torres, Douglas Leite, Rodrigo Pessoa, Argemiro Sobrinho, André Pereira,* Instituto Tecnológico de Aeronáutica, Brazil

Transition metal oxide heterostructures are crucial for advancing sustainable energy technologies, demanding precise control over interfacial charge dynamics and long-term chemical stability. This work presents a systematic study on the fabrication and optimization of an Iron Oxide (α-Fe_2O_3) a visible-light absorber heterojunction with a Tungsten Oxide (WO_x) as an electron-transport layer, serving as a band alignment at the interface. Junction formation is a powerful strategy to overcome intrinsic limitations like poor charge transport and high surface recombination in semiconductors [1]. The staggered band alignment creates an internal electric field that promotes efficient separation of photogenerated electron(e^-)/hole(h^+) pairs and facilitates electron extraction, significantly reducing surface charge recombination [1,2].

The structures were fabricated using scalable DC Magnetron Sputtering, depositing the α-Fe_2O_3 layer over FTO glass (SnO_2/F) followed by the WO_x transport layer. The study investigates tunable surface engineering by systematically varying the WO_x deposition time to precisely control the layer's thickness and potentially its stoichiometry (WO_{3-x}), thereby modulating the electronic band alignment and transport efficacy.

Comprehensive characterization, including XRD, SEM, EIS, and CV, was employed to correlate layer thickness with interfacial structure. Analysis confirmed WO_x crystallization at 550°C, showing a direct relationship between peak intensity and deposition time. Deposition of an optimal WO_x layer enhanced Fe_2O_3 optical modulation, resulting in a 15% lower visible transmittance minimum (at ≈ 600 nm).

Functional performance such as stability and charge transfer dynamics was assessed, revealing that the WO_x (180s) sample's highest carrier number and lowest flat band voltage directly correlate with superior electrochemical performance (Specific Power under light and Specific Energy in the dark), suggesting that the improved electronic structure drives enhanced charge storage and transfer capabilities.

This research presents valuable insights into controlled thin film deposition and advanced surface engineering of robust oxide structures. These findings support the development of next-generation photoelectrochemical cells (PEC) for water splitting.

Keywords: WOx/α-Fe_2O_3, Heterojunction, DC Magnetron Sputtering, Thin Film Deposition, Advanced Surface Engineering.

[1] N. Al-Aisaee et al., *Solar Energy Materials and Solar Cells*, 263 (2023).

[2] B. Liu et al., (Review article on heterojunctions and charge separation mechanisms) (2025).

9:20am **TS2-2-ThM-5 Thermal Treatment Effects on the Structural and Optoelectronic Properties of Nb2O5 Thin Films Deposited by DC Magnetron Sputtering**, *Rodrigo Prado Medeiros Leite da Silva, Natali da Silva Barbosa, Bianca Sartori,* Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Brazil*; Lucas Diniz Araujo,* Aeronautics Institute of Technology (ITA), Brazil*; Carlos Eduardo Gomes,* Instituto Federal de Educação, Ciência e Tecnologia de São Paulo, Brazil*; Filipe Caldatto Dalan, André Luis de Jesus Pereira,* ***Argemiro Soares da SIlva Sobrinho [argemiro@ita.br]***, Aeronautics Institute of Technology (ITA), Brazil

The development of efficient semiconductor oxides for solar-driven energy conversion is a key step toward achieving a sustainable hydrogen economy. Transition-metal oxides such as TiO_2, WO_3, and Nb_2O_5 have emerged as promising photoactive materials due to their chemical stability and suitable band-edge alignment for photoelectrochemical (PEC) water splitting. Among them, niobium pentoxide (Nb_2O_5) is particularly attractive for its abundance, low toxicity, and tunable optoelectronic properties associated with oxygen-vacancy engineering. Understanding how deposition and post-treatment conditions affect its structure and charge-transport characteristics is therefore essential for optimizing its functional performance. In this work, Nb_2O_5 thin films were deposited by DC magnetron sputtering onto Si, glass, and FTO substrates and subsequently annealed at 300 °C, 400 °C, 500 °C, and 600 °C for eight hours under two controlled atmospheres: air at atmospheric pressure and vacuum (~10^{-2} Torr). The films were characterized by X-ray diffraction, Raman spectroscopy, UV–Vis transmittance, and electrochemical techniques to evaluate the influence of temperature and ambient on crystallization, defect formation, and electronic behavior. Structural analyses revealed a transition from amorphous to orthorhombic (Pbam) Nb_2O_5 above 500 °C, while vacuum-treated samples exhibited more pronounced oxygen-vacancy-related Raman features and a narrower optical band gap. Electrical impedance and cyclic-voltammetry results indicated reduced charge-transfer resistance for oxygen-deficient films, evidencing the beneficial role of substoichiometry in enhancing carrier mobility. These results demonstrate that both annealing temperature and atmosphere strongly modulate the structural and optoelectronic properties of sputtered Nb_2O_5, providing valuable guidelines for tailoring its performance in PEC and photocatalytic applications.

10:20am **TS2-2-ThM-8 Interface-Driven Evolution and Electrochemical Behavior of CuO/WO_X Heterostructures Deposited by Magnetron Sputtering**, *Rafael Leal, Giovana Fazenda, Helen Barros, David Graves, Filipe Dalan, Mariane Murase, Marcilene Gomes,* Aeronautics Institute of Technology (ITA), Brazil*; Douglas Leite,* Aeronautics Institute of Technology, Brazil*; Argemiro Silva-Sobrinho,* ***André Pereira [andreljp@ita.br]***, Aeronautics Institute of Technology (ITA), Brazil

Heterostructures composed of copper and tungsten oxides have drawn increasing attention for solar-driven photoelectrochemical (PEC) hydrogen generation due to their complementary optical and electronic properties [1]. The interface between p-type CuO and n-type WO_x plays a critical role in charge separation and carrier transport; however, its efficiency strongly depends on the structural order and chemical composition of the WO_x layer [1,2]. In this work, CuO/WO_x heterostructures were fabricated entirely by DC magnetron sputtering. CuO films were first deposited onto FTO substrates and annealed at 450 °C for 2 h to promote crystallization and improve adhesion. WO_x overlayers were then deposited for 1, 5, and 10 min, followed by post-annealing at 450 °C for 2 h to obtain crystalline layers; as-deposited samples were kept amorphous. The WO_x layer thickness, determined by profilometry and ellipsometric modeling, increased linearly with deposition time (~15 nm min^{-1}), while the refractive index was slightly higher for crystalline samples, indicating greater density and lower porosity. Structural and vibrational analyses revealed distinct interface behaviors. For crystalline WO_x layers, Raman and XRD showed that samples with 5 and 10 min deposition underwent interdiffusion at the interface, forming $CuWO_4$, whereas the 1 min sample exhibited a substoichiometric WO_x layer. In contrast, amorphous WO_x overlayers preserved only CuO peaks. Electrochemical measurements confirmed the correlation between structure and functionality. Cyclic voltammetry and impedance spectroscopy revealed that crystalline samples containing $CuWO_4$ exhibit lower charge-transfer resistance and higher photocurrent under illumination, while amorphous heterostructures display slower carrier dynamics and greater capacitive behavior. The electrochemically active surface area (ECSA), estimated from non-faradaic capacitive current, was significantly larger for crystalline samples, particularly those with $CuWO_4$, indicating an increased density of electroactive sites and enhanced charge accumulation capability. Overall, the controlled formation of $CuWO_4$ or substoichiometric WO_x interlayers offers a promising strategy to improve PEC efficiency and long-term stability of CuO-based photoelectrodes for sustainable hydrogen generation.

Acknowledgments
We acknowledge the financial support from FAPESP (Grant No. 2022/02994-2) and CNPq (Grant No. 302823/2025-5).

[1] X. Wen et al., ACS Appl. Nano Mater. 7 (2024) 14936–14945. DOI: 10.1021/acsanm.4c00769.

[2] M. Castaneda Mendoza et al., Materials 18 (2025) 2896. DOI: 10.3390/ma18122896.

10:40am **TS2-2-ThM-9 Unlocking the Potential of Medium-Entropy Prussian Blue for Superior Electro-Fenton Oxidation***, **Sheng-Wei Lin [alec97622964@gmail.com]**, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Electro-assisted advanced oxidation processes, such as the electro-Fenton (EF) process, are gaining intensive attention recently. This work investigates the application of a medium-entropy Prussian blue analogue (designated as 3M-PBA) as a heterogeneous EF catalyst for the removal of organic pollutants from water. EF process can overcome the drawbacks of conventional Fenton process, such as the limited pH range and poor reusability. In this work, the 3M-PBA catalyst further enhances the EF performance by providing multiple redox-active sites, which accelerate electron transfer and improve structural stability during operation.

The phase, morphology, oxidation state, charge-transfer behaviour, hydroxyl-radical generation efficiency, and EF degradation performance were characterized using several techniques. UV-Vis spectroscopy analysis shows a continuous decrease in the characteristic TC absorption peak at 357 nm with time, confirming the molecular breakdown. The 3M-PBA catalyst achieves a high TC removal within a short time under an applied potential (0.6 V vs. Ag/AgCl). Iron leaching remains below 0.4 ppm throughout the five cycles, indicating strong structural integrity and environmental safety.

Keywords: electro-Fenton, high-entropy PBA, charge transfer, catalyst stability, wastewater treatment

11:00am **TS2-2-ThM-10 Non-Precious Metal Phosphide/Sulfide Heterostructure Electrocatalyst for SOR***, **Jian-An Wu [tommy772222@gmail.com]**, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

With the increasing discharge of wastewater containing sulfur compounds from various industries, the need for efficient sulfur removal and recovery is becoming more urgent. The Sulfion Oxidation Reaction (SOR), which converts sulfide ions (S^{2-}) into elemental sulfur (S_8), which is common for industrial use. Unlike the conventional oxygen evolution reaction (OER), which is thermodynamically challenging and energy-consuming, SOR operates at a much lower potential (-0.48 V vs. RHE), making it a more energy-efficient alternative for sulfur oxidation. Furthermore, the added economic value makes SOR an attractive option for wastewater treatment, as it reduces the need for costly disposal methods while turning a pollutant into a resource.

Herein, we have synthesized a non-precious metal phosphide/sulfide heterostructure catalyst with conductive backbone and abundant active site on the surface. The catalyst demonstrates an exceptional SOR performance in 1M KOH with 1M Na_2S, achieving a low potential of 0.278V at 100 mA cm^{-2} and 0.368V at 300 mA cm^{-2}, and a lower onset potential.

Keywords:Sulfion Oxidation Reaction (SOR), transition-metal based catalyst, heterostructure

11:20am **TS2-2-ThM-11 Defect-Engineered Copper-Based Materials for Electrocatalytic Nitrate Reduction***, **Ting- Chun Hung [jim8965976@gmail.com]**, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Electrochemical nitrate reduction reaction (NO_3RR) has emerged as a promising strategy for simultaneously addressing nitrate pollution and producing valuable ammonia via a carbon-free process. Ammonia is an important chemical feedstock, widely used in fertilizer production, and offers advantages such as an alternative energy source for replacing hydrogen due to its ease of storage and transport.

For NO_3RR, copper-based materials are known to be highly active catalysts by facilitating the conversion of nitrate (NO_3^-) to nitrite (NO_2^-), which is the rate-determining step. In this study, novel Cu-based heterostructure nanosheets rich in oxygen vacancies (Ov) were investigated as an effective electrocatalyst for NO_3RR. The catalyst was synthesized via a hydrothermal method, followed by chemical reduction for controlled creation of Ov. The catalyst exhibits excellent NO_3RR performance, achieving a Faradaic efficiency of ~95% at -0.2 V vs. RHE, a high ammonia yield rate of 0.92 mmol h^{-1} cm^{-2}, and outstanding stability over 1000 hours, demonstrating both superior activity and long-term durability. Density functional theory calculation was performed to support the experimental data.

Keyword: Electrochemical nitrate reduction, heterostructures, oxygen vacancy, high ammonia yield rate

Topical Symposium on Sustainable Surface Engineering
Room Town & Country A - Session TS1-ThP

Coatings for Batteries and Hydrogen Applications Poster Session

TS1-ThP-1 Hydrogen Permeation Testing: Electrochemical vs. Pressurized Methods, ***Phillip Rückeshäuser [phillip.rueckeshaeuser@tuwien.ac.at]***, TU Wien, Austria; *Szilard Kolozsvari, Peter Polcik,* Plansee Composite Materials GmbH, Germany; *Timea Stelzig,* Oerlikon AM Europe GmbH, Germany; *Konrad Fadenberger,* Oerlikon Balzers Coating Germany GmbH, Germany; *Klaus Boebel,* Oerlikon Balzers, Liechtenstein; *Tomasz Wojcik, Helmut Riedl,* TU Wien, Austria

The interactions between hydrogen and materials are subjects of significant interest in both research and industry. Consequently, the hydrogen charging of samples and following detection are crucial aspects of this field. Currently, there are two primary methods for hydrogen charging: electrochemical charging and pressurized hydrogen charging.

In electrochemical charging, atomic hydrogen is produced through the dissociation of water, while in pressurized charging, hydrogen is introduced in gaseous form and subsequently thermally dissociated. Although these two methods are based on fundamentally different principles, they ultimately achieve the same goal: the absorption and permeation of atomic hydrogen in the sample. However, most studies tend to focus on either one method or the other. Thus, it becomes essential to explore the correlation between these methods and identify equivalent charging conditions for specific hydrogen permeation characteristics.

In this study, we conducted hydrogen permeation tests using both electrochemical and pressurized setups. We applied nitride coatings such as TiN and CrN to steel substrates using physical vapor deposition (PVD) techniques and compared the permeation performance of the two charging methods. This comparison involved determining key parameters such as diffusion coefficients and permeation reduction factors. Additionally, we characterized the coating properties using secondary electron microscopy, X-ray diffraction, and linear sweep voltammetry.

TS1-ThP-2 Towards Defect-Free Laser-Induced Graphene Coating on Copper and Aluminum Foils for Anode-Free Li and Na Metal Batteries, ***Aarti Gunjal [aartitambe22@gmail.com]***, IISER PUNE, India; *Suparna Saha,* TCG-CREST Kolkata, India; *Swati Jadhav,* IISER PUNE, India; *Satishchandra Ogale,* TCG-CREST Kolkatta, India

Laser-induced graphene (LIG) is a very well-established process for realizing functional carbon coatings on different substrates. Depending on the laser processing parameters it yields structurally, morphologically and chemically interesting forms which are also adherent because of the thermal energy input. In most cases, however, a defect band (D band) is invariably observed in the Raman spectrum of such coatings, in addition to the so-called G-band corresponding to desired graphitic carbon. In this work we have applied CO2 laser processing to carbonize the coatings of the dried powder of aromatic eucalyptus (EU) leaves on metals. The effects of laser power density, scanning speed, substrate choice, and precursor coating thickness on the quality of carbon are carefully examined and optimized to obtain a unique almost defect-free few layers graphene coating, as reflected by a miniscule D-band and a significant 2D signature in the Raman spectra of few-layer graphene. Comparative studies on other aromatic leaves sample (e.g. lemon grass) and non-aromatic leaves suggest that aromaticity is important for realizing an enhanced 2D band, which could be due to internal turbulent cavitation upon laser-induced transient heating. In situ nitrogen doping is also achieved by applying the LIG process to a mixture of EU powder loaded with urea. Remarkably, the nitrogen incorporated coatings on copper and aluminum current collectors render far superior performance in anode-free Li and Na metal batteries, respectively, as against the defect-free few layers graphene coating. In fact, half cells with alkali metals show an impressive cycling stability of over 450 cycles for both Li and Na. Through thorough characterizations employing multiple techniques, an attempt is made to develop a mechanistic understanding of the issues involved.

TS1-ThP-3 HiPIMS Mo_xN and Cu-Mo_xN Thin Films for the Hydrogen Evolution Reaction, *Hung-I Wu,* Department of Electronic Engineering, National Yunlin University of Science and Technology, Taiwan; *Ying-Hsiang Lin,* Department of Materials Science and Engineering, National United University, Taiwan; *Shih-Hung Lin,* Department of Electronic Engineering, National Yunlin University of Science and Technology, Taiwan; *Fan-Bean Wu, Chi-Yueh Chang,* Department of Materials Science and Engineering, National United University, Taiwan; *Thi Xuyen Nguyen, Ruei-Chi Lin, Jyh-Ming Ting,* Department of Materials Science and Engineering, National Cheng Kung University, Taiwan; ***Wan-Yu Wu [wywu@nuu.edu.tw]***, Department of Materials Science and Engineering, National United University, Taiwan

Hydrogen produced by water electrolysis is a promising clean energy carrier, yet large-scale deployment is hindered by the high cost and limited durability of noble-metal catalysts. Transition-metal nitrides, particularly molybdenum nitride (Mo_xN), offer attractive corrosion resistance and electrical conductivity, enabling hydrogen evolution reaction (HER) catalysis in both acidic and alkaline media.

In this work, Mo_xN thin films were deposited and benchmarked using RF sputtering and high-power impulse magnetron sputtering (HiPIMS). In 0.5 M H_2SO_4, the HiPIMS-Mo_xN catalyst achieved an overpotential of 292 mV, corresponding to a ~61.2% improvement compared with pristine carbon paper (CP). The performance gain is attributed to the superior film adhesion achieved by HiPIMS, leading to a 9.7% reduction in charge-transfer resistance (R_{ct}) and the absence of large-area catalyst delamination after HER testing. Process optimization identified Cu addition is suggested to tune the Mo d-band center and improve overall conductivity, reducing the overpotential to 254 mV (~13.0% improvement vs. HiPIMS-Mo_xN) and decreasing the Tafel slope from 75.9 to 55.0 mVdec^{-1}, indicating accelerated HER kinetics via a synergistic effect. In 1.0 M KOH, HiPIMS-Mo_xN achieved the lowest overpotential (199 mV), while Cu addition deteriorated activity, suggesting Mo as the dominant active center in alkaline media and that secondary metals reduce accessible Mo sites.

TS1-ThP-4 Hydrogen Barrier Properties of Thin Oxide Films Prepared by Different Methods: Correlations of Thin Film Properties with Hydrogen Permeation Rates, *Dmitry Kalanov, Juergen W. Gerlach, Patrick C. With,* ***Yeliz Unutulmazsoy [yeliz.unutulmazsoy@iom-leipzig.de]***, *Ulrike Helmstedt,* Leibniz Inst. of Surface Eng. (IOM), Germany

Efficient hydrogen barriers are essential for the hydrogen economy, where minimizing hydrogen loss and ensuring material safety are critical. In the present study, we investigate thin oxide films, using TiO_2 as a model oxide system, deposited on PET substrates by UV photochemical conversion of metalorganic precursors under ambient conditions and by High-Power Impulse Magnetron Sputtering (HiPIMS) deposition without substrate heating. Using a dedicated gas-permeation measurement system, hydrogen permeation through the oxide films on PET was studied as a function of film thickness. Results demonstrate a strong thickness dependence of the barrier properties: 50 nm TiO_2 films exhibit a fivefold improvement, while increasing the thickness to 70 nm for HiPIMS grown thin films reduces permeation below the detection limit, highlighting the high barrier performance of dense, amorphous TiO_2 films. These findings are discussed in the context of current challenges in measuring hydrogen permeation in thin films on various substrates, compared to other oxide systems such as SiO_x [1], and in relation to differences in structural properties of the films arising from the distinct deposition methods.

[1] P.C. With, T. Pröhl, J.W. Gerlach, A. Prager, A. Konrad, F. Arena, U. Helmstedt, Hydrogen permeation through uniaxially strained SiO_x barrier thin films photochemically prepared on PET foil substrates,
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