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

Sustainable Processing and Materials Selection for Surface Solutions

Moderators: Denis Kurapov, Oerlikon Surface Solutions AG Pfäffikon, Liechtenstein, **Fan-Bean Wu**, National United University, Taiwan

1:40pm **TS2-TuA-1 Microplasma-Enabled Upcycling for Nanomaterials Synthesis and Applications***, **Wei-Hung Chiang (whchiang0102@gmail.com)**,* National Taiwan University of Science and Technology, Taiwan **INVITED**

Microplasmas are a special class of electrical discharges formed in geometries where at least one dimension is less than 1 mm. As a result of their unique scaling, microplasmas operate stably at atmospheric pressure and contain large concentrations of energetic electrons (1-10 eV). These properties are attractive for a range of nanomaterials synthesis and nanostructure engineering such as metal nanostructures and semiconductor nanomaterials [1]. Recently, we found that the energetic species including radicals, ions and electrons generated in the microplasmas were capable of initiating electrochemical-assisted reactions for the nucleation and growth of graphene quantum dots (GQDs), silicon quantum dots (SiQDs), and metal nanoclusters (MNCs). Moreover, we discover a simple and controlled synthesis of metal/metal, metal/QD heterostructures using our unique microplasma engineering. In this presentation, I will discuss these topics in detail, highlighting the advantages of microplasma-based system for the synthesis of well-defined nanomaterials for emearging appplications including detections of SARS-CoV-2 proteins [2], cancer and neurotransmitter biomarkers [3, 4], drug delivery [5] and environmental applications such as clean water production [6] and CO_2 adsorption [7]. These experiments will aid in the rational design and fabrication of nanomaterials for nanotechnology-enhanced biosensors and may also have significant impact in emerging applications for next generation biomedical applications.

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2:20pm **TS2-TuA-3 Enhancing Hydrogen Production in 2D Materials via Surface Modifications: An Atomistic Study***, N. Khossossi, S. Sagar, **Poulumi Dey (p.dey@tudelft.nl)**,* TU Delft, Netherlands

Hydrogen (H2) is one of the most potential candidates of sustainable energy produced in an eco-friendly manner. However, there are several challenges to be met before realization of H2 as an energy source. Known bottlenecks are slow kinetics and high overpotential associated with Hydrogen Evolution Reaction (HER), inefficient storage and H2 induced mechanical degradation of structural materials e.g., steels. To establish a viable 'H2-based economy', such bottlenecks could be addressed by designing materials with enhanced properties. To this end, the development of strategies for surface modification e.g., single-atom catalysts (SACs) supported on two-dimensional (2D) materials, are highly desirable. In this study, we perform Machine Learning (ML) assisted high-throughput screening of SACs supported on a 2D Ga-based system to expedite the prediction of HER overpotential. Firstly, Density Functional Theory (DFT) calculations are performed to investigate the catalytic properties of the system for HER. Our results reveal that, akin to many other 2D materials, the pristine Ga-based system is inert for HER due to its weak affinity towards hydrogen. However, the defective Ga-based system with surface sulfur-vacancy, exhibits highly desirable HER catalytic activity. Subsequently, we demonstrate the ML-accelerated prediction of HER overpotential for all transition metals on the system. By leveraging DFT calculations performed on 14 distinct SACs, we put forward a ML based model that maps the HER overpotentials to the atomic properties of the corresponding SACs. The trained ML model exhibits exceptional prediction accuracy and significantly reduces the prediction time compared to DFT calculations. Moreover, we identify an intrinsic descriptor that elucidates the relationship between the atomic properties of SACs and the overpotential. Our study thus provides valuable insights and a robust methodology for screening SACs on 2D materials, facilitating the design of high-performance catalysts for HER.

2:40pm **TS2-TuA-4 Surface Wettability Modification of Polymers for Use in Electrocaloric Heat Pumps***, **Maria Barrera (maria.isabel.barrera.marin@fep.fraunhofer.de)**,* Fraunhofer FEP, Germany*; D. Pinkal, M. Wegener,* Fraunhofer IAP, Germany*; F. Fietzke,* Fraunhofer FEP, Germany

Electrocaloric (EC) materials show a reversible temperature change in response to an external electric field, under adiabatic conditions [1]. In Germany, six Fraunhofer Institutes are working on the development of a refrigerant-free, energy-efficient electrocaloric heat pump, in which the heat transfer is done through latent heat when a fluid evaporates or condenses on the EC material. Due to their relatively high electrocaloric activity and mechanical flexibility, relaxor ferroelectric terpolymers such as P(VDF-TrFE-CFE) are being used as single thin films of a few micrometers thickness as well as multi-layer components to increase the thermal mass of the system [2].

In general, polymers have an intrinsic hydrophobic surface, which might have drawbacks for some applications. As an approach to overcome the poor surface wettability of the polymer components, there is a motivation to use superhydrophilic polyimide (PI) films for encapsulating the EC components, producing a complete wetting of the surface by the working fluid and hence improving the latent heat transfer for optimal performance of the electrocaloric heat pump. Additionally, PI also exhibits outstanding heat resistance and excellent chemical resistance [3], which makes it suitable as insulating material when the application of relatively high electric fields is required for inducing electrocaloric activity on the terpolymers.

For this purpose, the wettability of 12.5 µm thick PI films (Upilex-S, Ube Industries) has been modified by pulsed magnetron sputtering under O_2 atmosphere, combining surface roughening and deposition of metal oxide layers. It has been found that the hydrophilic nature of the coatings together with the appropriate surface topography ensure a durable superhydrophilic performance of the flexible PI foils for (up to now) more than 290 days after treatment.

Results about the influence of composition variation, treatment time, material deposited, and surface roughening on the wetting properties of the PI foils will be presented. Finally, the integration of the encapsulating PI film with the EC polymer components is discussed.

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3:00pm **TS2-TuA-5 High Volume Coating of Metallic Plates for Hydrogen Applications–A Challenge for Coating Machine Builders***, **Philipp Immich (pimmich@hauzer.nl)**, R. Bosch, K. Fuchigami, R. Jacobs, T. Karla, P. Broekx,* IHI Hauzer Techno Coating B.V., Netherlands*; T. Hurkmans, J. Ummels, F. Schuivens,* IHI Ionbond AG, Netherlands

The hydrogen market is growing rapidly. The industry is developing for technical solutions for hydrogen generation and hydrogen-based electricity generation for mobile and stationary applications, and universities and institutes are investigating solutions for the long term. Today's challenge is to bridge the gap between current low to medium technology maturity level and market demand: how to be able to produce hydrogen on large scale and how to scale fuel cell production to high volumes? IHI Hauzer and IHI Ionbond are working on this challenge for many years, developing low cost coatings to supply to the market either by machine solutions and coating services. Key components of electrolyzers and fuel cell stacks like bipolar plates, PTL sheets and CCM's need high quality coatings to enable good catalyst performance, good electrical conductivity and good corrosion properties. For bipolar plates and PTL sheets, Hauzer and Ionbond have developed coatings based on PVD and DOT technology. In the presentation, both technologies will be addressed, including the current status of market introduction and our expected further roll-out within the next years. For PVD, the current main challenges related to machine and process solutions for high speed inline coating will also be addressed. For DOT technology the current main challenges are related to upscaling production capacity in the near future and optimizing precious metal use further.We will further address the requests from the market especially the electrolyzer business and give an outlook about possible solutions to serve these demands.

4:00pm **TS2-TuA-8 Iron Aluminide-Based Coatings as Sustainable Alternative for High Temperature Wear Protection**, *H. Rojacz, K. Pichelbauer, M. Rodriguez Ripoll,* AC2T Research GmbH, Austria*; G. Piringer,* University of Applied Sciences Burgenland, Austria*; P. Mayrhofer,* TU Wien, Institute of Materials Science and Technology, Austria*;* ***Carsten Gachot (carsten.gachot@tuwien.ac.at),*** Vienna University of Technology, Austria

Strengthened iron aluminides show excellent mechanical properties up to 600°C. Therefore, coatings based on the intermetallic phase Fe_3Al are promising candidates to replace Co-, Cr- and Ni- rich coatings; critical raw materials with a high ecological impact. Different strengthening mechanisms can be used in order to increase the hardness of such coatings. Silicon can be used to for solid solution strengthening, whereas carbon as well as the combination Ti and B can be used to precipitate hardphases, intended to result in increased wear resistance. In this study, the influence of different amounts of alloying on the processing and moreover the wear resistance was evaluated. A thorough analysis of the materials and the present phases was conducted, using scanning electron microscopy, electron backscatter diffraction, hot hardness testing, nanoindentation as well as high temperature abrasion testing. Results show that the hardness can be significantly increased from ~260 HV10 to ~ 350 HV10 via solid solution strengthening with silicon or TiB_2 precipitations. Over 405 HV10 can be achieved by precipitating perovskite-type carbides $Fe_3AlC_{0.6}$. Hot hardness results show a good stability of the coatings >500°C. The wear results show a significant reduction of abrasive wear at high temperatures when strengthened, leading to lower wear rates at elevated temperatures due the increased formation of mechanically mixed layer. The obtained wear rates were used to estimate a lifetime utilised for ecological impact calculations from cradle to gate to compare the developed coatings with other wear protection coatings. Here, a reduction of the ecological impact of ~80% compared to cobalt based coatings can be assessed, showing the high potential of iron aluminide-based claddings as high temperature wear protection.

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