Topical Symposia
Room Town & Country A - Session TS1-1-MoM
Coatings for Energy Storage and Conversion - Batteries and Hydrogen Applications I

Moderators: Dr. Nazlim Bagcivan, Schaeffler Technologies GmbH & Co. KG, Germany, **Klaus Böbel**, Bosch Manufacturing Solutions, Germany

10:00am **TS1-1-MoM-1 The Effect of Microstructure on the Hydrogen Storage Capacity of Ti_xZr_{1-x} Thin Films***, **Ido Zukerman**, M. Buzaglo,* Divison of Chemistry, NRCN, Israel*; S. Hayun,* Department of Materials Engineering, Ben Gurion University of the Negev, Israel

Metal hydrides (MH_x) provide a promising solution for a future hydrogen-based energy system due to their high hydrogen storage density and safety advantages compared to compressed or liquefied hydrogen. Thin films were proposed to ease the absorption/desorption cycles by maximizing the surface-to-volume ratio. In this study, we suggest controlling the macro- and micro- structure of Ti_xZr_{1-x} thin films, in order to reduce the absorption/desorption temperature and to increase the rate and absorbed hydrogen volume. To achieve this goal, a series of Ti_xZr_{1-x} thin films were deposited using pulsed-DC magnetron co-sputtering technique. Low sputtering power, high working pressure, or floating bias conditions resulted in an open columnar structure (i.e., zone 1 microstructure). High negative bias (< -150 V), however, promoted a dense columnar structure (i.e., zone T microstructure). The thin film's hydrogenation was conducted as follows: The samples were held at 623 K under vacuum ($< 5x10^{-3}$ Pa) for 1 hr for surface activation, then the chamber was filled with pure hydrogen to $2.0±0.1x10^4$ Pa and cooled to room temperature. The samples were held under H_2 for additional 24 hours at room temperature. Temperature-Programmed Desorption (TPD), Glow Discharge Spectroscopy (GDS), and electron microscopy were used to study the microstructure of the films, hydrogen storage capacity, desorption temperature, and the durability for multiple absorption/desorption cycles.

10:20am **TS1-1-MoM-2 Transition Metal – Doped Ni/YSZ Anode Functional Layers for Solid Oxide Fuel Cells Produced via Magnetron Sputtering***, K. Steier,* Manchester Metropolitan University, UK*; I. Jang, A. Hankin,* Imperial College London, UK*; P. Kelly, **Justyna Kulczyk-Malecka**,* Manchester Metropolitan University, UK

Solid oxide fuel cells (SOFCs) convert the chemical energy stored in fuels, such as hydrogen and gaseous hydrocarbons, directly into electrical power and thermal energy through electrochemical reactions. State-of-the-art SOFC anodes consist of a cermet of nickel and yttria-stabilised zirconia (YSZ) to increase the reactive sites at the anode/electrolyte interface, generating so-called triple-phase boundaries. The quantity of triple-phase boundaries in nanostructured materials increases through finer particle sizes, resulting in enhanced performance. For that reason, the magnetron sputtering technique, which offers elemental distribution at the nanoscale, high deposition rates, reproducibility, scalability and excellent uniformity over large-area substrates has been chosen as the deposition method to fabricate anode functional layers (AFLs) for SOFCs.

Nanostructured NiO-YSZ thin films have been previously produced by reactive pulsed DC magnetron co-sputtering of metallic targets of zirconium-yttrium and nickel, defining the optimal deposition parameters to create state-of the-art AFLs. Based on recent studies, the future of oxide-based anode materials for SOFCs will greatly focus on reducing Ni catalyst content through alternative non-precious metal doping and increasing the cell performance by tailoring the microstructure of the AFL. This would allow Ni coarsening to be mitigated and maintain the nanostructure over the lifetime of the cell. Therefore, in this study complex transition metal oxides, such as vanadium, tantalum or manganese oxides, were doped into SOFC anodes to study their influence on the structural and morphological properties of magnetron sputtered AFLs. The effect of the dopant's concentration on the properties of Ni-YSZ films in as-deposited, pre-annealed and reduced state was analysed using SEM, EDS, XRD and XPS. To characterise the electrochemical performance of the deposited films, polarisation curves were obtained from SOFC single stack assemblies under hydrogen and air flows for anode and cathode, respectively, at operating temperatures of 750, 800 and 850 °C.

10:40am **TS1-1-MoM-3 Surface Modification of Graphite Felt Electrode for Vanadium Redox Flow Batteries by High Entropy Alloy Oxide Thin Films: Effect of Oxygen Gas Flow Ratios***, **Krishnakant Tiwari**, C. Wang,* National Taiwan University of Science and Technology, Taiwan*; B. Lou,* Chang Gung University of Technology, Taiwan*; J. Lee,* Ming Chi University of Technology, Taiwan

Vanadium redox flow battery (VRFB) is one of the most promising renewable large scale energy storage devices. Electrode is one of the key components of VRFB which has significant effect on the energy efficiency and cost of the system. Carbon-based materials are widely used as electrodes in VRFB due to their lower electrical resistance and better corrosion resistance. However, untreated carbon-based electrode shows poor catalytic activity for redox reaction towards vanadium ions and cannot meet the development needs of VRFB. Among several surface modification methods, deposition of nanoparticles on the graphite felt (GF) electrode has been widely used. However, the poor uniformity of deposited nanoparticles results in a low charge transfer rate and poor adhesion. In this work, we investigated a surface modification approach for the graphite felt electrode by depositing refractory VNbMoTaW high entropy alloy oxide (HEAO) films grown under different oxygen flow rates using a high power impulse magnetron sputtering (HiPIMS) system for improving the performance and economic competitiveness of VRFB. Surface morphology of HEAO modified GF electrodes were examine using FESEM, contact angle test, Raman analysis, XRD and XPS. The electrochemical performances of GF electrodes modified with HEAO films grown under different oxygen gas flow ratios were compared. The flow cell test of HEAO modified GF electrodes was performed to demonstrate the charge-discharge capacity, voltage efficiency and energy efficiency at different current densities. The cycling test illustrated the stability of the VNbMoTaWOx film layer on graphite felt, where no significant decay in efficiencies was observed. The effect of oxygen gas flow ratios on the phase, chemical compositions, and electrochemical performance of the HEAO films were also discussed.

11:00am **TS1-1-MoM-4 Temperature Dependency of Specific Electrical Conductivity of DLC Coatings***, S. Danninger,* University of Applied Sciences Upper Austria*; **Francisco Delfin**,* University of Applied Sciences Upper Austria, Argentina*; C. Forsich, D. Heim, M. Schachinger,* University of Applied Sciences Upper Austria*; B. Rübig, C. Dipolt, T. Müller,* Rubig GmbH & Co KG, Austria

DLC coatings show a favourable combination of both low friction coefficient and high wear resistance and are therefore widely used for technical applications. To increase the film's electrical conductivity for special applications (e.g., coatings for electrodes) common methodes are film doping with nitrogen or metals. This study, however, investigates the decrease of electrical resistivity of un-doped DLC coatings through an increase in deposition temperatures above 450 °C.

DLC coatings were produced by means of PA-CVD using pulsed DC discharge. Temperatures of 450 °C, 500 °C and 550 °C were used to deposit a-C:H and a-C:H:Si films on various steel substrates. Process gas consisted of a mixture of argon, acetylene, and HMDSO as silicon precursor. Additionally, coatings with process gas consisting of 20 % hydrogen were produced respectively. Afterwards, for coatings deposited at 450 °C a tempering was conducted at 550 °C to exclude only heat treatment related effects. An amorphous silicon interlayer was used as an electric insulator between substrate and coating. To measure the specific electrical resistivity of all coatings the van der Pauw method employing four contact points was performed. Further coating characterizations included GDOES and EDX analysis and the measurement of layer hardness through nanoindentation. Raman spectroscopy was performed, and the spectra were compared to estimate the hydrogen content and hybridization of the DLC coatings.

Silicon free DLC films showed a clear decrease of specific electrical resistivity with an increase of deposition temperature. Values dropped from 10^7 µΩ cm at 450 °C to under 10^4 µΩ cm at 550 °C, reaching levels comparable to graphite. While the specific electrical resistivity of these a-C:H films decreased with higher deposition temperatures, a hardness increase of more than 70 % was measured over the temperature range. The average hardness of 350 HV at 450 °C rises to 600 HV for 550 °C. Process gas consisting of 20 % hydrogen decreased specific electrical resistivity even more by at least 60 %, while also slightly raising surface hardness. For a-C:H:Si coatings the specific electrical resistivity exceeded the measurement setup's detection limit of about $1.9·10^7$ µΩ cm, as they seem to be highly electrically insulating. Hydrogen containing process gas did not show any effects on silicon doped coatings. With this new process approach electrically conductive and hard a-C:H coatings could be produced without metal- or nitrogen-doping with thicknesses up to 120 µm only through an increase of deposition temperature.

11:20am **TS1-1-MoM-5 High Efficiency of Metal Oxide Catalysts for Vanadium Redox Flow Battery*, Chen-Hao Wang,*** National Taiwan University of Science and Technology, Taiwan **INVITED**

The development of sustainable energy resources such as wind and solar is urgently needed to diminish the environmental impact of fossil fuels. Nevertheless, energy storage systems (ESS) are required to store and stabilize such intermittent and random clean energy sources. Among various energy storage devices**,** the vanadium redox flow battery (VRFB), first invented by Skylla-Kazacos and co-workers in the 1980s, is one of the most promising large-scale energy storage devices owing to its design flexibility, extended cycle life, and safe operation. Furthermore, VRFB avoids cross-contamination due to employing the same electroactive element (vanadium) for both half-cells. VRFB comprises three essential components: membrane, electrolyte, and electrode. To store energy, it uses the redox couples of the electrolyte, $V^{3+}/V^{2+,}$ and VO^{2+}/VO_2^{+}, on the negative and positive sides, respectively. The membrane behaves as a separator for the two half-cells and maintains electroneutrality by passing hydrogen ions through it. The electrode does not participate in the redox reaction but provides a reaction site for active species. Therefore, some active electrodes with metal oxide-based catalysts are used in the VRFB to enhance performance. In this talk, we will introduce metal oxides, e.g., $W_{18}O_{49}$, CeO_2, and $BiVO_4$, which have excellent electrochemical activities, making VRFB more powerful.

Keywords: Energy storage system, vanadium redox flow battery (VRFB), electrode modification, energy efficiency

12:00pm **TS1-1-MoM-7 Effect of Mg Doping on Characterization and Cycling Performance of $LiCoO_2$ Thin Film Cathode for Lithium-Ion Batteries*, Tai-Yan Liu,*** *J. Huang, C. Liu,* National Cheng Kung University (NCKU), Taiwan

Lithium-ion batteries (LIBs) are the most popular energy storage devices for portable electronics and electric vehicles due to their high energy density, long cycling lifetime and no memory effect. Lithium cobalt oxide ($LiCoO_2$, LCO) is the first commercialized cathode materials for LIBs. It has many advantages such as favorable rate capability, excellent capacity retention, and high theoretical specific capacity compared with other cathode materials. However, LCO has severe structural destruction due to irreversible phase transition under high cut-off voltage above 4.2V, which causes rapid capacity fading and structural instability during repeated cycling. Therefore, electrochemically inactive element doping is studied to improve structural stability. Among many dopants, Mg is regarded as a promising element to achieve better cycling performance for LCO. Hence, we deposited Mg-doped lithium cobalt oxide (Mg-LCO) thin films for cathode materials. Co-sputtering method and post annealing were utilized to grow Mg-LCO thin films. Firstly, Al foils were sequentially cleaned in 95% ethanol and DI water for 10 min, respectively. Secondly, $LiCoO_2$ (99.99%) and MgO (99.99%) targets were co-sputtered via RF magnetron sputtering system to deposit Mg-LCO thin films on Al foils at 250 °C for 60 min in Ar/O_2 mixed gas atmosphere. The RF power of the $LiCoO_2$ target was fixed to 100W and the RF power of the MgO target was varied from 0 to 60W. Afterwards, the Mg-LCO thin films were annealed at 600°C in air for 4h via a tube furnace. From XPS and sheet resistance measurement, Mg successfully doped into LCO thin films and replaced Li sites thereby increasing the sheet resistance. SEM images showed granular size and thickness in the Mg-LCO films decreased with the MgO working power from 0 to 60W. TEM and XRD investigations revealed that the Mg-LCO thin films were layered structure and polycrystalline with (003) preferred orientation. Finally, in half-battery test, the 60W Mg-LCO thin film cathode exhibited better voltage plateaus and capacity retention than 0W, 30W Mg-LCO in the voltage range of 3.0-4.2 V at 0.2 C rate after 30 cycles. According to the above results, the structure of LCO thin film after Mg doping was more stable during charge/discharge process. In future, we will study the electrochemical performance of LCO thin films with higher Mg doping amount. Further, we will do the high voltage cycling tests (above 4.5V) and combine electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) to investigate redox kinetics of high voltage Mg-doped $LiCoO_2$ thin film cathode.

Topical Symposia
Room Town & Country A - Session TS1-2-MoA
Coatings for Energy Storage and Conversion - Batteries and Hydrogen Applications II

Moderators: Dr. Nazlim Bagcivan, Schaeffler Technologies GmbH & Co. KG, Germany, **Klaus Böbel**, Bosch Manufacturing Solutions, Germany

2:20pm **TS1-2-MoA-3 Influence of Oxygen Content During the Deposition of Scandium Stabilized Zirconia Thin Films by Reactive High Power Impulse Magnetron Sputtering (R-HiPIMS)***, **Isabel Fernandez Romero,*** Corporate Sector Research and Advance Engineering- Robert Bosch, Germany*; S. Klein, C. Engel,* Corporate Sector Research and Advance Engineering - Robert Bosch, Germany*; J. Fleig,* Technical University of Vienna, Austria

Hydrogen is one of the key energy carriers in the fight against current climate problems as H_2 can be produced using electrical energy from renewable sources and directly used in production processes, eg steel production or in chemical industry. Solid Oxide Electrolysis Cells (SOEC) transform electricity and water vapor into hydrogen (and oxygen) with the highest energetic efficiency among electrolyzer technologies

The cells of the SOEC require a dense, gas-tight, and thin electrolyte layer which is at the same time ionic conducting and electron blocking. Doped zirconia materials have been broadly used as a suitable material. Over the last years extensive research has been done to investigate the suitability of reactive vacuum techniques for their mass production.

In this work dense Scandium Stabilized Zirconia (ScSZ) layers have been successfully deposited on Gadolinium Doped Ceria (GDC) pellets using reactive High Power Impulse Magnetron Sputtering (r-HiPIMS) technique. The ceria ceramic was as substrate to mimic the microstructural conditions of the SOEC fuel and air electrode surfaces: polycrystalline, rough, and porous

By varying the oxygen content in the chamber (from 1 % to 4 %) the deposition mode can be changed from a non-poisoned (metallic) mode to a poisoned mode, decreasing the discharge voltage as well as the deposition rate but improving the stoichiometry of the ScSZ layers. This process variation modifies the microstructure and crystallinity of the film, which are related to the ionic conductivity and electron blocking ability of the film, thus offering a means to investigate the feasibility of the film as electrolyte material

2:40pm **TS1-2-MoA-4 Comparison of the Impacts of High Entropy Oxide/Alloy Coatings for Lithium-Sulfur Battery Separators***, **Ming-Roe Wann,** Y. Lin, S. Chung, J. Ting,* National Cheng Kung University (NCKU), Taiwan

The repeating formation and irreversible diffusion of liquid-state lithium polysulfides (LiPSs) during the discharge and charge of lithium-sulfur batteries (LSBs) represent the major challenge for the development of the high-performance LSB. Therefore, it is essential to alleviate the shuttling of LiPSs that dissolve in the electrolyte and cause the loss of active material. Herein, high entropy oxide (HEO) as an additive in the separator for LiPS trapping is reported. The HEO exhibits single phase spinel structure having a unique core-shell morphology. The HEO is also de-alloyed for enhancing the electrical conductivity. Both the HEO and de-alloyed HEO are subjected to material characterizations, including X-ray diffractometry (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). Then, lithium polysulfide adsorption test is done by ultraviolet–visible (UV-vis) test. For electrochemical analysis, electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV) measurements as well as cycle and rate performance are analyzed. The effect of the alloy percentage in HEO on battery performance is also addressed and discussed.

Keywords：High entropy materials, lithium-sulfur battery, lithium polysulfides

3:00pm **TS1-2-MoA-5 $BaCeZrYO_{3-\delta}$ Coatings Deposited by Solution Precursor Plasma Spray (SPPS) for Sustainable Energy Application***, **Yen-Yu Chen,** W. Zeng, C. Liu, G. Yao,* Chinese Culture University, Taiwan

Pervoskite-type proton-conductive ceramic materials have high potentials for the application of sustainable energy fields, such as protonic ceramic fuel cell (PCFC), ammonia fuel synthesis, carbon dioxide conversion, etc. In this study, perovskite-type proton-conductive coatings, $BaCeZrYO_{3-\delta}$ (BCZY), were deposited on NiO/$BaZrYO_{3-\delta}$ (BZY) composite substrates by a solution precursor plasma spray (SPPS) method. The precursors were consisted the BCZY species of the nitrate salts, and dissolved into de-ionic water. The NiO/BZY substrates were prepared by a die-pressing method. Several properties of the coatings were analyzed, including crystal phases by X-ray diffraction (XRD), microstructures by scanning electron microscope (SEM), electrical properties by electrochemical impedance spectroscopy (EIS), etc. The results of XRD show the coatings after post-coating annealing over 600°C are mainly consisted of perovskite phases. The microstructure analysis of the BCZY coatings characterized by SEM show that the coatings are either consisted of overlapped splats of BCZY with a few of surface pores on the surface, or with porous structure by BCZY particle necking. The average thickness of the coating layers are about several microns. The formation mechanism of the BCZY coatings can be purposed as the BCZY precursor droplet breakup, liquid-phase evaporation, thermal pyrolysis of precursors, solid particles melting, and then the melting particles splatted and overlapped on the substrate to form the BCZY coatings. The details electrical property analysis of the BCZY coating samples are as mentioned in the following report.

3:20pm **TS1-2-MoA-6 Aluminum-Doped Non-Stoichiometric Titanium Oxide (Al-TiO_X) for Anode in Lithium-Ion Batteries***, **Guan-Bo Liao,*** National Cheng Kung University (NCKU), Taiwan*; Y. Shen,* Hierarchical Green-Energy Materials (Hi-GEM) Research Center, Taiwan*; J. Huang,* National Cheng Kung University (NCKU), Taiwan

Lithium-ion batteries (LIBs) are regarded as the most promising recyclable energy storage system nowadays. Among those anodes, TiO_2 is a candidate due to its excellent safety and cycling performance. Moreover, a recent report suggested that non-stoichiometric titanium oxide (TiOx) has the high-rate capability as the non-stoichiometry creates more oxygen vacancies creating voids for ion transportation thereby facilitating lithium-ion diffusion. The report exhibits the fast-charging potential of TiOx. Nevertheless, the low capacity is still a problem. In this study, an aluminum-doped non-stoichiometric titanium oxide (Al-TiOx) was used as an anode in LIBs. Here, we used the sol-gel method followed by annealing to synthesize Al-TiOx. First, the Aluminum precursor was incorporated into titanium-based sol to form Al-TiO_2 gel. After evaporation and grinding, the Al-TiO_2 powder was formed. Second, the Al-TiO_2 powder was annealed in a reduced atmosphere to synthesize Al-TiO_x to increase the capacity and the rate capability further. The TEM and XRD results (shown as supplementary file) showed that aluminum was successfully doped in TiO_2 lattice. The best electrochemical results showed that the first cycle capacities were 480 and 350 mAh/g for Al-TiOx and TiOx respectively, which both exceeded the theoretical capacity of pristine TiO_2 (335 mAh/g). The cycling test also shows a good performance. Both Al-TiO_x and pure TiO_x remain stable for more than 200 cycles. Al-TiO_x also showedbetter rate capability than pure-TiOx. The Al-TiOx specific capacities are 131, 125, 115, 86, 70,40,25 mAhg^{-1} while TiOx showed 137,120,80,62,27,7,3 mAhg^{-1} for 0.1,0.2,0.5,1,2,5,10C respectively. EIS and GITT will be used to measure the diffusivity of Lithium-ion later.

After this study, we had a preliminary understanding of the anode performance of Al-TiOx. Recently, we are preparing in-operando measurements (**e.g., in-situ XRD, in-situ Raman…etc.**). We will observe the crystal structure change during charging-discharging using in-situ XRD and the defect analysis by in-situ Raman, especially focusing on the normal speed and fast-charging behavior.

3:40pm **TS1-2-MoA-7 Unveiling Capacitive and Diffusion-Limited Li-Ion Storage in Semiconducting 2d-Mos_2 Composited with Aluminium Nitride Nanoflowers for Flexible Electrodes of Supercapacitors***, D. Kaur,* ***Gagan Kumar Sharma,*** Indian Institute of Technology Roorkee, India

A flexible supercapacitor electrode can be realised by combining the exclusive characteristics of two-dimensional MoS2 layered material with a conventional key material, aluminium nitride (AlN). We present a bendable electrode that is straightforwardly grown on stainless-steel foil via a binder-free sputtering route. The inherent merits of good conductive pathways among MoS_2 nanolayers and enriched pseudocapacitive and dielectric activity from AlN nanoflowers enable synergism of intermixed porous structure. This unique surface morphology facilitates sulfur and nitrogen edges to make insertion/de-insertion of Li-ions more feasible to store electrochemical energy. The MoS_2-AlN@SS hybrid working electrode achieves a gravimetric capacitance of 372.35 F/g at a 5 mV/s scan rate with a wide potential window of 2 V in 1 M Li_2SO4 electrolytic aqueous solution. The composite thin film of better adhesion with the current collector exhibits a remarkably high specific power of 28.05 W h/kg at a specific power of 0.26 kW/kg, simultaneously an advanced cycling lifespan of 91% over 5,000 charge-discharge cycles. The capacity of the hybrid electrode is almost unperturbed under bending from 0º to 175º, while only ~5% degradation in capacitance was noticed at a flexing angle of 175º. These distinctive features of this electrode material elucidate the practical applicability and recommend it as a promising candidate in wearable bendable supercapacitors.

References

[1]G.K. Sharma, B. Ranjan, D. Kaur, Appl. Phys. Lett. 121 (2022) 013901. https://doi.org/10.1063/5.0093681.

[2] G.K. Sharma, B. Ranjan, D. Kaur, Ceram. Int. 48 (2022) 23404–23414. https://doi.org/10.1016/j.ceramint.2022.04.332.

[3] G.K. Sharma, B. Ranjan, D. Kaur, Appl. Phys. Lett. 118 (2021) 203901. https://doi.org/10.1063/5.0045378.

4:00pm **TS1-2-MoA-8 Lithium Passive Diffusion and Surface Oxidation on Battery Materials at Room Temperature***, **Jozef Ociepa**,* OCI Vacuum Microengineering Inc., Canada

Passive Li diffusion is defined as the process of Li atom/ions migration under a concentration gradient and activated by thermal energy from atomic vibrations of the host structure at room temperature. This process of passive Li diffusion is important for a better understanding of the active diffusion processes that are happening in lithium-ion batteries (LIBs), where external energy component such as electrical potential is applied. It is expected that materials that exhibit good "natural" Li diffusion properties will perform much better under the external electrical potential. This approach offers a unique opportunity to observe the free movement of lithium atoms/ions into the solid structure and simplify the understanding of diffusion processes especially if single-crystal structures are used. The single-crystal structures are free from grain boundaries and the lithium diffusion process is limited to lattice diffusions such as interstitial, vacancies, and dislocations. This approach allows for categorizing materials that are attractive to lithium diffusion based on the pure lattice component. The characterizing techniques are Auger electron spectroscopy (AES) for tracing Lithium concentration on the surface (Li-KVV peak at 52eV) and Low Energy Electron Diffraction (LEED) for surface crystallography changes. The lithium concentration gradient is created on the surface of the host material by the evaporation of a thin film of lithium with an effective thickness from 5 Angstroms to 250 Angstroms under ultra-high vacuum conditions. The data obtained from these experiments are showing different lithium diffusion behavior on the selected materials and there is an indication of three categories of the characterized materials. 1-Rapid lattice diffusion of Li into HOPG and no change in the surface crystalline structure. 2-Moderate lattice diffusion of Li into CVD Diamond, SiC-6H, SiO2/Si(001, LiNbO3, and TiO2 and some changes in the surface crystalline structure. 3-No lattice diffusion of Li into Si single crystals, Ga2O3 and SrTiO3, and no long-range order in the surface crystalline structure. Comparison of the Li diffusion on SiC single crystals and polycrystalline structure shows faster Li diffusion on single-crystal. The exposure of lithiated SiC to an oxygen gas environment at 5x 10-6 Torr at room temperature indicates a Li diffusion toward the surface. This method simplifies the understanding of diffusion processes and limitations such as oxidation, plating, and the role of grain boundaries.

4:20pm **TS1-2-MoA-9 Development of Carbon-based PVD Coatings for Stainless Steel PEMFC's Bipolar Plates***, **Michaël Ougier**, M. Leroy,* IREIS/HEF group, France*; A. Chavanne,* HEF group, France*; H. Christophe,* IREIS/HEF Group, France

Proton Exchange Membrane Fuel Cells (PEMFC), employing dihydrogen as fuel, are promising energy sources (for their high energy conversion and near-zero emission), particularly for the automotive sector. In these electrochemical systems, bipolar plates (BPP) enable to electrically connect the cells and represent 20-30% of the total cost of the system, for about 70% of its mass and volume.

Stainless steel bipolar plates are widely used in fuel cell because of its combination of a good corrosion resistance and manufacturability. However, due to a native oxide layer they exhibit a high interfacial contact resistance. Additionally, in certain conditions, the harsh environment in a fuel cell is able to corrode stainless steel. By the deposition of coating onto the BPP surface, the electrical conductivity and the corrosion resistance can be greatly enhanced. Finally, the main objectives of coating are:

1. to ensure an efficient protection against corrosion, avoiding electrolytic membrane contamination with metallic corrosion products.
2. to minimize the electrical contact between the plate and the gas diffusion layer, guarantying low electrical losses.

A high-performance coating is therefore key to the durability and efficiency of the bipolar plates and of the fuel cell stack itself.

Among all deposition techniques, Physical Vapor Deposition (PVD) methods like magnetron sputtering and cathodic arc evaporation are able to deposit highly adherent, conductive and corrosion resistant coatings. PVD gold coatings have long been the reference solution to fulfill the above-mentioned requirements, and nowadays in heavy duty vehicles. However, treatment price is a sticking point for large volume commercialization and cost-effective alternative materials are now developed.

In this present work, we review the deposition methods and present experimental results on the performance of various PVD coatings such as gold, ceramic, and carbon-based coatings, with and without interlayer. Coupons of coated stainless steel are investigated both in simulated aggressive PEMFC environment (80°C, H_2SO_4 pH 3). Beyond these basic tests, accelerated corrosion stress tests are also be developed to simulate in a few hours the more detrimental conditions that can be encountered in the 7000 hours lifetime of the electrochemical system. Coating degradations mechanisms are evidenced by post-mortem coupons and plates analysis. Complementary to these corrosion tests, electrical contact resistance of the coated surface is also evaluated before and after corrosion tests.

Topical Symposia
Room Town & Country A - Session TS1-3-TuM

Coatings for Energy Storage and Conversion - Batteries and Hydrogen Applications III

Moderators: Dr. Nazlim Bagcivan, Schaeffler Technologies GmbH & Co. KG, Germany, **Klaus Böbel**, Bosch Manufacturing Solutions, Germany

8:20am **TS1-3-TuM-2 High-Performance Rechargeable Zinc Ion Batteries: From Surface Modification of Zn Anode and Structural Engineered Cathode to Deep Eutectic Solvent (DES)-Based Electrolytes***, **Yu-Lun Chueh,*** National Tsing Hua University, Taiwan

Rechargeable metal ion batteries have been widely studied as efficient energy storage systems for portable devices, such as electric vehicles, which have become the trend in the future. Among these candidates, zinc ion batteries exhibit superior advantages because of the abundance of zinc compared with lithium, while the cost of zinc is lower than that of lithium. Moreover, zinc has been characterized by multivalence in an ionic state, which provides approximately three times higher volumetric capacity than lithium. For Zn ion batteries, the uncontrollable dendrite growth and side reactions existed on the Zn anode seriously restrict the cycle stability of zinc ion batteries. In my talk, different strategies on the design of low dimensional materials on the surface metal anode or cathode for high-performance rechargeable Zn ion batteries will be reported. For example, organic hydrophobic polyvinylidene fluoride and inorganic Santa Barbara Amorphous-15 (PVDF-SBA15) hybrids were designed as a surface modification layer to stabilize the Zn anode, leading to an optimized Zn/electrolyte interface with large-scale feasibility.[1] In addition, an alternative electrolyte system based on the deep eutectic solvent (DES), because of their low cost, high stability, biodegradability, and non-flammability, making them optimal candidates for sustainable batteries, was demonstrated.[2]*Ex-situ* Raman, XPS, and TEM characterization results of the electrodes under different states confirm the reversible alloying conversion and intercalation hybrid mechanism during the discharge and charge cycles for Zn ion batteries. All possible chemical reactions were proposed by the electrochemical curves and characterization.

Reference:

1. Nano Energy 103, 107805, 2022

2. ACS Applied Materials & Interfaces 14, 7814-7825, 2022

8:40am **TS1-3-TuM-3 Electrochemical Performances of LiNi0.8Co0.1Mn0.1O2 Synthesized by Hydroxide Coprecipitation Method***, **Chia-Hsin Lo**, J. Huang,* National Cheng Kung University (NCKU), Taiwan*; C. Chang,* National University of Tainan, Taiwan

To meet the rising demand of electric vehicles, cathode materials of rechargeable lithium-ion batteries with high energy density and long cycle life are investigated. Lithium nickel cobalt manganese oxide ($LiNi_xCo_yMn_zO_2$) is a promising candidate to be the next generation cathode materials. A series of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ was successfully prepared by hydroxide coprecipitation method and calcination. The crystal structures and microstructures were characterized by X-ray diffraction and scanning electron microscopy. Charge/discharge cycling were also employed to investigate their electrochemical behaviours. XRD results show that pHvalue have an impressive effect on the crystal structure of the $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ powder. Among all the samples, the one prepared at pH=11.5 possessed the lowest degree of Li^+/Ni^{2+} disordering and the . Scanning electron microscopy with element mapping tests reveal that the homogeneous $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ solid solution has been achieved via this synthesis method. The $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ powder prepared at pH=11.5 can deliver a high initial discharge capacity of 182.9 mAh/g with coulombic efficiency of 66.0% at 0.5C-rate in the voltage range of 2.8−4.3 V.

9:00am **TS1-3-TuM-4 Pb-Free Halide Perovskite/TiO_2 Heterostructure for Enhanced Solar-Driven PFC***, **Yong Yu**, J. Ting,* National Cheng Kung University (NCKU), Taiwan

Photocatalytic fuel cell (PFC) isa promising technology that can simultaneously treat wastewater and generate electricity. Upon solar light irradiation, the photoanode generates electron–hole pairs, the holes degrade organic pollutants by formation of reactive oxidative species and the electrons go through the circuit to the cathode for oxygen reduction reaction (ORR) or hydrogen evolution reaction (HER), depending on the oxygen concentration in solution. Regarding the photoanode, TiO_2 is commonly used due to its low toxicity, low cost, and high stability. However, there are still problems need to be solved, such as low visible light absorption and fast electron-hole recombination rate.

In the present study, we use all-inorganic lead (Pb)-free halide perovskite to form a heterostructure with TiO_2 to tackle the above issues. The heterostructure increases the absorption of visible light, reduces the recombination of electron–hole pairs, and improves the efficiency of PFC. Halide perovskite is chosen due to the easy synthesis, narrow energy gap, and high carrier mobility. The Pb is replaced by bismuth. The photodegradation performance is investigated using tetracycline antibiotic as organic pollutant and reported.

9:20am **TS1-3-TuM-5 Inline PVD Coating of Bipolar Plates for Electrochemical Energy Converters***, K. Böbel, M. Mueller,* Bosch Manufacturing Solutions, Germany*; D. Beisenherz, S. Huebner,* Singulus Technologies AG, Germany*; J. Jiao, S. Wetzel,* Bosch Automotive Products (Suzhou) Co., Ltd., Germany*; **Rafael Gryga**,* Matthias Mueller, Bosch Manufacturing Solutions, Germany

Electrochemical energy converters are key components for a broad establishment of green hydrogen economy. The relevant technologies have been applied for decades in several niche applications. Recently many countries and companies pursue the mass production of fuel cells and electrolyzers. Hence, great efforts are made towards cost efficient systems, components and fabrication methods.

In practice single fuel cells and electrolyzer cells are stacked to a powerful system consisting of up to several hundred cells. The single cells are separated and electrically connected via bipolar plates. Those plates must withstand different electrochemical and temperature conditions without significant deterioration of their performance. Widely applied performance indicators are interfacial contact resistance and corrosion current. Those properties can be perfectly controlled by means of noble metal coatings applied onto steel or other bipolar plate materials. In order to replace this expensive solution, many coating systems and a wide variety of coating techniques have been suggested so far.

The paper reports on the optimization of both, bipolar plate properties as well as production efficiency based on PVD coating technology. Different coating designs have been tested and promising candidates have been optimized in terms of process parameters and coating thickness. The coating process has been transferred from batch to inline systems with a cycle time of a few seconds. This results in a competitive solution for the mass production of cost efficient bipolar plate coatings.

9:40am **TS1-3-TuM-6 Studies on the TiO_2 Thin Film on the Silicon Nanowire Arrays using Taguchi - Grey Method for Heterojunction Solar Cell***, A. Chiou, H. Liao, **Jun-Luo Wei**,* National Formosa University, Taiwan

In recent years, the problem of energy has become more and more serious, and renewable energy is the most important.Among the renewable energy sources, solar energy is the best developed. Many different materials have been applied to solar cells by scholars. One way to produce large-area, easy-to-process thin films is to use radio frequency magnetron sputtering. In this study, P-layer silicon nanowire arrays were prepared by electroless etching method to replace the previous multilayer films. TiO_2-SiNW Arrays heterojunctions were formed by preparing TiO_2 as N layer by magnetron sputtering method. In this paper, the Grey-Taguchi method was used to analyze and optimize PN heterojunctions with TiO_2 films. The effects of sputtering process parameters (RF power, process pressure, deposition temperature and deposition time) on surface morphology, material structure, photoelectric conversion efficiency and reflectivity were investigated.An AZO window layer is then added and annealed.

The gray correlation analysis shows that the reflectivity is reduced from 8.02225% to 7.72081%, and the photoelectric conversion efficiency is increased from 0.01915% to 0.082%. In the confirmation runs, the TiO_2 film was amorphous and wound around an array of silicon nanowires.After adding the AZO window layer, the reflectivity increased to 18.04712%, and the photoelectric conversion efficiency increased to 0.124%.Confirmation runs show that the AZO film is polymorphic. The experimental results demonstrate the effectiveness of the RF magnetron sputtering method, which provides good reflectivity and photoelectric conversion efficiency.

10:00am **TS1-3-TuM-7 Impacts of Mutual Phase Interactions on Crystal Polarity and Photocatalytic Hydrogen Evolution Reactions***, **Jrjeng Ruan**,* National Cheng Kung University (NCKU), Taiwan

The secondary molecular interactions are well known able to influence the organization behaviors and electrooptical responses of dispersed molecules. Whereas, for dispersed phase domains of organic and inorganic components, including amorphous and crystalline phases, mutual polarization/interactions are much less recognized. In general, the interactions among phases, especially crystalline phases, have not been envisaged yet as a factor of crystal engineering and the electrooptical features of phase domains.

Upon the coalescence and mutual drawing behaviors, arrayed stacking of PVDF-TrFE ferroelectric lamellar crystals has been achieved, and, with activated mutual polarization, the dielectric constants of a monolayer of oriented lamellar crystal are able to be enhanced above 80 at room temperature. As the roughness of FTO substrate is tailorable upon the deposition of PMMA molecules, various degrees of coalescence and thus thickening of PVDF-TrFE lamellar crystals are achievable. Following this result, crystal surface potentials and piezoelectric responses of lamellar crystals were found critically dependent on reached lamellar thickness, exhibiting the relationship between crystal dimension and crystal polarity for the first time. Surprisingly, simply with the spread of P3HT-wrapped MoS2 or graphene quantum dots on PVDF-TrFE ferroelectric lamellar crystals, the piezoelectricity of stacked ferroelectric polymer crystals has been dramatically enhanced. These results have been viewed to unveil mutual interactions between the ferroelectric lamellar crystals and deposited 2D materials. Furthermore, depending on reached crystal polarity/surface potentials of underneath ferroelectric polymer crystals, the capability of P3HT-wrapped MoS2 in catalyzing hydrogen evolution upon water splitting under the irradiation of visible light is able to be activated and enhanced. The mutual polarization between dispersed ZnO nanorods crystals and nearby polymer ferroelectric lamellar crystals has been identified also, which causes one order of magnitude increases of piezoelectric responses, and dielectric constants of hybrid thin films. The antiparallel interactions of crystal dipole have been realized able to serve as a new type of phase interactions, which gradually decay with the increase of separation distance between interacting crystals.

The impacts of phase evolution and dispersion on phase interactions have been investigated in this research, which are expected to indicate a new direction for the preparation of hybrid crystalline materials capable to overcome the current bottlenecks of materials applications.

10:20am **TS1-3-TuM-8 Systematic Investigation of the Piezocatalysis–Adsorption Duality of Polymorphic Mos$_2$ Nanoflowers***, **Hsun Yen Lin**,* National Tsing Hua University, Taiwan

This study theoretically and experimentally investigates the piezocatalytic and adsorption effects of different phases of polymorphic MoS$_2$ NFs. To verify whether the polymorphic MoS$_2$ NFs would exhibit adsorption or piezocatalytic effects, the electrostatic surface charge of these NFs and the RhB solution is varied using sodium hydroxide and nitric acid solutions. The cationic dye is adsorbed on the surfaces of the 1T MoS$_2$ NFs; however, the few-layer 2H MoS$_2$ NFs generate a considerable quantity of hydroxyl species for degrading RhB molecules through the mechanical-force-induces piezopotential. This study discovers that the polymorphicMoS$_2$ NFs exhibit a piezocatalysis–adsorption duality.

10:40am **TS1-3-TuM-9 Improving Urea Oxidation Reaction Performance by Enhancing Gas Releasing***, **Ming Feng Tsai**, J. Ting,* National Cheng Kung University (NCKU), Taiwan

Urea electrolysis, or urea oxidation reaction (UOR) on nickel is considered to be one of the high overpotential routes for water splitting. However, the rate determining step (RDS) during the reaction is related to the release of gas molecule from the active site. In this study, we aim to directly release the creamy gas at the anode via investigating a group of metal organic framework (MOF) electrocatalysts based on nickel.We demonstrate an Ni-based MOF electrocatalyst having a current density of 1 A▪cm^{-2} at 1.48 eV (vs. RHE), which is comparable to that of the commonly used noble metal catalyst like Rh and Pt. A mechanism is proposed to explain the excellent performance of the Ni-based MOF electrocatalyst.

Topical Symposia
Room Pacific F-G - Session TS2-TuA

Sustainable Surface Solutions, Materials, Processes and Applications

Moderators: Justin Cheney, Oerlikon Balzers Coating, USA, **Prof. Fan-Bean Wu**, National United University, Taiwan

1:40pm **TS2-TuA-1 Application of High Entropy Spinel Oxides on Photodetector***, **Jyun-Yi Li**, K. Kuo,* National Cheng Kung University (NCKU), Taiwan*; T. Nguyen,* National Cheng Kung University (NCKU), Taiwan, Viet Nam*; P. Hsiao, C. Chen, J. Ting,* National Cheng Kung University (NCKU), Taiwan

Photodetector as a widely use application in daily life, such as environmental monitoring, biological /chemical analysis, and communication, is often to be constricted to work in the certain wavelength due to the materials inside. Recently, a new concept of high entropy oxides (HEO) has been proposed, which is consisted of more than five metals with concentration of each metal in range of 5-35% and having a calculated configurational entropy $\Delta S \geq 1.5R$. Although there have been many studies on high entropy oxides, few of them have focused on photodetectors. Herein, we synthesized a series of high entropy spinel oxides with hydrothermal method and apply on photodetector. The crystal structure of materials were confirmed using X-ray diffraction (XRD). The morphology was characterized with scanning election microscope (SEM). Besides, the material were also characterized using inductively coupled plasma (ICP), X-ray photoelectron spectroscopy (XPS), transmission electron microscope (TEM), …. .The optical performance of HEO photodetector were evaluated by UV-VIS-NIR, responsivity(R), external quantum efficiency (EQE), detectivity (D), rise time and decay time.

Keywords: high entropy oxide(HEO), spinel,photodetector, responsivity, EQE, detectivity

2:00pm **TS2-TuA-2 Euro 7/VII – Challenges for Surface Solutions in ICEVs and EVs***, J. Vetter,* Oerlikon Balzers Coating Germany GmbH, Germany*; **Justin Cheney**,* Oerlikon Balzers Coating, USA*; J. Becker,* JB, Germany*; M. Esselbach,* Oerlikon Surface Solutions AG, Liechtenstein

The upcoming Euro 7 standards are aimed to further reduce pollutant emissions from vehicles and improve air quality. Euro 7 is valid not only for passenger car but also for heavy-duty vehicles. The proposed standard will influence the development of internal combustion engine vehicles (ICEVs) and electric vehicles (EVs) alike.

After all the drivetrain of ICEVs and EVs is quite similar and the requirements with respect to improved long-life performance and reduced particle emission may be even more challenging with EVs. Surface solutions are ready to work as an enabler to reach the goals. E. g. coatings allow a longer lifetime of drive train components which otherwise suffer from the higher torque of an electric motor.

Besides the well-known tribological coatings for engines and drive-train other coatings are of interest. Examples are coatings which allow to measure stress, pressure, or temperature, insulating coatings or conducting coatings for connectors of batteries.

Coatings for hydrogen applications will be discussed. Hydrogen applications can be found in fuel cells, the periphery of fuel cells, but also in hydrogen ICEs.

Whatever coating solution may come up, the requirements of a circular economy need to be an integral part of a system.

2:20pm **TS2-TuA-3 Surface Technology as a Key Technology for New Energy Systems***, **Yashar Musayev**, L. Dobrenizki,* Siemens Energy Global GmbH & Co. KG, Germany **INVITED**

Siemens Energy is one of the world's leading energy technology companies. The company works with its customers and partners on energy systems for the future, thus supporting the transition to a more sustainable world. With its portfolio of products, solutions and services, Siemens Energy covers almost the entire energy value chain – from power generation and transmission to storage. The portfolio includes conventional and renewable energy technology, such as gas and steam turbines, hybrid power plants operated with hydrogen, and power generators and transformers. More than 50 percent of the portfolio has already been decarbonized. An estimated one-sixth of the electricity generated worldwide is based on technologies from Siemens Energy.

Using renewable electrical energy like wind or solar power for "green electrons" from the power sector to decarbonize energy across all sectors unlocks enormous environmental and business benefits. Through Power-to-X technologies, sectors beyond power generation will benefit from renewable power and become increasingly green over the total chain from production to application.

Siemens Energy will provide optimum solutions in order to contribute to the realization of a carbon-neutral society in countries and regions around the world by utilizing our hydrogen related technologies, business and global network. The joint vision of the two companies is to advance the technology to produce green hydrogen from innovative PEM (Proton Exchange Membrane, Fig.1) water electrolysis using renewable energy systems. PEM water electrolysis (Fig.2) enables the production of high-purity green hydrogen. The resulting green hydrogen can not only be used for large-scale power generation and other electric power applications, but also for sector coupling such as heat, transport, and industrial applications.

An PEM-electrolysis cell consists of a MEA (Membrane Electrode Assembly; Catalyst Coated Membrane) as well as porous structures (gas diffusion layer & fleece) on both sides for the distribution of product gases. The cells are separated in the segment by bipolar plates. The PEM-systems have been further developed regarding efficiency, service life and cost-effectiveness. The key performance indicators (KPIs) of an electrolysis stack can be derived from the current-voltage and voltage-time curves.

4:00pm **TS2-TuA-8 Progress on Piezoelectrocatalysis for Hydrogen Production and Environmental Science***, **Jyh-Ming Wu**,* National Tsing Hua University, Taiwan **INVITED**

Continual technological advancements have substantially improved peoples' quality of life; however, excessive energy consumption and improper waste management have caused tremendous environmental disruption. Unrestricted fossil fuel exploitation contributes to greenhouse gas emissions, precipitating climate change, and the discharge of large amounts of industrial wastewater has deteriorated natural ecologies and contributed to severe health problems. Solutions involving the remediation of water pollutants, water splitting, and clean energy alternatives have been widely investigated. Specifically, electrocatalytic and photocatalytic water splitting are potentially promising strategies for hydrogen gas production and polluted dye decomposition.

This talk will report how 2D transition metal dichalcogenides can be used for piezocatalyts for highly efficient wastewater treatment and hydrogen production without applied light irradiation. Furthermore, we will report that a new generation of piezocatalyts — A self-powered photoelectrochemical microsystem comprising quartz prism microrods assembled with TiO_2 nanoparticles or MoS_2 nanosheets developed and demonstrates a marked catalytic effect on organic dye degradation and hydrogen evolution through a piezopotential sensitized catalytic activity. The induced piezopotential not only tilted the band structure to accelerate the separation of photoexcited carriers but also restrained their recombination, contributing to a more efficacious catalytic reaction. A self-poweredelectrochemical microsystem realizes the remarkable coupling effect of piezocatalysis and photocatalysis on different applications, introducing a potential material and strategy to environmental science and renewable energy fields.

References:

1. J. M. Wu*, W. E. Chang, Y. T. Chang, C. K. Chang, Advanced Materials 28 (19), 3718-3725, 2016.
2. Y. T. Lin, S. N. Lai, J. M. Wu*, Advanced Materials 32 (34), 2002875, 2020.
3. M.-C. Lin, S.-N. Lai, K. T. Le, and J. M. Wu*, Nano Energy, 91. 106640, 2016.

4:40pm **TS2-TuA-10 Visible Light Activated Photocatalytic Coatings by Reactive Magnetron Sputtering for Environmental Applications***, **Peter Kelly**,* John Dalton Building, Chester Street, UK*; M. Ratova, J. Redfern,* Manchester Metropolitan University, U.K.

Photocatalytic coatings and materials have many potential applications, such as removal of organic pollutants in water and air supplies, antimicrobial and anti-viral surfaces, self-cleaning glass and building materials and the production of hydrogen via water splitting. However, the most widely known photocatalytic material, titanium dioxide in the anatase form, is limited by its low quantum efficiency and wide band gap (3.2 eV), which means it requires UV light for activation. Band gap narrowing can be achieved by doping the anatase, but this can increase the recombination of the holes and electrons produced by exposure to ultra band gap radiation and lead to an overall reduction in activity.

We report the development of a series of bismuth oxide and bismuth oxide-based coatings with band gaps in the 2.4 to 2.6 eV range and, consequently, significant visible light activity. The coatings were produced by reactive magnetron sputtering and have been deposited onto planar substrates and also particulates including PC500, P25 and 2mm diameter glass beads to demonstrate the flexibility of the deposition process and to allow a wide range of applications to be explored. Coating types investigated include bismuth oxide, bismuth tungstate and bismuth molybdate. The coatings were analysed using SEM, EDX, XRD, XPS, and UV–vis spectroscopy. The photocatalytic properties have been determined by dye degradation tests under visible light irradiation and an acetone degradation test. The antimicrobial efficiency of the coatings was tested via inactivation of E. coli.

It was found that the performance of bismuth oxide for both dye degradation and bacterial inactivation experiments under visible light was superior to that observed for either bismuth tungstate, bismuth molybdate or titanium dioxide coatings also produced for comparison purposes. Additional tests have been carried out against cyanobacteria and free-floating genomic DNA to demonstrate the water treatment potential of the bismuth oxide coatings. Further trials have demonstrated the capability of selected coatings to breakdown microplastics in water.

5:00pm **TS2-TuA-11 A Covalent Organic Framework-Based Ionic Diode Membrane for Ultrahigh Blue Energy Generation***, **Yu-Chun Su**, L. Yeh,*
National Taiwan University of Science and Technology, Taiwan

Blue energy has recently attracted significant attention due to the growing energy demand and increasing awareness on environmental protection. Electric eels can convert ionic concentration gradients into a high-efficiency electric power when facing enemies via sub-2 nm biological transmembrane channels, which can exhibit high ion selectivity and strong diode-like ion rectification property. Inspired by this, a heterogeneous ionic diode membrane, composed of an ultrathin (~110 nm) two-dimensional covalent-organic framework (COF) membrane with well-oriented sub-2 nm ion transport channels and a highly ordered alumina nanochannel membrane (ANM), is reported for highly efficient blue energy harvesting. Higher ionic flux can be obtained due to well-ordered ion transport channels which achieves lower membrane resistance. Moreover, as verified by our experimental and simulation results, the heterostructured COF/ANM membrane is capable of strong ionic diode behavior due to asymmetric charges and pore sizes in two aligned COF (1.1 nm) and ANM (100 nm) channels that can enhance current density. Thus, an unprecedented power density of up to 27.8 W/m^2 is achieved by mixing the artificial salt-lake water and river water. This study will open new avenues of using the rectified ion channel-mimetic nanofluidic membrane as a new platform towards the exploration and development of an ultrahigh osmotic power generator.

Topical Symposia
Room Town & Country B - Session TS3-WeA

Processes of Materials for Printed and Flexible Film Technologies

Moderators: Prof. Panos Patsalas, Aristotle University of Thessaloniki, Greece, **Dr. Demosthenes Koutsogeorgis**, Nottingham Trent University, UK

2:00pm **TS3-WeA-1 Upscalable Nanomanufacturing of Thin-Film Electronics***, **Thomas Anthopoulos,*** King Abdullah University of Science and Technology (KAUST), Division of Physical Sciences and Engineering, Saudi Arabia **INVITED**

Adapting existing manufacturing methods to emerging forms of large-area nanostructured electronics presents major technological and economic challenges. Despite the difficulties, however, a number of new processing concepts have been gaining ground, transforming the broader marketplace and relevant manufacturing infrastructure. In this talk, I will discuss our recent efforts toward scalable manufacturing of emerging forms of large-area nanostructured electronics. I will show how the development of innovative patterning technologies in tandem with engineered nanomaterials, can lead to more sustainable forms of optoelectronics with high-performance characteristics. Particular emphasis will be placed on the development and evolution of adhesion lithography (a-Lith) and self-forming nanogap lithography techniques and their use in an expanding range of applications from ultra-fast optoelectronics to new forms of chemical reactors.

2:40pm **TS3-WeA-3 Plasma Technologies for Sustainable Packaging Materials***, **Glen West,*** Manchester Metropolitan University, U.K.*; T. Cosnahan, C. Struller, N. Copeland,* Bobst Manchester Ltd., UK*; P. Kelly,* Manchester Metropolitan University, U.K.

The sustainability drive in the plastics packaging market has, in recent years, been propelled to public attention and incorporated into corporate strategies. In response, most major market players, from resin producers to brand owners and retailers are aligned to have only fully recyclable packaging by 2025, and to reduce carbon dioxide emissionsfor this 141 MTonne market. Other requirements in development from various regulatory and statutory bodies present an environment of increasing demand on producers throughout the sector. From an equipment manufacturer perspective, these environmental sustainability pledges will require technological development.

The industry is moving away from multi-layer, multi-chemistry structures which were used to adhere various coating layers to each other, as mono-material plastic packets are being targeted due to their recyclability. Substantial research attention is focused on promoting the surface energy of polyolefin materials, including the utilization of plasma in the early converting steps. Plasma techniques are favored within the industry, as they are operator independent processes. The plasma surface treatment of kilometers-long reels of polymer to prepare them for subsequent deposition steps is now understood to be vital to achieve the required interfacial bond strength. This is understood to promote barrier and adhesion performance to parity with historical non-recyclable structures (i.e. <1 cc/m2.day oxygen transmission and > 3 N/15mm adhesive failure).

Within the flexible film packaging market, thin film SiOx and diamond-like-carbon are deposited using plasma enhanced chemical vapor deposition – as these thin films create robust environmental barriers to oxygen and water vapor on plastic packaging for food and medical products, although one drawback of DLC is the use of acetylene which comes with various safety hazards. One of major issues when using plasma is the control of arcs that can damage the polymer web. For successful plasma enhanced chemical vapor deposition, two key parameters required: high enough ionization percentage of large input gas flow, and sufficient energy of deposition. These create the high reaction rates required and the energy for surface reorganization (and reaction) of the deposit on the surface to create a correctly reacted and structured bonding which has the balance of properties of barrier, flexibility and toughness. The plasma technologies for achieving effective surface treatment and consistent barrier film deposition on large areas with sufficient processing speed will be discussed in this paper.

3:00pm **TS3-WeA-4 Transition Metal Nitride Colloids: From PVD Targets to Laser-Ablated Nanoparticles***, N. Pliatsikas, S. Panos, I. Fekas, S. Kassavetis, **Panos Patsalas,*** Aristotle University of Thessaloniki, Greece

Transition metal nitrides (TMN), such as TiN, ZrN, HfN, VN, NbN, TaN, MoN, WN, have been the cornerstone of hard coating industry for several decades. Some of them have been considered as electronic materials of substantial importance, mostly as diffusion barriers in transistors. Recently TMN have been revisited as important plasmonic materials and biomaterials for emerging applications in the printed electronics and biomedical sectors. TMN share unique traits such as refractory character, electronic conductivity, notorious chemical stability, and miscibility among them facilitating the formation of ternary (e.g. $Ti_{1-x}Zr_xN$, $Ti_{1-x}Ta_xN$, and $Ti_{1-x}Sc_xN$, among others) and quaternary (e.g. $Ti_{1-x-y}Zr_xAl_yN$, $Ti_{1-x-y}Ta_xAl_yN$, among others) alloys. TMN collectively cover a wide range of values for their electron conductivity, work function and plasmon resonance spectral location. While they are routinely produced in thin-film form by PVD (mostly sputtering) and CVD/ALD, the formation of colloidal nanoparticles of TMN has been proven exceptionally challenging, especially for the case of ternary TMN. In this work we exploit the knowledge of various sputtering variants (including HIPIMS) to produce thick TMN films to be used as targets for laser ablation in liquids (LAL) to produce TMN colloids and inks. We attempt to correlate the crystal structure and chemistry of the film materials with the LAL conditions (laser wavelength, pulse duration, liquid solvent), and with the traits of nanoparticles by implementing a variety of experimental techniques such as optical transmission spectroscopy, AFM, SEM, XPS, and Raman spectroscopy.

3:20pm **TS3-WeA-5 Fully Inkjet-Printed Gas Sensing Antenna Based on Carbon Nanotubes for Wireless Communication Applications***, **Hsuan-Ling Kao,*** Chang Gung University, Taiwan*; L. Chang,* Ming Chi University of Technology, Taiwan*; Y. Tsai,* Chang Gung University, Taiwan

Sensors have been widely used in wearable electronic devices for various detection such as gas, strain, or temperature. The sensor incorporates wireless transmission to reduce the bulkiness and inconvenience caused by the cable. Wireless sensors that embedded sensing film into wireless communication devices such as resonators or antennas has been proposed to achieve small size, simple fabrication, high energy efficiency, and low cost for real-time remote monitoring. In order to embedding sensing film into wireless devices, the conductivity of sensing film is important. Fully inkjet printing technology promotes the green process using by digital controlled pattern in required location due to the advantages fast fabrication, material saving, low cost, high substrate selectivity, and low annealing temperature, which is one of the green process technologies. Carbon nanotubes (CNTs) have been attention for gas sensing applications owing to their high specific surface area and high structural porosity, which enable fact response, high sensitivity and low operating temperature. Inkjet printing technology can precisely control the density carbon nanotubes by droplet spacing (DS) and multi-pass to provide various resistive-type samples to study gas response. However, the relationship between the density of carbon nanotubes and gas sensing response has not been discussed yet. In this work, various DSs and passes were used to control the density of CNTs by pattern rotation. The sensing film and conductive film were printed by commercially carbon nanotube ink (Nink-1000, Nano Lab.) and nanoparticle silver ink (DGP-40LT-15C, Advanced Nano Products Co., Ltd.), respectively. The gas sensing properties were studied by resistance response to validate its feasibility, repeatability, and reversibility. After optimize the CNTs sensing film, wireless sensing antenna composite was designed and fabricated. The appropriate carbon nanotube sensing film was embedded into the dipole antenna by changing the transmission characteristics of antenna. The CNT films allows the electromagnetic transduction of antenna during gas sensing. The appropriate carbon nanotube sensing film was embedded in the dipole antenna to use microwave characteristics to obtain multi-dimensional values for providing high precision detection, which is also more stable than DC resistance value. In addition, it can also reduce the connection-induced loss and the area required for matching to obtain compact area and low power consumption. The wireless antenna sensor can be used in portable electronic products for its light, thin, and compact size and detection in anytime and anywhere.

3:40pm **TS3-WeA-6 Characterization and Evaluation of PVD-Coatings on Bipolar Plates for PEMFC***, **Julian Kapp**, V. Lukassek, V. Mackert, J. Wartmann, H. Hoster,* ZBT Zentrum für BrennstoffzellenTechnik GmbH, Germany*; R. Cremer, P. Jaschinski,* KCS Europe GmbH, Germany

As a result of the steadily increasing demand for energy and the associated need for the responsible use of global energy resources, efficient and sustainable energy conversion and storage is becoming increasingly important. Promising solutions in this context are new developments in fuel cell technology. Here, the chemical energy of an energy carrier (e.g. hydrogen) is directly converted into electrical energy, resulting in high efficiency.

The development of novel techniques for improvement of Proton Exchange Membrane fuel cell (PEMFC) components has to be addressed. One of those components is the bipolar plate (BPP) which has various functions within the PEMFC, such as cell separation, fuel and oxidant gas distribution, collection and transport of generated electricity as well as water and heat management. Therefore, with respect to all those functions, an ideal BPP has to fulfill a number of material requirements, such as high compressive strength, sufficient electrical and thermal conductivity, along with good electrochemical stability. Although metal-based BBPs meet all necessary requirements, the main weak point of these is their susceptibility to corrosion in acid environment, as during PEMFC operation. While formation of the passive layer prevents further corrosion, it often results in electrode catalyst poisoning and contamination of the membrane. Furthermore, an increase in electrical resistance is a typical behavior induced by a passivation process of the metallic surface.

One goal of this work is the suitable series production of corrosion protection coatings with an excellent electrical conductivity on metallic BPP from a PEMFC. The Physical Vapor Deposition (PVD) processes arc and sputtering are used to generate these layers. When selecting the material for the BPP, attention is paid to inexpensive steel and aluminum alloys. The coating material is completely deposited without precious metals for cost reasons. At the same time, the task is to develop a continuous coating process that meets the demands for large-scale production of BPPs.

The developed coating systems were investigated using material characterization (XPS, SEM/EDX, CLSM and Contact Angle Measurements) and in-situ electrochemical analysis. Interfacial-electrical contact resistance (ICR) of coated BPP samples were measured before and after they were exposed to electrochemical corrosion testing. The ICR values and the corrosion rate were compared to United States Department of Energy (DOE) values. Promising coating systems were finally subjected to in-situ diagnostic studies.

4:00pm **TS3-WeA-7 Towards Large Area Scalable Organic Solar Cells using Solution Processing***, **S. Ravi P. Silva**,* Advanced Technology Institute, University of Surrey, UK **INVITED**

The rise in global energy consumption and demand requires a faster expansion in renewable energies. The world at present is powered from energy generated by burning coal/oil and gas to sustained industry, domestic heating and electricity [1]. The world now needs to change from the fossil fuels and march towards a net carbon zero position, with changes urgently needed to the energy mix, all manufacture, including the electronic device industry as well as powering devices during its operational lifetime.

Electronic devices have evolved into nanoscale architectures that could be powered via mW power management systems. The envisioned future sustainable societies will be intrinsically inter-connected: humans to transport to homes to cities etc. driven by inexpensive nano-scale electronics, most likely in the form of inexpensive flexible devices that are connected to everything – the Internet of Everything (IoE) -.This lends itself to delocalized power sources, that can operate under variable conditions. Plastic electronics are ideally suited to produce such devices with some of the lowest carbon footprints. We will examine next generation designs for sustainable nanodevices and renewable energy harvesting systems to help reduce the impact on the carbon foot-print. This will include energy harvesting systems such as plastic photovoltaics and Triboelectric generators.

Hybrid organic-inorganic halide perovskite solar cells (PSCs) show great potential for future solar, due to their incredible efficiency growth in last decade, which now reached as high as 25.7%, competing with the commercially available Si solar cells. Perovskites benefits from superior light absorption coefficient, long carrier diffusion length, high mobility, low exciton binding energy, and high defect tolerance. The solution processability of perovskite materials to form high-quality polycrystalline thin films provides the possibility of low-cost fabrication of PSCs on both rigid and flexible substrates. This can significantly cut the final price of solar energy harvesting. Roll-to-roll (R2R) production of flexible solar cells can also reduce the cost of transferring and storing and makes it possible to easily deliver the solar cells to less developed regions in the world with higher needs for energy.

[1] Silva, S.R.P. (2021), EDITORIAL: Now is the Time for Energy Materials Research to Save the Planet. Energy Environ. Mater., 4: 497-499. https://doi.org/10.1002/eem2.12233

4:40pm **TS3-WeA-9 Rational Design of Perfluorocarbon-Free Oleophobic Textiles***, **Sadaf Shabanian**,* University of British Columbia, Canada*; K. Golovin,* University of Toronto, Canada

Water- and oil-repellent fabrics have global applications within the textile industry and as technical apparel. Fabric finishes utilizing perfluoro compounds (PFCs) are known to render textiles both water and oil-repellent uniquely. However, PFC-based finishes are not sustainable because they compromise environmental and human health, and garment factories have accordingly begun to phase out PFC usage. This is problematic, as all previous studies on fabric finishes indicate that oil repellency cannot be achieved without perfluorination. Here we develop design parameters for fabricating oil-repellent textile finishes using PFC-free surface chemistries. In this work, we demonstrate that oil repellency is possible using PFC-free finishes by controlling a finish's texture size, porosity, and surface chemistry, based on a design framework rooted in wettability theory. For example, a PFC-free, oil-repellent jacket fabric is fabricated that exhibits oleophobicity towards canola, olive, and castor oil in addition to synthetic sweat. The textile remains non-wetted for liquids with surface tension as low as 23.9 $\mathrm{mN\,m^{-1}}$. The equations developed in this work allow for the rational design of oil-repellent textile finishes that do not utilize perfluorinated substances.

Topical Symposia
Room Golden State Ballroom - Session TS1P-ThP

Coatings for Energy Storage and Conversion - Batteries and Hydrogen Applications - TS1 Poster Session

TS1P-ThP-1 Bacezryybo$_{3-\delta}$ Coatings Deposited by Colloidal Coating Process for Sustainable Energy Application*, **Chien-Ming Lei**, P. Lin, Y. Chen,* Department of Chemical and Materials Engineering, Chinese Culture University, Taiwan

BaCeZrYYbO$_{3-\delta}$ (BCZYYb) is one of the high temperature proton-conductive materials, which widely applied in protonic ceramic fuel cell, alkane and alkene reforming, water-gas shifting, ammonia synthesis, CO_2 reduction, etc. The main purpose of this research is to fabricate the BCZYYb coatings on NiO/yttria stablished zirconia (YSZ) substrate via a colloidal coating process. The BCZYYb powders were prepared by solid-state reaction method. The powders were well-dispersed in de-ionic water to prepare the BCZYYb colloidal suspensions. The suspensions were spin-coated on a pre-sintered NiO/YSZ substrate to obtain BCZYYb coating samples for the sequent sintering processes. Several properties of the as-prepared coating samples were analyzed including the crystal phases by X-ray diffractometer (XRD), microstructures by scanning electron microscopy (SEM), electrical properties by electrochemical impedance spectra (EIS). The results show that the main crystalline phase of BCZYYb powders are a single-phase perovskite structure, when the calcination temperature is higher than 1500°C. According to the observation results of SEM microstructures, the BCZYYb coating sample were formed a dense layer on the substrate when the sintering temperature higher is than 1500 °C. But there are still a few pores found from the surface of the coating layer. The average thickness of the coating layer is around 3.3 µm. After the second coating cycle, the pores on the surface were obviously eliminated, and the average thickness of the coating layer is around 5.7 µm. The results of electrical analysis show that the conductivity of BCZYYb single-coating samples are 0.0134 and 0.11261 S/m tested at 500 °C and 800 °C, respectively, and the activation energies are 0.299 eV and 0.292 eV, respectively. The conductivity of the double-coated samples is similar with that of the single-coating sample.

TS1P-ThP-2 PVD Core-Shell-Catalysts for Use in Electrolyzers*, **Jan-Ole Achenbach**, S. Cremer, R. Cremer,* KCS Europe GmbH, Germany

Up-scaling of electrolyzers is necessary to provide sufficient quantities of hydrogen for fuel cells in the future. Alkaline polymer membrane water electrolysis (APM-WE) in particular offers promising potential for the production of hydrogen. However, a requirement for the widespread use of this technology is the cost-effective production of suitable quantities of catalyst.

KCS Europe is pursuing the approach of replacing the usual expensive catalysts containing precious metals with cheaper core-shell particles within the research project AlFaKat. In this approach, particles of a suitable low-cost material are activated by the deposition of a more expensive catalyst material by means of physical vapor deposition (PVD). To realize this, various PVD technologies were evaluated at the beginning of the project with regard to the aspects of 'basic suitability', 'deposition rate' and 'homogeneity'. In a feasibility study on a commercially available batch coater, it was demonstrated that a homogeneous coating of the core particles is possible by PVD process. Furthermore, an economical production of core-shell particles appears possible. The gained knowledge was transferred to a demonstrator, aiming mass production of core-shell catalyst powders on an industrial scale in the future.

Keywords: PVD, Core-shell, Electrolyser, Hydrogen, Catalyst

TS1P-ThP-3 Repressing Noble Metal Ruthenium Target to Reduce the Cost of Bipolar Plate Manufacture in Fuel Cells*, **Jing Yang,*** SCI Engineered Materials, inc, USA

Bipolar plates, as the key component, contribute up to 60% of cost in a proton exchange membrane fuel cell. The most expensive part in bipolar plates is the noble metal coating for catalyst layers. Although there is research and development work done on non-noble metal catalyst, the noble metal coating on stainless steel, is still one of the most widely used combinations due to its good electrical and phonon conductivity, and corrosion resistance.

Sputtering is a preferred coating technique for bipolar plates catalyst layer due to its uniformity, as well as little chance to introduce impurity. However, due to the high price of the noble metal powder and the low usage of a planar sputtering target (15%-30%), the target is one of the costly factors for the process. At SCI, we have developed a process for adding a small portion of the metal powder on top of a spent target to fill in the sputtered area. SCI's process produces a high-density target with an interface between the original target and additional powder that doesn't interfere with the sputtering process. Depending on the target geometry, a spent target backer can be repressed up to ten times before the noble metal backer would need to be fully reclaimed. The repressing process can have a cost reduction on a noble metal powder costs up to 50%.

TS1P-ThP-4 Corrosion Protection of Bipolar Plates in Electrolysers*, M. Welters,* KCS Europe GmbH, Germany*; N. Kruppe,* Schaeffler Technologies GmbH & Co. KG, Germany*; **Peter Jaschinski**, T. Breuer, S. Yang, R. Cremer,* KCS Europe GmbH, Germany*; M. Öte, N. Bagcivan,* Schaeffler Technologies GmbH & Co. KG, Germany

By 2050, 80% of the total energy supply in Germany is to be converted to renewable energies. Since renewable energy generation fluctuates significantly, possibilities for storage and cross-sectoral use must be developed. The direct conversion of regeneratively generated electricity into a secondary energy medium such as hydrogen represents an elementary solution for the technical implementation of the energy transition.

Bipolar plates (BPP), which are combined into stacks, are an essential component of electrolysers in terms of functionality and service life. Currently, both untreated and coated steel and titanium BPP are used. Thereby, a coating can extend the operating conditions and increase the service life. Two main approaches are currently being pursued with regard to corrosion protecting coating systems: carbon-based and metal-based coatings. With regard to the technologies utilized for the production of coatings, there has only been little experience in order to be able to specifically assess the advantages and disadvantages of individual process variants. In addition to the functional suitability of the coatings, in this context the economic process efficiency and suitability for large-scale production are essential aspects. Corresponding aspects often correlate with the coating system to be synthesized.

For this reason, KCS Europe carried out fundamental analyses as part of the StacIE joint project, in which physical vapor deposition (PVD) processes, were compared. Both, the layer morphology and the deposition rate of metallic and non-metallic coatings were investigated and compared. The coated samples were provided to Schaeffler and analyzed with regard to the interfacial contact resistivity using through plane voltage (TPV) measurements. The corrosion stability was investigated using electrochemical cell tests in laboratory scale adapting electrolyzer cell conditions. These findings provide the basis for the development of new concepts, which can be used in the environment of industrial coating of bipolar plates by PVD technology.

Keywords: PVD, Electrolyser, Hydrogen, Corrosion, Protection

TS1P-ThP-5 MOF-Derived Molybdenum Carbide-Copper as an Electrocatalyst for The Hydrogen Evolution Reaction*, W. Chen, **Yu-Chin Shen**, J. Huang,* National Cheng Kung University (NCKU), Taiwan*; S. Wang,* Southern Taiwan University of Science and Technology, Taiwan*; Y. Shen,* National Cheng Kung University (NCKU), Taiwan

The only side product of water electrolysis for hydrogen production is water, which is a clean and environmentally friendly process. However, the HER efficiency is quite low, and the electrocatalyst is required to improve the reaction efficiency. Molybdenum carbide has good catalytic activity and acid resistance. However, high temperature is generally required to prepare molybdenum carbide and the high temperature process leads to excessive growth of nanoparticles. To solve this problem, one of the solution is to combine it with conductive substrates to avoid excessive growth and agglomeration of nanoparticles, and to improve the conductivity of electrons.

In this study,Mo-Cu-MOF was used to confine the growth of molybdenum carbide nanoparticles, and Cu with high conductivity in Mo-Cu-MOF served as the electron transporter through the change of the gas flow (nitrogen → 20% CH_4/H_2) during the annealing process, MoO_2-Cu transformed to η-MoC-Cu. And then with the increase of temperature(800°C→1000°C), η-MoC phase disappeared and β-Mo_2C phase appeared, leading to the transformation from η-MoC-Cu to β-Mo_2C-Cu. Electrochemical performance results show that the overpotential at -10 mA/cm^2 of η-MoC-Cu carbonized at 800°C is -233 mV and the Tafel slope is 73 mV/dec. Finally, some analysis were taken by XRD, TEM, XPS and BET.

TS1P-ThP-7 rGo-SiOx Nanocomposite as Anode Material in Lithium Ion Battery*, **Sheng Hsu**, J. Huang,* National Cheng Kung University (NCKU), Taiwan*; B. Sanjaya,* National Cheng Kung University (NCKU), Taiwan, India

Research to develop negative electrode materials in lithium ion batteries is an emerging topic. Graphite, the most commonly used anode in LIBs, may be useful to operate typical electronic equipment but the theoretically capacity(372mAhg^{-1}) is quite low for applications in advaced devices such as electric hybrid vehicles. Recently, silicon has been leading as a key material of choice owing to its easy availability, low discharge voltage vs. Li/Li+, and outstanding capacity(3580mAhg-1). However, challenges remain due to the significantly high volume change(~400%) which leads electrode degradation and a quick decline in capacity. Recently, SiOx have emerged as one of the promising high capacity anode materials due to lower cost, less volume expansion(~200%), high cyclic stability and rate performance than pure Si making it more suitable material for applications in power batteries. However, SiOx has lower electrical conductivity that requires a high-level conductive agent to fabricate the anode. So far, top-down approach and complicated synthesis procedure at high temperature is usually used to prepare SiOx-C composite. We have expertise in the synthesis of metal oxide and reduced graphene oxide nanocomposite at room temperature that delivered very good reversible capacity, cyclic stability and rate capability when used as anode in LIB. Therefore, we explore a room temperature, low temperature and bottom-up approach for the synthesis SiOx-rGO, Si/SiOx-rGO nanocomposite and apply them as anode material in LIB.

Topical Symposia
Room Golden State Ballroom - Session TS2P-ThP

Sustainable Surface Solutions, Materials, Processes and Applications - TS2 Poster Session

TS2P-ThP-1 The Study of Different Crystalline Moissanite: Nucleation and Growth of Nanoparticle Gold Coatings*, **Tsung-Jen Wu**, S. Song, W. Chen,* Institute of Geosciences, National Taiwan University, Taiwan*; W. Lin,* Department of Materials and Mineral Resources Engineering, National Taipei University of Technology, Taiwan

The localized surface plasmon resonance effect (LSPR) of gold nanoparticles (Au NPs) causes color diversity at the nanoscale, which is often applied to form color of material appearance. Particles below 10 nm of Au NPs show pink-red on coating surface. Results from the analyses of spherical aberration-corrected transmission electron microscopy (AC-TEM) with electron energy loss spectroscopy (EELS) methods, the pattern of nucleation and growth of Au NPs coatings on moissanite (silicon carbide, SiC) with different crystalline are highly variable.

When the Au NPs coating is grown on the amorphous interface layer produced by the CVD method, it is suitable for growth but not nucleation. Under the TEM observations show that the atomic structure is disordered, and only a few inconspicuous lattice fringes form the quasi-granular shapes. On the contrary, the Au NPs coating is directly grown on the moissanite matrix of 4C-SiC or 6C-SiC structures, which is more suitable for nucleation than growth. Therefore, images of TEM with EELS show that the Au-crystal has a pronounced particle shape in the coating surface. The lattice fringes of nanoparticles are prominent and unevenly distributed in coating layers.

Color coating of moissanite needs to be stable and not easy to peel off for different usages. Therefore, the Au NPs coating on the amorphous SiC interface is less prone to exfoliation due to the different surface energy. That is why it is the most suitable way for color coating.

TS2P-ThP-2 Multilayered Structure of PE-Based Polymer Film Composites*, **Marcin Bilewicz**,* Silesan University of Technology, Poland

Polymer processing of films becomes widely developed recent years and evolved in different directions to obtain more complex structures includingmono- and multilayer films and films filled with different fillers like micro- and nano-sized particles. Achievements in polymer chemistry and polymer processing through more advanced technologies equipped with precise sensors and computer controlled brings possibility to obtain more advanced structures of polymer composites. Multilayered films are used recently for many applications like packaging, materials with special barrier properties or with resistance for specific liquids or radiation, e.g. UV. The investigation aims to obtain the composite in form of 3-layer polymer film (fig. 1). Structure of the composite contains polymer based layers. To obtain the film was used blow molding technology on 20 meter high machine with advanced, rotating basket, gravimetric dosing and precise sensors. Tensile strength of 3-layer layer films can be even doubled comparing to single layer film. Additionally material composition and arrangement can brings additional improvement of properties.

TS2P-ThP-3 Understanding the Mechanical Behavior of Nanoporous Si by Molecular Dynamics Simulations*, B. Crutchfield, **Robert Fleming**,* Arkansas State University, USA

Nanoporous materials are of great interest for developing low-density, high-strength materials for a variety of applications, such as zeolites, light-weight structural elements, and scaffolds for biomaterials. These materials are often created from a ceramic or oxide matrix, with porosity generated by sacrificial polymer inclusions that are burned out during thermal processing. As a result, there is much interest in fine-tuning the structure of nanoporous materials and understanding how the mechanical properties are influenced by the porosity volume fraction. In this project, molecular dynamics (MD) simulations have been performed to better understand how porosity affects the stress-strain behavior of nanoporous crystalline silicon (c-Si) as function of crystalline orientation, as well as amorphous silicon (a-Si). From these simulations, the elastic modulus and strength-to-weight figure of merit were determined as a function of porosity and applied strain rate. These results give insights into the mechanical behavior of porous Si-based materials, and can be used to improve the understanding of structure-property-processing relationships for nanoporous materials.

Topical Symposia
Room Golden State Ballroom - Session TS3P-ThP

Processes of Materials for Printed and Flexible Film Technologies - TS3 Poster Session

TS3P-ThP-1 Organic and Perovskite Solar Cells based on 3D-Printed Transparent Conducting Electrodes*, H. Lee, B. Tyagi, **Jae-Wook Kang**,* Jeonbuk National University, Republic of Korea

The photovoltaic performance of organic/perovskite solar cells (OSCs/PSCs) are directly governed by the optoelectronic properties of the transparent conducting electrodes (TCEs) used. However, there exists a classic trade-off the optical transmittance and sheet resistance (R_{sheet}) in most of the TCEs which limited their usage in photovoltaic devices. Moreover, most of the solution-process based TCEs suffer from poor scalability, making them incompatible with large-area device application. To overcome these limitations, we demonstrate the innovative use of three-dimensional direct-ink writing (3D-DIW) techniques for the scalable fabrication of bottom/top transparent conducting electrodes (TCEs) in photovoltaic devices.The 3D-DIW technique allows us to use a wide selection of inks/pastes to form TCEs with various structures. A layer-by-layer printing strategy through 3D-DIW technique can produce TCEs with high aspect ratio and excellent optoelectronic properties unbounded by the transmittance-R_{sheet} trade-off.

TS3P-ThP-2 Development of a Microfluidic System for Oxygen Environment Detection in Cell Culture*, **Wen-Cheng Kuo**, L. Wu, J. Wang,* National Kaohsiung University of Science and Technology, Taiwan

The development of bioreactors based on microfluidic chips has been the focus in the field of drug screening in recent years. In this study, a MEMS process was used to integrate a flexible Clark-type dissolved oxygen sensor into a wafer, and graphene materials with high mechanical strength were used to fabricate electrodes, and the surface modification properties of oxygen plasma were studied. Nano-silver particles (AgNPs) are doped, and electrodes are prepared based on the suction filtration method on a biocompatible Parylene substrate, and Nafion is coated on the electrodes as a selective thin film and a solid electrolyte layer. The bottom and outer layers are encapsulated with biocompatible Parylene, which can avoid cell rejection when implanted in the body, and integrate electrodes into the flow channel of PDMS material, which is conducive to monitoring the dissolved oxygen concentration of the cell environment. Electrode performance analysis was performed using an electrochemical analyzer. The measurement results show that at the two groups of flow rates, it can be seen that the linear range of dissolved oxygen concentration is 0.4-2.08 mg/L, the difference of current density is about 0.1 μA/cm^2, and the reliability is above 0.99. Sensitivity increases slightly with an increasing flow rate of approximately 3%. The response times were about 1.5 and 1.6 seconds, respectively, demonstrating the excellent sensor's response and repeatability.

TS3P-ThP-3 Radiation Effect on Trapping States Modification for Nanowire Junction-less Charge Trapping Flash Memory Devices*, **Che-Wei Lin,*** National Tsing Hua University, Taiwan*; D. Ruan,* Fuzhou University, China*; K. Chang-Liao,* National Tsing Hua University, Taiwan

Recently, charge trapping (CT) flash memory architecture has become the most mature non-volatile memory in commercial market. Following with the scaling trend, the high-energy extremely ultraviolet would be applied on development of high density memory integration and fabrication. Therefore, radiation effect for charge trapping (CT) flash memory will be one of the most important issues in the coming years. Notably, the radiation damage plays a completely different role for different trapping layer material, which may be strongly related to the original trapping states in trapping layer. It seems that the radiation illumination can provide a promising method to optimize the trapping level without complicated band-gap engineering.

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