

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 für 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 $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (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. $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) is one of the oxide-based electrolyte materials and was developed in our previous investigation. After sintering at 1100°C 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°C 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°C . 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°C 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, Arditia 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 $\Gamma_{\text{Si-B-C-N-O/TiN}} = 2:3$ multilayer reached PRF values of ~ 5300 by embedding crystalline TiN within amorphous Si–B–C–N–O layers, yielding a dense, columnar-free architecture without continuous diffusion channels. These

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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.

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