Topical Symposia
Room Town & Country A - Session TS5-MoM
Sustainable Surface Solutions, Materials,Processes and Applications

Moderators: Jyh-Wei Lee, Ming Chi University of Technology, Taiwan , **Noora Manninen**, Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein

10:00am **TS5-MoM-1 Innovative Processes for High Performance Materials for Low Carbon Energy in a Circular Economy Approach***,* ***Frederic Schuster (frederic.schuster@cea.fr)****,* CEA, France **INVITED**

Innovative materials and coatings in particular are at the core of innovation process for energy transition. They are not the sole technological challenges but they are often the link that makes progress happen or not, sustainability possible or not, economically feasible or not, ecologically meaningful or not. Metallurgical coatings and thin films have been developped in the field of low carbon energy since a long time ago. This surface functionalization, more and more integrated from the beginning in the steps of design of efficient architectures having to work in environments sometimes harsh and often complex, is the result of the implementation of surface treatment processes sometimes quite old, sometimes revisited, sometimes much more emerging. In a Green Deal approach, sustainability and in particular durability, are the main drivers for the development of surface engineering in energy field. The coatings must often operate under combined stresses such as: mechanical and corrosion, oxidation and irradiation, corrosion and irradiation. In general, the design of a coating must be done on the basis of precise specifications and the choice of the method of elaboration must be made taking into account a certain number of scientific, technological, economical and environmental criteria. Material efficiency, especially when it comes to using for example critical metals as well as the recyclability of scarce resources can also in some cases become one of the criterion of choice. Hybridation of processes is also a strong driver for breakthrough innovation. Surface engineering has made many advances in the past two decades, making possible applications that were not in the past. This is particularly the case with developments for the nuclear energy sector. In the PVD field, the development of ionized PVD such Hipims technology is now very close to the production of protective coatings for EATF (Enhanced Accident Tolerant Fuels) but is also under development in the field of nuclear fuel reprocessing. This very generic technology is also developped in renewable sector, for example for hydrogen production through electrolysis. In the field of CVD, the great diversity of organometallic chemistry offers real opportunities for the development of DLI-MOCVD or Atomic Layer Deposition, and recent advances concerning the upscaling of technology will be presented as well as the great versatility of the process.As for other development of Materials Science and Engineering, surface engineering benefits greatly from digital technologies progresses, in particular Artificial Intelligence, that makes the optimization of complex processes faster.

10:40am **TS5-MoM-3 Pathways for Sustainable Surface Solutions***, J. Vetter, J. Becker, C. Scholz,* Oerlikon Balzers Coating Germany GmbH, Germany*; F. Rovere,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein*; A. Barth,* Oerlikon Metco AG, Switzerland*; M. Esselbach,* ***Noora Manninen (Noora.Manninen@oerlikon.com)****,* Oerlikon Balzers, Oerlikon Surface Solutions AG, Liechtenstein

Surface solutions are enablers of an ecological transformation of production and consumption. The goal is to reach sustainability for instance by product enhancement, efficient materials management, waste reduction, pollution prevention, or energy saving in different applications fields.

Sustainable Surface Solutions are now mostly applied for wear and/or friction reduction, e.g. for tools and automotive components. There are also various deposition or treatment processes which enable different pathways for sustainable solutions for energy conversion and storage. Examples can be found in the field of energy conversion like wind power, fuel cells, electrolyzers, batteries, or supercapacitors. The applications include also thermal insulation, self-cleaning surfaces (e.g. photocatalytic effect, lotus effect), coatings on plastics, optical coatings, medical coatings, decorative coatings, antifouling coatings, corrosion protection coatings, sensoric and electronic coatings.

Also aspects of life cycle assessment "cradle to grave" are of interest for surface solutions beginning with the material selection and ending with the "recycling" (circular economy, cradle to cradle). This analysis has to be intensified besides the pure cost calculations.

The potential and typical dedicated applications of coating solutions based on Oerlikon coating technologies, e.g. for general engineering, emission reduction of cars, including EV and Hydrogen-ICE, and green manufacturing are presented.

11:00am **TS5-MoM-4 Selection of Laser Processing Parameters for Cleaning of Aluminum and FRP Sheets***,* ***Bartłomiej Przybyszewski (Bartlomiej.Przybyszewski.dokt@pw.edu.pl)****, R. Kozera, A. Boczkowska, D. Kuczyńska, H. Garbacz, J. Pura,* Warsaw University of Technology, Poland

This study presents the laser cleaning of grade aluminium alloy sheets as well as Glass Fibre Reinforced Plastics (GFRP) covered with standard paint systems as an alternative for commonly used mechano-chemical stripping methods. A SPI20W laser with wavelength of 1064 nm was applied to remove a variety of painting systems from 2024-T3 alloy sheets with a pure aluminium-clad layer or from composite materials. The paint removing effect from substrates at a laser speed of 500–4000 mm/s, distance of passes of 40-80 µm and different number of passes was studied. Based on detailed substrate examination the best speed for paint stripping was 1000 mm/s with beam distance 40 µm and number of passes strongly depending on the structure of the coating system. The results showed that interaction of laser beam does not cause any significant changes in microstructure or mechanical properties of aluminium alloy, pure aluminium clad or GFRP matrix.

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Topical Symposia
Room Town & Country A - Session TS6-1-MoA
A Session to Acknowledge the Contributions of Joe Greene to the ASED, ICMCTF, AVS, and IUVSTA I

Moderators: Michael Stüber, Karlsruhe Institute of Technology, Germany, **Samir Aouadi**, University of North Texas, USA

1:40pm **TS6-1-MoA-1 Low-Temperature Growth of Epitaxial and Polycrystalline Thin Films Under High-Fluxes of Low-Energy Gas Ions***, **Ivan G. Petrov (petrov@illinois.edu)**,* Linköping University, Sweden, University of Illinois at Urbana-Champaign, National Taiwan University of Science and Technology, Taiwan*; J. Sundgren,* Swedish Association of Engineering Industries, Sweden*; L. Hultman,* Linköping University, Sweden*; J. Greene,* inköping University, Sweden, University of Illinois at Urbana-Champaign, National Taiwan University of Science and Technology, Taiwan **INVITED**

From its inception the benefits of sputter deposition have stemmed from the presence of plasma in the vicinity of the growing film. Bombardment with charged particles and energetic photons affect the substrate initial condition and all stages of film growth: nucleation, coalescence, competitive growth, and recrystallization. Measuring and controlling the fluxes and energy of the charged particles to the substrate is essential in achieving low-temperature growth of high-quality thin films. Under typical conditions during direct current magnetron sputtering (DCMS), the dominant ion species incident at the growth surface while sputtering with N_2/Ar gas mixtures optimized to obtain stoichiometric films is typically Ar^+, while the ratio of the gas-ion flux to deposited metal flux $J_i/J_{Me} \leq 1$. Densification is achieved by increasing the ion energy $E_i$commonly above 100 eV.[1] However, at higher ion energies, a steep price is extracted in the form of residual ion-induced compressive stress resulting from both recoil implantation of surface atoms and trapping of rare-gas ions in the lattice.An alternative approach is offered by strongly magnetically-unbalanced magnetron sputter deposition system, which allows ion-to-neutral flux ratios J_i/J_{Me} incident at the growing film to be varied over extremely wide ranges (up to > 20) at very low (below the lattice displacement threshold) ion energies (E_i ~ 10-20 eV).[2] Using high-flux low energy ion irradiation during deposition opens new kinetic pathways to independently control the texture (from completely 111 to completely 200) and microstructure (from underdense to fully dense) in transition metal (TM) nitride films grown on amorphous substrates as well as to achieve low-temperature epitaxy of refractory materials as well as of metastable alloys.

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2:20pm **TS6-1-MoA-3 Advanced Materials, A Key for the Green and Digital Transformations and for Industrial Competitiveness (Virtual Presentation)***, **Jan-Eric Sundgren (jesundgren@gmail.com)**,* Swedish Association of Engineering Industries, Sweden **INVITED**

Large resources are allocated world-wide to the green and digital transitions. It is also obvious that research and development in close cooperation between different sectors in society play a crucial role for this twin transition. Another important part to achieve the necessary change is access to advanced materials and new innovative processes for sustainable production of these materials.

In this talk we will describe a mapping study that have conducted of the Swedish broad field of advanced materials. The results show that the value added for Swedish Industries manufacturing advanced materials has continuously increased in the years studied (2011-2019). The field is also expected to globally grow with 5-10% annually. In addition to the industry sector Sweden has also a strong academic community, with several research groups at the international forefront to which Prof Joe Greene has contributed significantly. Based on the mapping conducted and other recent studies we will present recommendations aimed to further boost the field of advanced materials both in Sweden and elsewhere.For example, an increased coordination and cooperation between different sectors and disciplines as well as the use of computational and AI methods are necessary to reduced lead times for industrial impact and thus to industrial competitiveness in the field.

3:00pm **TS6-1-MoA-5 Industrial Magnetron Sputtering: Interfaces & More***, **Wolf-Dieter Münz (W_DM@gmx.at)**,* Consultant, Austria **INVITED**

Magnetron sputter deposition of wear resistant hard coatings has found broad acceptance in many industrial applications serving e.g. the automotive, micro mashining, aeronautical and biomedical but also decorative industry. Perfect adhesion is a dominant precondition to meet reproducible production conditions. The paper discusses three types of substrate pretreatment prior to the actual film deposition: intensive Ar etching, metal ion etching by cathodic arc and HIPIMS technology respectively. Particular attention is paid to ion implantation during metal ion etching and the related epitaxy of the growing film. The resulting enhanced adhesion guarantees successful deposition of very hard and highly stressed e.g. TiAlN based superlattice coatings. The industrial realization of these methods of pretreatment is outlined by verification in a double (twin) cathode, combined cathodic arc/unbalanced magnetron and combined HIPIMS/unbalanced magnetron approaches. Two industrialized applications will be discussed in detail: (1) performance of superhard C-DLC coatings utilizing a five cathode batch type coater and (2) a simultaneous HIPIMS/UBM process depositing multilayer TiAlN/CrN coatingsproduced in a large scale multi cathode equipment.

3:40pm **TS6-1-MoA-7 Applying Thin Film Synthesis and Characterization Methods to Improving Photovoltaics***, **Angus Rockett (arockett@mines.edu)**,* Colorado School of Mines, USA **INVITED**

Prof. Joe Greene has been an amazing mentor and teacher to me. Without his help and patience, I would never have succeeded as I have. My career is entirely thanks to Joe both during my graduate study and more importantly afterward. This talk briefly reviews how the synthesis and characterization of thin films, particularly by sputter deposition, as I learned from or with the support of Joe, has been applied to the full spectrum of materials applied to photovoltaics. Film materials studied include silicon, binary, and ternary materials and alloys. Novel dielectrics and contact materials have been developed including a metastable alloy of 30% Cu in bcc Mo. Characterization methods include microstructural, microchemical, and optoelectronic approaches. The results have been simulated with continuum elasticity, finite element, Monte Carlo, and density functional methods. The result is a detailed picture of how defects in semiconductors affect the performance of photovoltaics and how they are related to process conditions.

4:20pm **TS6-1-MoA-9 May the Interatomic Forces be with You; Self-Organized Nanostructure Design in Functional Nitride Alloy Films (Virtual Presentation)***, **Lars Hultman (lars.hultman@liu.se)**, G. Greczynski,* Linköping University, Sweden*; I. Petrov, J. Greene,* Linköping University, Sweden; University of Illinois at Urbana-Champaign, USA; National Taiwan University of Science and Technology, Taiwan **INVITED**

During ~40 years our group has developed strategies for thin film formation during physical vapor deposition, spanning epitaxial growth and crystallographic texture control to self-organization of nanostructures. Both primary and secondary phase transformations from the vapor phase and in the as-deposited state, respectively, are explored. Self-organization from surface and bulk diffusion is used to enhance mechanical and electronic properties of functional ceramics by structural design, here exemplified by transition metal and group-III nitride metastable alloy model systems: TiAlN, ZrAlN, HfAlN, TiSiN, MoVN, VWN, and InAlN. Material characterization is performed by XRD, analytical STEM, FIB, and isotopic-substitution APT. Molecular dynamics simulations, *Ab initio* calculations, and phase-field modelling are employed to assess phase stability, diffusion, and decomposition behavior from lattice mismatch and electronic band structure effects. Our concept of age hardening is reviewed, where spinodal decomposition is established for TiAlN by the formation of cubic-phase nm-size domains in a {100}-checker-board pattern of TiN and AlN at temperatures corresponding to cutting tool operation. 2-D-nanolabyrinthine structuring in ZrAlN is obtained from intergrowth of non-isostructural phases *c*-ZrN/*w*-AlN: {110}║{11-20} interfaces. Superhardening in TiN/Si_3N_4 nanocomposites takes place due to Si segregation forming a few-monolayer-thick SiN_x tissue layer, which is shown to be vacancy-stabilized cubic-phase SiN_x. A hardness maximum at 34 GPa – short of ultrahard – is observed in TiN/SiN_x(001) superlattices at the epitaxial-to-amorphous thickness-limit for the SiN_x layers. For $In_xAl_{1-x}N$, we report inherently-curved-lattice epitaxial growth of nanospirals with controllable chirality as well as core-shell nanorod formation. The emerging inherently nanolaminate family of so-called MAX phases is briefly reviewed with examples from Ti_2AlN including for non-van-der Waals intercalation of noble metals. More recently, we discovered transmorphic heteroepitaxy between CVD-grown AlN epilayer and SiC(0001) wafer substrates. The atomic configuration transits over two atomic layers from SiC ® $(Al_{1/3}Si_{2/3})_{2/3}N$ with ordered vacancies on 1/3 of the Al and Si positions ® $(Al_{2/3}Si_{1/3})N$ ® AlN. The resulting special epitaxial AlN layer has state-of-the-art low lattice defect density, enabling growth of high-quality thin GaN HEMT heterostructures for superior power electronics.

5:00pm **TS6-1-MoA-11 From Thin Films to Solid Oxide Fuel Cells***, Scott Barnett (s-barnett@northwestern.edu),* Northwestern University, USA **INVITED**

This talk will start with a brief history of how my background in thin films in Joe Greene's group helped lead to a new approach to making practical solid oxide fuel cells (SOFCs). Although thin film vapor deposition techniques have not supplanted conventional ceramic processing of SOFCs, this talk will highlight vapor deposition methods likely to play an increasing role going forward. Recent developments in SOFCs and solid oxide electrolysis cells (SOECs) will be discussed. SOFCs are being increasingly applied for clean efficiency electrical generation, and produce highly concentrated CO_2 exhaust that is nearly sequestration-ready. SOECs have potential for highest efficiency conversion of renewable electricity to hydrogen and other renewable fuels. The devices can also be operated in both SOFC and SOEC modes to allow large-scale electrical energy storage – a key technology needed for enabling increased utilization of renewable wind and solar energy resources. Current research areas will be highlighted including improving device performance via reduced electrolyte thickness and highly-active nano-scale electrodes, and determining the mechanisms that limit device long-term stability.

Topical Symposia
Room Town & Country A - Session TS6-2-TuM

A Session to Acknowledge the Contributions of Joe Greene to the ASED, ICMCTF, AVS, and IUVSTA II
Moderator: Scott Barnett, Northwestern University, USA

8:00am **TS6-2-TuM-1 Metal-Ion-Controlled Thin Film Growth: What Have We Learnt During the Last Decade?***, Grzegorz (Greg) Greczynski (grzegorz.greczynski@liu.se),* Linköping Univ., IFM, Thin Film Physics Div., Sweden*; I. Petrov, J. Greene,* University of Illinois at Urbana Champaign, USA*; L. Hultman,* Linköping University, IFM, Thin Film Physics Division, Sweden **INVITED**

Ion irradiation is a key tool for controlling the nanostructure, phase content, and physical properties of refractory ceramic thin films grown by magnetron sputtering. Up until recently, gas ion irradiation was used to enhance adatom mobility in the surface region. Development of high power pulsed magnetron sputtering (HiPIMS), which provides metal-ion plasmas with tunable degree of ionization, enabled systematic studies of the effects of metal-ion irradiation on properties of refractory ceramic thin films. The original motivation for the use of metal-ions stems from the fact that they are film constituents, hence they can provide the benefits of ion-mixing (film densification at low film-growth temperatures) without causing the high compressive stresses associated with trapping of gas ions in interstitial sites. Since 2012 we have explored several pseudobinary TM nitride model systems including TiAlN, TiSiN, VAlN, TiTaN, TiAlTaN, and TiAlWN.[1] Experiments were carried out in a hybrid HiPIMS/DCMS configuration.[2]A substrate bias V_s was synchronized with the metal-ion-rich portion of the HiPIMS pulses to allow for a control of metal-ion energy, based on the input from time-resolved mass spectrometry analyses. This enabled us to suppress the role of gas ion irradiation and allowed us to study the influence of intense M_1^+ andM_2^+ metal-ion fluxes on film growth kinetics, microstructure, and physical properties over a wide range of M_1M_2N alloy compositions. We established that the effects of metal-ion irradiation depend on the mass of incident ion with respect to that of film constituents.Irradiation with lower-mass metal-ions (e.g. Al^+ or Si^+) results in the near-surface trapping with the depth controlled by the V_s amplitude. This enabled unprecedented control over the phase content of metastable ternary nitrides and the growth of NaCl-structure M_1M_2N solid solutions far above the M_1N concentration range achieved with DCMS.[3] At the other extreme, bombardment of the growing film surface with pulsed high-mass metal ion fluxes (e.g., W^+ or Ta^+) during HiPIMS/DCMS deposition of $Ti_{1-x}Ta_xN$, $Ti_{1-x-y}Al_xTa_yN$, and $Ti_{1-x-y}Al_xW_yN$ alloys provides fully-dense, low stress, films without intentional substrate heating. The high metal-ion mass irradiation leads to effective low-energy recoil generation that provide sufficient adatom mobility, necessary to obtain high-quality fully-dense films, in the absence of conventionally used resistive heating. Thus, the process energy consumption is greatly reduced, while the new possibilities open up for coating temperature-sensitive substrates.

8:40am **TS6-2-TuM-3 Predictive Kinetics-based Epitaxial Film Growth Modeling for the SiGe, Si:B and SiGe:B Systems***, Glenn Glass (glenn.glass@intel.com),* Intel Corporation, USA **INVITED**

CVD growth of Si-based epitaxial thin films continues to hold relevance in industrial applications as well as a model system for scientific discovery. Observation of thin film growth rate trends from hydride precursors combined with quantitative temperature-dependent surface measurements of dangling bond reaction-site densities are combined as input parameters. We demonstrate a model with no fitting parameters that predicts film growth rates across a wide range of temperature, gas flow and flow ratios. The combination of surface bond density measurements (activation energy and frequency factor in the Polanyi–Wigner formalism) and growth rates provides insight into surface segregation behavior that can drive significant second-order effects including roughening and relaxation.

9:20am **TS6-2-TuM-5 Growth Kinetics of Spontaneous Superlattices, and Single Wall Carbon Nanotubes Using Gas Phase Precursors***, Yonglim Foo (Yonglim.Foo@SingaporeTech.edu.sg),* Singapore Institute of Technology, Singapore **INVITED**

The segregation of C during $Si_{1-y}C_y$/Si(001) growth during gas-source molecular beam epitaxy, using Si_2H_6 and CH_3SiH_3 has a strong influence on the growth kinetics. During growth of the initial Si-rich layer, strain-driven C segregation to the subsurface results in charge transfer from surface Si atom dangling bonds to C backbonds. This decreases the Si_2H_6 sticking probability, and, hence, the instantaneous deposition rate, thereby enhancing C segregation. This results in an interesting observation, where alloy superlattice structures consisting of alternating Si-rich and C-rich layers form spontaneously during constant Si_2H_6 and CH_3SiH_3 precursor fluxes at Ts = 725–750 C. The Si-rich layer continues until a critical C coverage is reached allowing nucleation of a C-rich layer which grows until the excess subsurface C is depleted. The process then repeats with periods tunable through the choice of Ts and $y_{avg.}$

The second section of the talk will be on the early career research work by author, which is heavily influenced by Professor Joe Greene's attention to growth kinetics. The growth dynamics of a single-walled carbon nanotube (SWNT) was observed in real-time using an in situ ultrahigh vacuum transmission electron microscope at 650 °C. SWNTs preferentially grow on smaller sized catalyst particles (diameter ≤ 6 nm) with three distinct growth regimes (incubation, growth, and passivation). All of the observed SWNTs grow via a base-growth mechanism with C diffusion on active Ni catalyst sites. Under the same experimental conditions, formation of carbon nanocages was observed on larger Ni catalyst particles. The evolution of SWNTs or nanocages is dependent on catalyst size, and this can be rationalized from both energetics and kinetics considerations.

10:00am **TS6-2-TuM-7 Engineering of Soft Materials for Stretchable Electronics***, Nae-Eung Lee (nelee@skku.edu),* Sungkyunkwan University, Korea (Republic of) **INVITED**

Stretchable electronics is promising for wearable sensor applications. In particular, wearable sensor devices with a form factor of skin-attachable patch which can sense skin strains, monitor vital signs and detect biomarkers from collected body fluids for disease diagnostics, and can be also used to detect the hazardous environmental factors around human have been extensively investigated. For successful implementation of various components into such stretchable skin-attachable sensor patches, engineering of soft substrates and functional materials is of great importance for skin-conformality, durability, stability, and minimal strain-induced signal interference. In this presentation, structural engineering of conventional elastomeric substrates and synthesis of intrinsically stretchable materials for application to stretchable electronics will be discussed. Firstly, structurally engineered substrates of mogul-patterned, trench-patterned, or skin-mimicking elastomers which can mitigate the stress level on the functional layers on them have been designed and developed. The applications of the structurally engineered elastomeric substrates to stretchable physical sensors (strain, pressure, and temperature), chemical sensors (gases) and biosensors (protein, enzyme) by employing low-dimensional nanoscale materials (0D, 1D and 2D), nanocomposites and their hierarchical nanohybrids onto them will be highlighted. Secondly, I will present the synthesis of intrinsically stretchable, transparent, and tough copolymer substrate with excellent temperature and chemical resistance applied to stretchable substrate and microfluidics. In addition, other forms of intrinsically stretchable functional materials such as stretchable solid or hollow microfibers with biodegradability or conductivity will be also demonstrated for electrode materials or microfluidic channel materials for stretchable bioelectronics.

Topical Symposia
Room Pacific C - Session TS2-1-TuA
Thin Films on Polymer Substrates: Flexible Electronics and Beyond

Moderators: Oleksandr Glushko, Erich Schmid Institute of Materials Science, Austria, **Barbara Putz**, Montanuniversität Leoben, Leoben, Austria

1:40pm **TS2-1-TuA-1 in Situ Observation of Strain Transfer and Crack Formation in Evaporated and Printed Thin Films and Devices on Compliant Substrates***, **Patric A. Gruber (patric.gruber@kit.edu)**, N. Misra, T. Haas , S. Yi, B. Kim,* Karlsruhe Institute of Technology (KIT), Germany **INVITED**

Compliant substrates enable the fabrication of flexible electronics for numerous applications like flexible displays, solar cells, batteries or wearable/biocompatible electronics. However, the reliability of such devices is limited by the stretchability of the inorganic components. So far, little experimental work has been carried out to investigate the mechanical properties of thin inorganic films on compliant substrates at high strains and cyclic loading. Here, we present experimental results for the flow stress, fracture strain and fatigue behavior of evaporated and printed Ag films as well as printed thin film transistors on compliant substrates. The film systems have been tested by a synchrotron-based tensile testing technique (up to 10% total strain) as well as cycling loading (50 Hz, strain amplitude up to 2.5%) and have been characterized by SEM and FIB microscopy. The synchrotron experiments yield the stress evolution and strain transfer within the film systems whereas the cyclic tests give the fatigue lifetime. On the other hand, *in situ* electro-mechanical testing, *in situ* tensile tests in the SEM and stationary FIB investigations reveal the evolution of electrical performance, crack morphology and crack density as well as fatigue damage in the individual films. First, results of electro-mechanical testing of printed and evaporated Ag films will be presented. Electrical conductivity and mechanical reliability are investigated with respect to the inherently nanoporous microstructure, and are compared to those of evaporated Ag films of the same thickness. It is shown that there is an optimized nanoporous microstructure for inkjet-printed Ag films, which provides a high conductivity and improved reliability. It is argued that the nanoporous microstructure ensures connectivity within the particle network and at the same time reduces plastic deformation and the formation of fatigue damage. Furthermore, results on printed In_2O_3 thin film transistors are presented. Here, the interplay of the polymer substrate and solid polymer electrolyte with the metallic and ceramic interlayers within the transistor structure will be discussed based on the strain evolution within the individual layers determined from the in situ synchrotron experiments.

2:20pm **TS2-1-TuA-3 Electrical Resistance During Cyclic Loading of Conductive Coatings – What Information is Hidden in the Data?***, **David Gebhart (david.gebhart@oeaw.ac.at)**, M. Cordill,* Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria

An increase in electrical resistance during cyclic loading of metallic films on polymer substrates is mainly a function of crack density in the film, mean crack length (and its distribution), and mean crack depth. Those factors cannot be separated in a single data point but an ensemble of datapoints may show trends that can be attributed to single factors. With a material system of a 150 nm Au coating on polyimide (Upilex-S; 50 µm), with and without a 30 nm Cr interlayer, a thorough analysis was done on information contained within electrical data obtained during cyclic tensile straining. With strain-controlled sinusoidal loading, twenty 4-wire resistance data points were recorded per cycle. By analyzing peak shape evolution, i.e. full width at half maximum values, cycle amplitudes, and curves fitted to minima and maxima points of each cycle, various damage initiation and propagation events could be identified and a distinction could be made between through-thickness cracking and surface necking. The findings are validated with imaging and characterization methods. Easy to implement and easily automated methods are presented, which can be used retroactively on acquired data, to make an argument for the effectiveness of deep analysis of electrical resistance data in fatigue investigations of conductive coatings.

2:40pm **TS2-1-TuA-4 Plasma Surface Activation of Epoxy Painted Polymer Composites to Enhance Adhesion of PVD Coatings***, **Nicolas Ranger (nicolas.ranger@oerlikon.com)**,* Oerlikon Balzers/IRCER, France*; C. Jaoul, P. Tristant,* IRCER, France*; T. Maerten,* Oerlikon Balzers, France*; S. Belveze,* Oerlikon Balzers , France*; S. Guimond,* Oerlikon Balzers, Liechtenstein*; M. Cavarroc,* Safran Tech, France

Polymer-based composites materials are increasingly employed in aircraft industry as replacement of metallic components due to their excellent specific properties (strength- and stiffness-to-density ratios). But aircraft surfaces are subject to harsh environmental conditions (rain, sand, gas, etc.) detrimental to polymer composites lifetime. As a result, deposition of hard ceramic films is required to protect them. PVD coating are envisioned but adhesion of such films is known to be low on these substrates [1].

Surface pre-treatments are therefore critical to improve the adhesion of coatings on polymer composite. Nowadays, it is commonly accepted that the enhancement of the adhesion of a coating is related to the density of nucleation sites at the polymer surface [2-3]. One simple way to quantify the increase of nucleation sites is by measuring surface energy.

The aim of the present study is to evaluate the effect of low pressure Ar, N_2 and O_2 plasmas on epoxy painted carbon fiber reinforced composite surface as adhesion-promoting treatment. Various plasma conditions are tested by changing parameters like gas mixture, bias voltage and duration. The surface energy is measured by contact angle measurements. These measurements are complemented by chemical analysis (XPS) and surface morphology observations (Profilometer, SEM, confocal microscopy) to understand the surface modification mechanisms.

Finally, the most promising plasma conditions as adhesion-promoting treatment are applied prior to the deposition of a titanium film deposited by magnetron sputtering. The adhesion is, then, evaluated using conventional methods (scratch and pull-off tests) to quantify the benefit of the pre-treatment.

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3:00pm **TS2-1-TuA-5 MOKE-XRD Experiment for the Study of Magnetomechanical Properties of Thin Films Deposited on Stretchable Substrates***, H. Mahmoud,* Université Sorbonne Paris, Université de Poitiers—CNRS, France*; **Damien Faurie (faurie@univ-paris13.fr)**,* Université Sorbonne Paris, France*; P. Godard,* Université de Poitiers—CNRS, France*; D. Thiaudière,* Soleil Synchrotron, France*; P. Renault,* Université de Poitiers—CNRS, France*; F. Zighem,* Université Sorbonne Paris, France

Stretchable/flexible electronics has been a rapidly growing field for several years. In particular, magnetic systems realized on stretchable/flexible substrates are of increasing interest for their potential applications [1-2]. These will be subjected to large strains during their use. It is therefore important to understand the different phenomena involved at very large strains in order to estimate the durability of their functional properties, through the study of elementary magnetomechanical phenomena [3].

In this context, we have developed an original experiment coupling *in situ* Magneto-Optical Kerr Effect (MOKE) magnetometry, biaxial traction, digital image correlation on the DiffAbs beamline of the SOLEIL synchrotron, in order to follow the evolution of the magnetic quantities at different mechanical regimes (elastic domain, plasticity, multicracking) (figure 1 (a), supplementary material). This device has been used to study model thin films of Cobalt (20 to 100 nm) deposited on Kapton (polymide) substrate. The evolution of the magnetization curves as a function of the applied strain was analyzed in order to estimate the evolution of the coercive field, the remanent magnetization and the saturation field. This analysis has been correlated to the different deformation micromechanisms estimated thanks to the monitoring of the elastic strains by X-ray diffraction (figure 1 (b), supplementary material).

Through this presentation, we will show the instrumental development of the device (biaxial tensile machine coupled to the magnetometer) as well as the mechanisms underlying the measured properties according to the type of loading (equibiaxial or complex). The perspectives of these first studies will also be discussed (understanding of the physical mechanisms, effects of lateral nanostructuring, ...).

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4:00pm **TS2-1-TuA-8 Nanoscale Deformation Mechanisms in Thin Film Metallic Glasses Explored by in-Situ SEM With Digital Image Correlation***,* ***Oleksandr Glushko (oleksandr.glushko@unileoben.ac.at)****, C. Mitterer, J. Eckert,* Montanuniversität Leoben, Austria

Digital image correlation (DIC) is a powerful technique allowing detailed mapping of local strain distributions from the images of deformed surface. Spatial resolution of DIC is restricted only by the pixel size of the image and quality of random speckle pattern on the surface. Here we demonstrate the capabilities of DIC to capture propagation of shear bands in thin film metallic glasses with spatial resolutions down to few tens of nanometers.

PdSi metallic glass films were sputter deposited on polyimide substrate and then covered with randomly distributed nano-sized Indium islands. Additionally, the films were pre-structured with specific FIB-milled patterns in a way that the formation of cracks is locally prohibited but in-plane shear bands can freely propagate. Straining experiments were performed in-situ in SEM and GOM Correlate software was employed for DIC analysis. Shear bands propagating within the film plane do not necessarily lead to appearence of surface traces and thus cannot be detected on the SEM images with a naked eye. With DIC analysis shear bands are clearly visualized as bands of extremely localized strains, significantly exceeding the strains in the rest of the film. Local strains before and after generation of shear bands were carefully measured and an analogue of von Mises yielding criterion is formulated. Additionally, provided analysis proved that shear bands are “cold” during operation, i. e the temperature on the surface stays far below the glass transition temperature. Demonstrated technique of combining pre-patterned polymer-supported films with in-situ SEM straining and DIC is shown to be extremely effective to capture microplasticity phenomena with nanoscale resolution.

Topical Symposia
Room Town & Country A - Session TS6-3-TuA

A Session to Acknowledge the Contributions of Joe Greene to the ASED, ICMCTF, AVS, and IUVSTA III

Moderators: Ivan G. Petrov, University of Illinois at Urbana-Champaign, USA, **Angus Rockett**, University of Illinois at Urbana-Champaign, USA

1:40pm **TS6-3-TuA-1 Perspective on Thin-Film Metallic Glasses: Road to Industrial Production (Virtual Presentation)***,* ***Jinn P. Chu (jpchu@mail.ntust.edu.tw)****,* National Taiwan University of Science and Technology, Taiwan **INVITED**

This presentation provides brief overviews on the recent application-oriented researches on thin film metallic glasses (TFMGs) in various fields such as biomedical, biosensors, and nanotube arrays. For instance, TFMGs have been shown to improve the mechanical properties and the surface properties (such as non-stick characteristics) of the underlying substrates. The surface topography of TFMGs has also been revealed to affect chemical activity, cell-adhesion, and wetting-related properties of surfaces. In addition, the first-ever metallic-glass nanotube array on Si has been successfully fabricated by a widely-used lithography and sputter deposition process for very large-scale integration. These research works actually suggest that thin film is the most suitable approach to answer many unrevealed questions on its bulk metallic glass counterpart. Nevertheless, the remaining question is where the researches on TFMGs are headed. This article also highlights future challenges and opportunities associated with the further development of TFMG for the industrial production.

2:20pm **TS6-3-TuA-3 Hollow Cathode Discharges: The Influence of the Electrode Material and Cathode Geometry***,* ***Stephen Muhl (muhl@unam.mx)****,* IIM UNAM, CDMX, Mexico*; R. Sangines,* CNyN (CONACYT) UNAM, Ensenada, BC, Mexico*; J. Cruz,* CNyN UNAM, Ensenada, BC, Mexico **INVITED**

I first meet Joe Greene in 1999 in a Mexican Vacuum Society meeting, and in 2011 he invited me to submit a review article on my hollow cathode work to Thin Solid Films. That task greatly increased my knowledge of hollow cathodes, but also showed me that I did not really understand how they worked.

Traditionally, in a low-pressure gas discharge, electrons emitted from the cathode are accelerated by the cathode sheath. They produce light emission in the cathode glow, then stop producing it in the cathode dark space until they get to the edge of the negative glow. The secondary electrons and ions are accelerated by the sheath producing additional ionization and this avalanche maintains the discharge. However, recent work has shown that this is wrong in that the cathode glow is not generate by electrons, and that the basic description has many problems.

Hollow cathodes include almost any cathode with a cavity-like geometry, cylindrical, planar or spherical. In 1916, F. Paschen showed that such a system can produce a high electron flux and plasma density, in part, by reducing the loss of electrons in the similar way as in a magnetron. In general, there are three types of hollow cathode discharge, at low power and/or low gas pressures, it is a typical low-current high-voltage plasma. For certain combinations of gas pressures and hollow cathode diameters, with high applied powers, the negative glow of the plasma almost completely fills the interior the cathode and the plasma current, and density can be orders of magnitude greater than that of a typical discharge. Finally, if the cathode material is not cooled the discharge can transform into a dispersed arc, the hot electrode produces thermal-field electron emission as an additional source of electrons, and this even further increases the plasma density and current.

The conventional explanation for the hollow cathode effect involves high-energy “pendulum” electrons which are reflected between the opposing sheaths on either side of the inside of the cathode; the long trajectory of these electron is considered to produce an increased number of secondary electrons, with this resulting in the higher plasma density and current. Here we describe some problems associated with this well-accepted model and present an alternative explanation based on doubly charged ions. Finally, we report the results of recent studies of the dependence of the I-V characteristics of an argon discharge on the geometry of a cylindrical cathode, the metal used to make the cathode, spatially resolved optical emission spectroscopy of the hollow cathode and measurements of the ion flux as a function of the experimental conditions.

4:00pm **TS6-3-TuA-8 Ti-Nb Based Alloy Coatings Produced by Magnetron Co-sputtering***,* *D. Gonzalez,* Universidade Federal de Sao Carlos, Brazil*; V. Amigo-Borras,* Universitat Politècnica de València UPV, Spain*; V. Mastelaro,* Universidade de Sao Paulo, Brazil*; **Pedro Nascente (nascente@ufscar.br)**,* Universidade Federal de Sao Carlos, Brazil **INVITED**

The AISI 316L stainless steel (SS) has been widely used as implant material due to its adequate biomechanical and biocompatibility properties. Its advantages compared to other used metallic materials, such as the CoCr alloys and titanium and its alloys, are its formability, weldability, and affordability. One of its main disadvantages is the release of harmful corrosion products in the human body. This limitation can be overcome by the coating of the SS with an alloy that has a higher corrosion resistance and a better biocompatibility. Ti, Nb, and Zr are non-toxic and non-allergenic elements that exhibit excellent biocompatibilityand low cytotoxicity; in addition to these qualities, they have total solubility among themselves. We report on binary Ti-Nb and ternary Ti-Nb-Zr alloy coatings deposited on AISI 316L SS by magnetron co-sputtering. The composition, phase formation, structure, morphology, texture, film growth, and mechanical and tribological properties of the $Ti_{80}Nb_{20}$, $Ti_{75}Nb_{20}Zr_5$, $Ti_{60}Nb_{20}Zr_{20}$, $Ti_{50}Nb_{20}Zr_{30}$, and $Ti_{40}Nb_{20}Zr_{20}$ (at.%) coatings are investigated. For low Zr content, two phases are detected: Predominantly the β phase and, in a lesser degree, a nanoscale metastable ω phase. For Zr amounts equal or higher than 20 at.%, only the β phase is detected. The coating with higher Zr content presents lower elastic modulus and hardness values. The coating morphology is affected by the increasing addition of Zr, from a growth characteristic of the zone I to a growth characteristic of the zone T of the structure zone diagram (SZD). The texture also is influenced by the Zr amount, going from {111} to {101} for the direction of the film growth, due to the increase in the strain energy and the total mass of the species in the plasma. The Ti-Nb-Zr coatings exhibit high ductility and high adhesion,, which are characteristics of a high combined plastic deformation on the coating/substrate system, and no delamination is observed. These findings indicate that the Ti-Nb-Zr coatings are promising candidates for biomedical applications.

4:40pm **TS6-3-TuA-10 Bill Sproul Award and Honorary ICMCTF Lecture: Modelling Reactive Sputtering: Back to the Future***, **Diederik Depla (Diederik.Depla@ugent.be)*** [1] *, J. Van Bever, K. Strijckmans,* Ghent University, Belgium **INVITED**

When looking back on our endeavor in the field of reactive magnetron sputtering, the authors may conclude that the technique is conceptual simple. This simplicity however conceals the underlying complex relationships between the simultaneously occurring processes. Hence, experimental results are often surprising or unexpected. Modelling of reactive magnetron sputtering is therefore indispensable to unravel this complexity. This conclusion was also drawn by others in the early days when this technique was first applied. Though less complete as compared to the historical research by J. Greene, a short historical overview of modelling attempts will be presented. However, it will provide a framework to discuss some essential and common features of the models, including the Reactive Sputter Deposition (RSD) model developed by our team. For the latter model the implemented processes will be reviewed. Some important results, such as the double hysteresis behavior and the presence of non-reacted oxygen atoms will be discussed. If these results are confronted with experiments, the general trends can be explained. If it either comes to the details, it is clear that new developments will be needed in the future. In this way our endeavor in modelling is luckily not finished.

[1] **Bill Sproul Awardee**

Topical Symposia
Room Town & Country B - Session TS3-WeA
Electrochemical Cells – Hydrogen and Batteries

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

3:20pm **TS3-WeA-5 Current and Future Trends in Materials for Advanced Lithium Batteries**, *O. Kahvecioglu, **Carrie Siu (b294370@anl.gov)**,* Argonne National Laboratory, USA **INVITED**

The story behind lithium-ion batteries is nothing less than a quest for a new better performing materials and more reliable, safer devices. As far back as the late 1970s, a team of pioneering scientists began research on an invention that is known today as the lithium-ion battery or LIB. This rechargeable electrical energy storage device powers everything from hand-held electronics to power tools to electric vehicles and, in the near future, possibly even large vehicles and aircrafts. In 2019, the three brilliant minds behind LIB development, John B. Goodenough, M. Stanley Whittingham, and Akira Yoshino were recognized for their discovery with the award of the Nobel Prize in Chemistry. Like any other great discovery, early LIBs were not perfect. The first experiments that used electrodes made from titanium disulfide and lithium metal were less than successful. After these early batteries short-circuited and caught fire, it was decided to halt the experiments. Not for long. John B. Goodenough came up with another idea. In the early 1980s he substituted lithium cobalt oxide (LCO) for the cathode instead of titanium disulfide. This new material was so successful that modern-day cell phone batteries still use it.

To satisfy market demands, the quest for new materials rages on. Although Li-ion batteries are proven and reliable technologies, they are not perfect, and suffer from performance degradation over time, limited shelf life and most importantly, some hazards associated with their use. Scientists and engineers are constantly making improvements to mitigate these issues, however performance decay and thermal runaways have not entirely been solved. Most of today's research effort is focused on cathode active materials. Coating and doping are the most frequently used techniques to improve material performance. Atomic layer deposition (ALD), for example, is by far most the popular technique for depositing nano-scale conformal layers on powder surfaces.

Current and future battery materials development for electric vehicles (EVs) must address the range limits (longer), cycle performance (stable), energy density (higher) and safety (flammability). Achieving all of these parameters at the desired level with a single material is challenging. Li-ion battery fires seen all over the world drive battery researchers to discover safer materials. One promising technology is the all solid state battery (ASSB), which can potentially address all these issues. Massive efforts seek to address the interfacial problems between the cathode and electrolyte.

The presentation will discuss current trends in battery materials.

4:00pm **TS3-WeA-7 Application of Bipolar Hipims to Enhance the Durability Performance of Carbon Coatings in Metallic Bipolar Plates**, *J. Santiago , I. Fernandez, **Pablo Diaz-Rodriguez (pablo.diazr@nano4energy.eu)**,* Nano4Energy, Spain*; M. Panizo, M. Morales-Furio, C. Molpeceres,* Technical University Madrid, Spain*; J. Sanchez-Lopez,* CSIC-University Sevilla, Spain*; L. Mendizabal,* Tekniker, Spain*; G. Sevilla, M. Sanchez, N. Rojas,* Spanish Hydrogen National Center, Spain

Metallic bipolar plates (BPPs) are a promising candidate to replace conventional graphite BPPs due to higher power density and lower costs in proton exchange membrane fuel cells (PEMFCs). However, great challenges still exist for the application of metallic BPPs since they are working in acidic, humid, warm and polarized environment that reduce the lifetime of BPPs. The application of coatings is essential to enhance interfacial conductivity and corrosion resistance.

In this study, four different metal-doped amorphous carbon coatings (a-C:Cr, a-C:W, a-C:Nb and a-C:Ti) have been deposited by bipolar HiPIMS on stainless steel. The influence of HiPIMS parameters on coating-substrate interface, as well as the coating properties have been evaluated. SEM and TEM microscopy have been used to evaluate the coating interface. Raman analysis has been carried out to analyze the influence of metal content on carbon structure. The sp3-sp2 ratio has also been assessed with EELS spectroscopy. XPS analysis was used to evaluate the formation of metal carbides. Potentiodynamic and potentiostatic tests have been conducted to evaluate the corrosion resistance of the coated samples. Interfacial contact resistance (ICR) has been measured before and after corrosion tests.

Coatings deposited by bipolar HiPIMS improve coating-substrate contact interface and allow optimizing sp3-sp2 carbon structure, reducing ICR and enhancing corrosion resistance, as compared with carbon coatings deposited by conventional sputtering techniques. The results show that coatings follow the requirements established by DoE and are of great potential for application in PEMFC.

4:20pm **TS3-WeA-8 Coatings for Fuel Cells and Electrolyzers: From Materials to Processes, Challenges and Opportunities**, ***Etienne Bouyer (etienne.bouyer@cea.fr)**,* Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA), Grenoble, France **INVITED**

Hydrogen technologies are booming according to the benefit such technologies can bring for decarbonisation of as an example energy intensive industry and mobility sectors.

One has to distinguish between hydrogen conversion to produce electricity and hydrogen production in itself for further valorization of this carbon free fuel. The first topic concerns fuel cells for electricity generation from hydrogen and oxygen whereas the second topic is related to electrolyzers that allow to produce clean hydrogen through water splitting. Both electrochemical devices are based on a multilayer system.

The first illustration relates to fuel cell that convert the chemical energy contained in a fuel into electrical energy. As all electrochemical devices, a fuel cell is composed by two electrodes (anode and cathode) separated by an electrolyte. Between the two electrodes, ions pass through the electrolyte (ionic conductor and electronic insulator). Fuel cell is an open electrochemical generator (unlike batteries that are closed systems). Proton Exchange Membrane Fuel Cell (PEMFC) is a fuel cell operating at around 60 to 80°C and, to maintain a reasonable kinetic noble-metals catalyst are needed.

The second illustration focuses on high temperature electrolyzers that are made of multilayer ceramic materials. It has the same structure (anode/electrolyte/cathode) than a PEMFC. The hydrogen production reaction is not spontaneous, therefore electrical energy must be supplied to the system to produce hydrogen in an electrolyzer. Such system operate at high temperature (600-800°C): increasing the temperature decreases electricity demand thanks to thermodynamics and improves electrochemical kinetics.But limitations due to materials are occurring.

An overview of materials as well as associated processes to shape such components as layers or coatings will be presented and discussed. A special emphasis will be put on the remaining challenges (which slow down development of such technologies) and on the potential solutions. This contribution will also pay attention on the use of the so-called critical raw materials, on the way to minimize their content or -even better- to substitute them by more abundant materials and to save material through an optimization of the shape forming processes.

5:00pm **TS3-WeA-10 Electrochemically Stable PVD Coatings With Low Interfacial Contact Resistance for Proton Exchange Membrane Electrolyzer Bipolar Plates**, ***Nathan Kruppe (kruppnth@schaeffler.com)**, E. Schulz, M. Öte, N. Bagcivan, J. Hackner, S. Rüth,* Schaeffler Technologies GmbH & Co. KG, Germany

In the scope of worldwide energy transition, the industrial availability of alternative energy sources is increasingly becoming the focus of attention - not least due to urgent legislative requirements. In the proton exchange membrane water electrolysis (PEMWE) water is electrochemically decomposed by an applied current. In this way, hydrogen is produced. PEMWE is characterized by its high-power density, the lack of hazardous chemicals and - a major advantage for the production of green hydrogen in particular - its ability to follow load changes almost instantaneously.

The core of the electrolyzer is the stack, in which numerous cells are stacked and interconnected via bipolar plates. The load collective acting on these bipolar plates is particularly harsh. Under warm and humid conditions, high electrochemical potentials, simultaneously low pH values, i.e. acidic environment as well as oxygen formation on the anode side and hydrogen formation on the cathode side, the materials are exposed to corrosive attacks on the one hand and hydrogen embrittlement on the other. The use of expensive solid materials such as titanium is not sufficiently suitable for the large series production of scalable, efficient, durable and robust PEMWE electrolyzers. Especially on the anode side, corrosive loading on stainless steel leads to reduced performance of the entire stack.

Surface technology offers a solution when stainless steel, which is significantly less expensive than titanium, is protected from corrosive attacks and hydrogen embrittlement by thin high-performance coatings. At the same time, a low contact resistance can be achieved in the long term. Within the scope of this contribution, it will be shown which requirements are placed on coating systems for PEMWE bipolar plates in order to realize electrochemical stability on the one hand and a sufficiently low interfacial resistance on the other hand. Results will be presented which prove the high potential of Schaeffler Technologies coating solutions for this application.

Topical Symposia
Room Pacific E - Session TS4-ThA
Big Data, Machine Learning, Artificial Intelligence and High-Throughput Methods
Moderator: Igor Abrikosov, Linköping University, IFM, Sweden

1:20pm **TS4-ThA-1 New 3D and 2D Metal Borides from Materials Synthesis Guided by High-Throughput Simulations***, **Johanna Rosen (johanna.rosen@liu.se)**,* Linkoping University, Sweden **INVITED**

Exploratory theoretical predictions in uncharted structural and compositional space are integral to materials discoveries. A more recent addition to the family of laminated metal borides, so called MAB phases, is new types of chemically ordered quaternary borides, *i*-MAB ($M'_{4/3}M''_{2/3}AlB_2$) and *o*-MAB ($M'_4M''SiB_2$), in which the M-atoms are in-plane and out-of-plane chemically ordered, respectively. Both types of phases have been identified in high-throughput simulations followed by experimental synthesis, and they can be chemically exfoliated into 2D sheets, and selectively prepared in multilayer form, as delaminated single-layer sheets in colloidal suspension, or as additive-free filtered films. For example, Ti_4MoSiB_2*o*-MAB can be used to derive 2D TiO_xCl_y of high yield. $(Mo_{2/3}Y_{1/3})_2AlB_2$ and $(Mo_{2/3}Sc_{1/3})_2AlB_2$ *i*-MAB can be used for realization of so called boridene in the form of single-layer 2D sheets with ordered metal vacancies, $Mo_{4/3}B_{2-x}T_z$(T_z = -F, -O, -OH). The present talk will summarize the results to date of our predictive theoretical approach that have led to 2D materials synthesis from 3D quaternary metal borides, the mechanisms behind the realization of these 3D/2D materials, and evaluation of selected properties.

2:00pm **TS4-ThA-3 Machine Learned Moment Tensor Potentials for Hard Coatings***, **Ferenc Tasnádi (ferenc.tasnadi@liu.se)**, F. Bock, M. Odén, I. Abrikosov,* IFM Linköping University, Sweden

Refractory nitrides (TiN, Hf N , NbN etc.) nitride alloys ($Ti_{1-x}Al_xN$, etc.) or high-entropy alloys, such as TiZrHfTa are materials with high industrial relevance for hard coatings o f cutting tools [1] even for superconducting and plasmonic-based devices. M ajor objectives for their performance are the high-temperature the rmodynamic, dynamic and elastic properties. A recently developed combination of quantum mechanical calculations with machine-learning interatomic potentials (MLIP) [2], is utilized to calculate high temperature properties with high accuracy. On-the-fly training of moment tensor potentials allows us to perform the calculations with more than two orders less computational effort than using state-of-the-art ab initio molecular dynamics simulations. The calculated elastic constants are used to simulate surface acoustic waves and Brillouin light scattering (BLS) spectra. The results are compared with experiments. Furthermore, we investigate high-temperature bcc phase of titanium and predict very weak temperature dependence of its elastic moduli [3], called Elinvar effect, similar to the behavior observed for the so-called GUM metals . The effect in bcc-Ti is intrinsic and therefore unique.

[1] See, for example, F. Tasnádi et al., Phys. Rev. B 85, 144112 (2012); F. Tasnádi et al., Appl. Phys. Lett. 97, 231902 (2010); D. Holec et al. Phys. Rev. B 90, 184106 (2014); F. Tasnádi et al., Mater. Des. 114, 484 (2017); H. Huang et al., Adv. Mater. 5, 1701678 (2017). [2] I. S. Novikov et al., Mach. Learn.: Sci. Technol. 2 025002 (2021). [3] A. Shapeev et al., New. J. Phys. 22, 113005 (2020).

2:20pm **TS4-ThA-4 High-Throughput Rapid Experimental Alloy Development (HT-READ)***, **Kenneth Vecchio (kvecchio@eng.ucsd.edu)**,* UC San Diego, Dept. of NanoEngineering, USA **INVITED**

The development of high-throughput materials development strategies in the thin-film field have moved forward more quickly than bulk material high throughput strategies, primarily due to the need in bulk materials to account for microstructure effects on properties.In addition, the current bulk materials discovery cycle has several inefficiencies from initial computational predictions through fabrication and analyses. Much of the information and knowledge generated existed in isolated data silos making integrated approaches more challenging. This was the motivation for the 2011 Materials Genome Initiative, which sparked advances in many high-throughput computational techniques related to materials development. However, computational techniques ultimately rely on experimental validation.However, bulk materials are generally evaluated in a singular fashion, relying largely on human-driven compositional choices and analysis of the volumes of generated data, thus also slowing validation of computational models. Thus, increasing the rate of materials experimentation is fundamental to improving materials research, and requires parallelizing, automating, and miniaturizing key steps in experimental materials research, including computation, synthesis, processing, characterization, and data analysis.To overcome these limitations, we developed a High-Throughput Rapid Experimental Alloy Development (HT-READ) platform and methodology that comprises an integrated, closed-loop material screening process inspired by broad chemical assays and modern innovations in automation. Our method is a general framework unifying computational identification of ideal candidate materials, fabrication of sample libraries in a configuration amenable to multiple tests and processing routes, and analysis of the candidate materials in a high-throughput fashion. An artificial intelligence agent is used to find connections between compositions and material properties.New experimental data can be leveraged in subsequent iterations or new design objectives. The sample libraries are assigned unique identifiers and stored to make data and samples persistent, thus preventing institutional knowledge loss.This integrated approach paves the way for compositionally accurate and microstructurally informed bulk materials development in a highly-accelerated manner.

3:00pm **TS4-ThA-6 Finding Thermally Robust Superhard Materials with Machine Learning***, **Jakoah Brgoch (jbrgoch@Central.UH.EDU)**,* University of Houston, USA **INVITED**

Superhard materials with a Vickers hardness >40 GPa are essential in applications ranging from manufacturing to energy production. Finding new superhard materials has traditionally been guided by empirical design rules derived from classically known materials. However, the ability to quantitatively predict hardness remains a significant barrier in materials design. To address this challenge, we constructed an ensemble machine-learning model capable of directly predicting load-dependent hardness. The predictive power of our model was validated on eight unmeasured metal disilicides and a hold-out set of superhard materials. The trained model was then used to screen compounds in Pearson's Crystal Data (PCD) set and combined with our recently developed machine-learning phase diagram tool to suggest previously unreported superhard compounds. Finally, industrial materials often experience tremendous heat during application; thus, we are building a method for predicting hardness at elevated temperatures.

3:40pm **TS4-ThA-8 Rational Composition Optimization: Coupling Mixture Designs, Combinatorial Methods and Machine Learning***, **Elise GAREL (elise.garel@grenoble-inp.fr)**, H. VAN LANDEGHEM, J. PAROUTY, M. VERDIER, S. COINDEAU, R. MARTIN, F. ROBAUT, R. BOICHOT,* SIMAP, Grenoble-INP, CNRS, France

Multinary optimization has been at the heart of recent developments, either for High Entropy Alloy or for metallic glasses, amongst others. It represents a challenge that requires overcoming the usual method of "one sample at a time". Combinatorial approaches have been applied many times to N-element systems, and this study proposes to couple it to mixture design, in order to guarantee a uniform and systematic screening of the composition space, by elaborating and characterizing magnetron sputtered films with controlled gradients of composition.

This method was applied to the refractory high entropy alloy system Nb-Ti-Zr-Cr-Mo, on as-grown and annealed samples, as well as on a nitride pseudo-ternary, Ti-Al-Nb-N. The mechanical properties were measured by nanoindentation for both, while crystallinity was assessed using XRD — and EBSD in the case of the HEA. Conductivity measurements were performed on the nitride system. This high-throughput screening resulted in an experimental database covering the properties of 460 HEA compositions and 140 nitride compositions that was used to train Machine Learning models linking compositions, structures and properties.

In order to explore the possibilities offered by Machine Learning, several databases and different models were used. Raw experimental data and statistically processed database allowed delineating the performances of Machine Learning. Models with increasing complexity were tested: multilinear regression with interactions, Support Vector Machine, Random Forest and Neural Network, with previously adjust hyper-parameters. Random Forest and Neural Network show a very good accuracy, either on regression or on classification, for property prediction over the entire composition space. Multilinear regression, performing adequately as well, allows a rapid understanding of the weights of each component on the properties, as well as their interactions, which can be used to rationally examine the largely discussed hypothesis of the cocktail effect. For instance, the elastic modulus of as-grown RHEA system is well fitted by multilinear regression and coefficients show that it almost only results from a linear combination of the effect of pure elements. Hardness presents on the contrary much more complexity, with a high positive effect of binaries and principally a negative effect of ternaries and quaternaries, leading to higher values at the edges of the composition space than at its center.

Based on Machine Learning predictions, isovalue hulls and Pareto-optimal domains can be determined inside the composition space and used to identify the composition sets that show the best property compromises.

4:00pm **TS4-ThA-9 Transfer Learning of Thermodynamic and Elstic Properties of Hard-Coating Alloys**, ***Henrik Levämäki (henrik.levamaki@liu.se)**, F. Tasnadi, D. Sangiovanni,* Linköping University, IFM, Sweden*; L. Johnson,* Sandvik Coromant, Sweden*; R. Armiento, I. Abrikosov,* Linköping University, IFM, Sweden

Accelerated design of novel hard-coating materials requires state-of-the-art computational tools, which include data-driven techniques, building databases, and training machine learning (ML) models against the databases.

We present a development of a heavily automated high-throughput workflow to build a database of industrially relevant hard coating alloys, such as disordered binary and ternary nitrides [1].

We use Vienna Ab initio Simulation package (VASP) as the density functional theory calculator and the high-throughput toolkit (httk) to automate the calculation workflow.

One of the key quantities in the computational study of hardness is the elastic tensor, and the challenge we face is that calculating the elastic tensor for disordered supercells is resource intensive, which makes building a large database of disordered hard-coating alloys slow.

We therefore explore ways for ML techniques to support and complement our databases.

We find that the crystal graph convolutional neural network (CGCNN) model [2] trained on ordered compounds from the Materials Project [3] has sufficient prediction accuracy for the disordered nitrides.

This suggests that the existing public or commercial databases provide important data for predicting mechanical properties of qualitatively different types of material systems, which in our case are disordered hard-coating alloys that are not included in the original dataset.

[1] Can be found in arXiv under the title: "Predicting properties of hard-coating alloys using ab-initio and machine learning methods"

[2] Xie, Tian and Grossman, Jeffrey C., "Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties", Physical Review Letters 120, 145301 (2018), doi: 10.1103/PhysRevLett.120.145301

[3] Jain, Anubhav and Ong, Shyue Ping and Hautier, Geoffroy and Chen, Wei and Richards, William Davidson and Dacek, Stephen and Cholia, Shreyas and Gunter, Dan and Skinner, David and Ceder, Gerbrand and Persson, Kristin A., "Commentary: The Materials Project: A Materials Genome Approach to Accelerating Materials Innovation", APL Materials 011002 (2013), doi: 10.1063/1.4812323

4:20pm **TS4-ThA-10 Data-Driven Search for Thermal Insulators Guided by Anharmonicity: From First Principles to Machine Learning**, ***Florian Knoop (florian.knoop@liu.se)**,* Linköping University, IFM, Sweden*; M. Langer,* Technical University of Berlin, Germany*; C. Carbogno,* NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Germany*; M. Rupp,* University of Konstanz, Germany*; M. Scheffler,* NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Germany

We present a systematic first-principles search for thermal insulators in materials space which covers hundreds of compounds, five lattice types and seven space groups, including simple rocksalt and zinc blende structures, up to complex perovskites. Using the high-throughput framework FHI-vibes [1] and a recently developed measure for the strength of anharmonicity [2], we identify 120 candidate materials with potential for low thermal conductivity at room temperature. We investigate the 60 most promising candidates with the ab initio Green Kubo method (aiGK) [3], enabling data-driven extraction of design principles for bulk materials with low thermal conductivity. The aiGK method provides an accurate framework to obtain thermal conductivities for materials, in particular strongly anharmonic ones such as thermal barrier coating ceramics like zirconia, since all anharmonic effects responsible for low thermal conductivity are included.We subsequently demonstrate how the first principles calculations can be complemented with the help of machine learning potentials to remove the computational bottleneck. For this task, we use message passing neural networks, a class of models that can accommodate implicit long-range interactions as well as directional information [4]. We present a systematic account of their performance for calculating the thermal conductivity of solid semiconductors and insulators and discuss implications for high-thoughput heat transport simulations and the discovery of novel thermal insulators.

[1] F. Knoop et al., J. Open Source Softw. 5, 2671 (2020)
[2] F. Knoop et al., Phys. Rev. Mater. 4, 083809 (2020)
[3] C. Carbogno, R. Ramprasad, and M. Scheffler, Phys. Rev. 118, 175901 (2017)
[4] K.T. Schütt et al., J. Chem. Phys. 148 241722 (2018)

4:40pm **TS4-ThA-11 2D Phase Mapping of Hf-Al-Si Refractory Complex Concentrated Alloy Produced using High-Throughput Magnetron Sputtering**, ***Sophia Cooper (sophiacooper@my.unt.edu)**, M. Dockins, M. Young, A. Voevodin,* University of North Texas, USA*; A. Ghoshal, V. Blair,* U.S. Army Futures Command, USA*; S. Aouadi,* University of North Texas, USA

Topical Symposia
Room Golden State Ballroom - Session TS1P-ThP
Anti- and De-Icing Surface Engineering - TS1 Poster Session

TS1P-ThP-1 A Fracture Mechanics Approach to Ice-Shedding Surfaces*,*
Michael Wood (michael.wood3@mail.mcgill.ca)*, P. Servio, A. Kietzig,* McGill University, Dept. Chemical Engineering, Canada

The adhesion of ice to external structures has been a persistent engineering challenge. This includes the accumulation of ice on metallic structures such as aircraft wings and power transmission equipment. There has therefore been considerable effort put into the development of passive ice-shedding surfaces in the past few decades. To-date there have broadly been two prevailing research paradigms for the engineering of low ice adhesion strength surfaces: (i) application of low surface energy chemical coatings / infusion of sacrificial lubricants; and (ii) limiting ice-substrate contact through superhydrophobic texturing. The results of these efforts have been overall mixed with coatings and lubricants needing continual reapplication and superhydrophobic texturing often leading to ice-substrate interlocking effects. We take a decidedly different approach to the design of low ice adhesion surfaces by choosing microstructures which induce interfacial cracking in combination with cohesive failure of ice within microstructure pores, an approach that allows for ice-shedding surfaces to be made of bare metal. Specifically, in this work we test the ice adhesion characteristics of an ultra-fine woven stainless-steel wire cloth, which we show has an extremely low ice adhesion strength of 12.5 kPa. Our testing shows that the low ice adhesion strength stems from the three-dimensional microstructural network formed by the woven stainless-steel wires which make up the cloth. Compared to a monolithic metal surface, the cloth structure possesses pores at each weaving point which induce the formation of micro-cracks during the ice freezing process. The cloth also possesses microstructural compliance of each woven wire segment which leads to facile opening of each of these micro-cracks. Rather than relying on few cracks which must open from edge-to-edge of the ice-substrate interface on monolithic materials, cracks at the interface with the woven wire cloth need only open from one weaving point to the next. Starting first with this fracture mechanics approach to ice-shedding surface engineering and only then tuning the surface chemistry, we may see new benchmarks set for low ice adhesion strength surfaces.

Topical Symposia
Room Golden State Ballroom - Session TS3P-ThP
Electrochemical Cells – Hydrogen and Batteries - TS3 Poster Session

TS3P-ThP-1 Ionic Conductive Polymer Electrolyte for High-Performance Flexible Solid-State Supercapacitors*,*
Haylay Ghidey Redda (ghaylay12@gmail.com)*, W. Su, R. Chen, B. Hwang,* National Taiwan University of Science and Technology, Taiwan

In recent years, high-performance ionic conductive polymer electrolytes have emerged as a crucial research target within flexible solid-state supercapacitors (FSSC). In this study, a flexible ionic conductive gel polymer electrolyte is designed to enhance FSSC's electrochemical stability and effectiveness. The ionic conductive gel polymer electrolyte is manufactured from 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfony)imide as ionic liquid (IL), poly(vinylidene fluoride-co-hexafluoropropylene) (PVdF-HFP) as host polymer and $Li_{1.5}Al_{0.33}Sc_{0.17}Ge_{1.5}(PO_4)_3$ (LASGP) as ceramic filler. The scanning electron microscope (SEM) image confirms that a homogeneous uniform phase with a smooth surface is achieved as the ionic liquid is added into the host polymer solution. The X-ray diffraction (XRD) patterns show that the PVdF-HFP blend has a semi-crystalline structure, and its amorphous nature extends with increasing IL and LASGP ceramic fillers. In light of this, the GPE film is used as the electrolyte and separator due to its high ionic conductivity 78 mS cm^{-1}), excellent thermal stability up to 346℃. Finally, the AC||LASGP/IL/PVdF-HFP||AC FSSC cell achieves a remarkable high specific capacitance of 115.45 F g^{-1}, and its corresponding specific energy density reaches 27.10 Wh kg^{-1} at 1 mA. These results suggest that GPE films with activated carbon electrodes are candidate materials for nanotechnology systems and FSSC applications.

Topical Symposia
Room Town & Country B - Session TS1-FrM
Anti- and De-Icing Surface Engineering

Moderators: Kevin Golovin, University of Toronto, Canada, **Jolanta-Ewa Klemberg-Sapieha**, École Polytechnique de Montréal, Canada

8:00am **TS1-FrM-1 Penguin-Inspired Anti-Icing Surfaces***, **Anne Kietzig (anne.kietzig@mcgill.ca)**, M. Wood,* McGill University, Canada **INVITED**

Over the past decades considerable research efforts have been made to provide novel and ideally passive anti-icing strategies. Broadly these efforts have either started off from aiming at reducing the amount of water present for solidification on a given surface or at facilitating the dislodging of already grown ice. In our work, we have addressed both aspects by taking inspiration from the South American penguin *Spheniscus humboldti* which exhibits strategies to not only shed water but also already accreted ice. The biomimicry of the Penguin feather's functionality is achieved by using a compliant finely woven wire cloth to mimic the microstructure of the feather in combination with using laser-micromachining to further decorate the latter with nanogrooves. Laser-micromachining in combination with selective post-processing techniques further allowed us to render the surface chemistry of our biomimetic surface either hydrophilic or hydrophobic, which allowed us to selectively identify the role of surface chemistry on our anti-icing surface. Our results from this biomimetic surface not only highlight that different physical mechanisms are at play when considering water and ice shedding, but also emphasizes the role of the hierarchical surface structure. Laser-machined nanogrooves with hydrophobic surface chemistry clearly support water shedding. Whereas, the porosity and compliance of the microstructure favors a multitude of evenly spaced crack initiation locations with facile and short pathways for crack propagation, which accordingly leads to exceptionally low ice adhesion strengths. In conclusion, our biomimetic approach highlights that having learnt from a natural example and abstracting the relevant features and functionalities to engineering provided us with a framework that exploits fracture mechanics to design the ice-shedding property and wetting science to separately design the water-shedding property.

8:40am **TS1-FrM-3 Screening of Anti-Icing Strategies Against Aeronautic Secondary Icing***, **Paloma García (garciagp@inta.es)**, J. Mora, F. Carreño, M. González, A. Agüero Bruna,* Instituto Nacional de Técnica Aeroespacial (INTA), Spain

Ice protection is an important issue in the aeronautic field, which has been traditionally faced by the use of active systems (systems that need energy support). In last decades, the use of several passive solutions, based on surface engineering strategies, has been explored to replace the active systems, or to decrease their energy consumption. However, so far the idea of completely avoiding ice accretion with a passive system seems utopic. In addition, ice accretion affects different sections of aircrafts, but to present, a single method efficient in all possible icing locations, has not been found. Thus different solutions must be designed for each specific application, and testing should be undertaken attending to the different location issues.

For instance, electrothermal active systems are widely used to protect sensible areas on aircrafts, i. e. leading edges. Those systems increase the surface temperature to avoid ice accretion or release or melt the ice once it has been accreted. As a result, icing in the downstream area of the wing's chord is caused by exposure to this ice-melted water droplets as well as to direct supercooled water. This is considered as secondary or runback icing resulting in an important challenge in aviation, and the use of anti-icing solutions can perhaps contribute to avoid or reduce this issue.

In this work, 12 materials and references, attending to 5 different anti-icing strategies have been tested using a common methodology. These include Slippery Liquid Infused Porous Surfaces (SLIPS), elastomer coatings, superhydrophobic surfaces and low surface energy materials. The test methodology includes the evaluation of ice adhesion after impact icing in an icing wind tunnel (IWT) as well as ice accretion through direct impinging of supercooled droplets and after melting or heating in an active system in the IWT.

Among the studied materials, several coatings showed ice accretion reduction and some of them also significantly reduced ice adhesion. In general, 2 strategies showed more promising results in terms of anti-icing features: SLIPS and elastomeric coatings. In addition, low roughness, low surface energy and high water droplet mobility (low contact angle hysteresis) were correlated with anti-icing behaviour. These are easy to measure properties which do not require complex equipment that can be considered as indicators of potentially good anti icing and de-icing performance. Results also showed that superhydrophobic solutions reduced runback icing as a result of a reduced interaction of the melted ice droplets with the surface.

9:00am **TS1-FrM-4 Influence of Organosilicon Based Modification on Ice Adhesion and Wettability of Unsaturated Polyester Gelcoats Surfaces***, **Rafal Kozera (rafal.kozera@pw.edu.pl)**, B. Przybyszewski, K. Zolynska,* Warsaw University of Technology, Materials Science and Engineering, Poland*; B. Sztorch, R. Przekop,* Adam Mickiewicz University of Poznan, Poland*; A. Boczkowska,* Warsaw University of Technology, Materials Science and Engineering, Poland

In recent years, the world of science and industry has paid a lot of attention to coatings as a functional materials.Used as the outer layer on an composite elements, they fulfill a number of extremely important functions.Starting with protection against weather conditions, through improving mechanical properties, and ending with decorative functions. One of the significant problem in many industries is accumulation and build-up of ice and snow what is a negative and unwanted phenomenon. Ice formation and accretion present serious, sometimes catastrophic, safety issues for all kinds of industry where application of the composites components has already become common e.g. wind turbines blades, aircrafts, electric and telecommunication infrastructure as well as other composite constructions exposed to supercooled water droplets both on the ground and in the air. In example, ice on wind turbine blades or aircrafts disrupts airflow by altering the shape of the wing surface, which leads to increased drag and decreased efficiency of the systems what cause necessity for more often servicing and utilization of energy consuming systems.

In the present work, composite materials based on unsaturated polyester resin and authors' chemical modifications were prepared and characterized in order to find compromise between hydrophobic and icephobic properties. Studies were conducted by means of goniometer to investigate contact angle, hysteresis and roll of angle, ice adhesion tester in order to find correlation between modified surface and ice and profilometer for roughness characterization.

Presented work is conducted in the frame of the project entitled"ICEphobic SURfaces for components based on polymER composites- IceSurfer" (no. LIDER/16/0068/L-9/17/NCBR/2018) under the LIDER program of the National Center for Research and Development, Poland.

9:20am **TS1-FrM-5 Quasicrystalline Coatings Exhibit Durable Low Interfacial Toughness with Ice***, **Kevin Golovin (kevin.golovin@utoronto.ca)**,* University of Toronto, Canada

Ice accretion can adversely impact many engineering structures in commercial and residential sectors. Although there are many reports of low-ice-adhesion-strength materials, a scalable and durable deicing solution remains elusive, as ice detachment is dominated by interfacial toughness for large interfaces. In this work, two durable quasicrystalline coatings (QC1 and QC2) were applied on aluminum substrates using HVOF thermal spray. XRD confirmed the quasicrystalline phases. Except for the roughest QC2 sample (root-mean-squared roughness ≈ 7 µm), a toughness-mediated regime of fracture was observed when detaching longer lengths of ice from the quasicrystalline coatings. The interfacial toughness was calculated to be 0.9 J/m^2 for the smoothest QC1 sample (root-mean-squared roughness ≈ 1.5 µm) and 1.1 J/m^2 for the smoothest QC2 sample (root-mean-squared roughness ≈ 0.3 µm), demonstrating that low-interfacial toughness coatings are possible to fabricate from metallic materials. Apparent shear strengths as low as 30 and 80 kPa at an ice length of 20 cm were observed for QC1 and QC2, respectively. A small imposed deflection could also dislodge 20 cm-long pieces of accreted ice adhesively. Interfacial toughness increased with surface roughness in line with the concept of a shielding factor that hinders crack propagation. Finally, the mechanical durability of the smoothest QC1 and QC2 samples was confirmed using abrasion, UV irradiation, pencil scratching, elevated temperature, and chemical contamination. Overall, thin quasicrystalline coatings exhibit the unique combination of low interfacial toughness and high durability, leading to long-lasting ice protection applicable to many different surfaces.

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