Fundamentals and Technology of Multifunctional Materials and Devices
Room Golden West - Session C3+C1-WeM

Thin Films for Energy-related Applications I/Optical Metrology in Design, Optimization, and Production of Multifunctional Materials

Moderators: Per Eklund, Linköpings Universitet, **Tushar Shimpi**, Colorado State University, USA

8:20am **C3+C1-WeM-2 Avoiding Blistering of Magnetron Sputtered Thin Film CdTe Photovoltaic Devices***, J Walls, F Bittau, R Greenhalgh, A Abbas,* ***Peter Hatton****, R Smith,* Loughborough University, UK

Magnetron sputtering is an industrially scalable technique for thin film deposition. It provides excellent coating uniformity and the deposition can be conducted at relatively low substrate temperatures. It is widely used in the manufacture of solar modules. However, its use for the deposition of thin film CdTe photovoltaics results in unusual problems. Blisters appear on the surface of the device and voids occur in the CdTe absorber. These problems appear after the cadmium chloride activation treatment at 400^{0}C. The voids often occur at the p-n junction interface causing catastrophic delamination. This problem has been known for more than 25 years, but the mechanisms leading to blistering have not been understood. Using High Resolution Transmission Electron Microscopy we have discovered that during the activation process, argon trapped during the sputtering process diffuses in the lattice to form gas bubbles. The gas bubbles grow by agglomeration particularly at grain boundaries and at interfaces. The growth of the bubbles eventually leads to void formation and blistering. Switching the working gas to xenon overcomes these problems.

8:40am **C3+C1-WeM-3 Electrochromic Device Based on WO_3/NiO Complementary Electrodes Prepared by Using Vacuum Cathodic Arc Plasma***, Po-Wen Chen,* Institute of Nuclear Energy Research, Taiwan

Smart windows based on electrochromic (EC) materials, which are controlled to change their optical properties of reflectance, transmittance, and absorption can be effectively reduced the heating or cooling loads of building interiors. Electrochromism can produce interesting phenomenon based on redox reaction that gives a reversible, persistent changing in color, thus with an optical modulation by a small applied DC voltage pulse difference. In this study, we prepared a complementary electrochromic device (ECD) with ITO/WO_3/$LiClO_4$-PC/NiO/ITO structure was assembled. This work focues on the influence of thickness of NiO layers on the ECD electrochemical and optical properties. For the fabrication of ECD, WO_3 and NiO electrode films were used as the cathodic and anodic coloring materials, which are fabricated by vacuum cathodic arc plasma (CAP). We achieve a high performance electrochromic elecrode, producing porous deposited by the CAP technique is promising smart window for potential electrochromic application. Our results are observed the highest oxidation/reduction ion diffusion coefficient ($9.38x10^{-9}$ / $8.12x10^{-8}$ cm^2/s, respectively) with NiO(60 nm)/ITO films, meaning that enhanced electrochromic properties compared to the other samples. The performance of the 5×5 cm^2 ECD demonstrated optical contrast of 52 % and switching times 4.6 sec and 8.1 sec for coloring and bleaching state at the wavelength of 633 nm. During the durability test, the transmittance cahnge (ΔT) of ECD remained 45% after 2500 cycles, which was about 85% of original state.

9:00am **C3+C1-WeM-4 Influence of Film Thickness on Growth, Structure and Properties of Magnetron Sputtered ITO Films***, Andrius Subacius,* Manchester University, UK*; É Bousser,* École Polytechnique de Montréal, Canada*; B Baloukas,* Polytechnique Montreal, Canada*; S Hinder, M Baker,* Surrey University, UK*; D Ngo,* Manchester University, UK*; C Rebholz,* Cyprus University, Cyprus*; A Matthews,* Manchester University, UK

Indium tin oxide (ITO) is one of the most widely used transparent conducting oxides due to its electrical conductivity and optical transparency, and it can be used for many applications, such as LEDs, flat-panel displays, smart windows and architectural windows. As typical for transparent conducting films, there is a trade-off between conductivity and transparency.

In this work, the effect of film thickness on the evolution of growth, microstructure and electrical and optical properties was studied. ITO coatings with different thickness values (200, 800 and 3000 nm) were deposited onto unheated soda lime glass substrates by r.f. sputtering from a ceramic (In_2O_3:SnO_2, 90:10 wt.%) target. X-ray diffraction (XRD), transmission Kikuchi diffraction (TKD) and transmission electron microscopy (TEM) analysis revealed an increase in crystallinity with growing ITO film thickness. While the 200 nm thin film appeared amorphous in XRD measurements, the 800 and 3000 nm coatings were found to be crystalline. The 3000 nm thick film displayed preferred orientations in the (440) and (400) directions. In the case of the 200 nm film, TKD results showed local crystallinity with 50-200 nm grains imbedded in an amorphous or possibly nanocrystalline matrix. The luminous transmittance in the visible range was found to decrease with increasing film thickness from 81.7 % for the 200 nm film down to 70 % for the 800 nm one and 44.6 % for the 3000 nm film. On the other hand, electrical resistivity values only slightly decreased with increasing film thickness from 6.15×10^{-4} Ω·cm to 5.36×10^{-4} Ω·cm and 5.23×10^{-4} Ω·cm for 200 nm, 800 nm and 3000 nm films, respectively.

9:20am **C3+C1-WeM-5 Metal/Semiconductor Superlattice Metamaterials: A New Paradigm in Solid-State Energy Conversion***, Bivas Saha,* Jawaharlal Nehru Centre for Advanced Scientific Research, India **INVITED**

Since the 1960s, researchers exploring the potential of artificially-structured materials for applications in quantum electronic devices have sought combinations of metals and semiconductors that could be combined on the nano-scale with atomically-sharp interfaces. Early work with multilayers of polycrystalline elemental metals and amorphous semiconductors showed promise in tunneling devices. More recently, similar metal/semiconductor multilayers have been utilized to demonstrate novel optical metamaterials. These metal/semiconductor multilayers, however, are not amenable to atomic-scale control of interfaces. We developed the first epitaxial metal/semiconductor multilayer and superlattice heterostructures that are free of extended defects. These rocksalt nitride superlattices have atomically sharp interfaces and properties that are tunable by alloying, doping and quantum size effects. Furthermore, these nitride superlattices exhibit exceptional mechanical hardness, chemical stability and thermal stability up to ~1000̊C.

In this presentation, I will describe the growth, structural characterization and transport properties of nitride metal/semiconductor superlattices including (Ti,W)N/(Al,Sc)N and (Hf, Zr)N/ScN. ScN and $Al_xSc_{1-x}N$ (x < 0.82) are rocksalt semiconductors in thin film and bulk form that can be doped preferentially with *n*-type or *p*-type carriers. $Al_xSc_{1-x}N$ can also be stabilized in rocksalt phase for high AlN mole fractions by lattice-matched epitaxy. TiN, ZrN, HfN and similar transition metal nitride films can be good metals with carrier concentrations approaching 10^{22} cm^{-3}. Potential applications of these single crystalline superlattice and thin films in thermoelectric devices and plasmonic metamaterials will be discussed. Furthermore, recent experimental efforts to employ these superlattices as model materials for investigating the fundamentals of heat transport in nanostructured materials will be addressed.

Reference:

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Fundamentals and Technology of Multifunctional Materials and Devices
Room Golden West - Session C2-WeA
Novel Oxide Films for Active Devices

Moderators: Vanya Darakchieva, Linkoping University, Sweden, **Alyssa Mock**, Naval Research Laboratory

2:00pm **C2-WeA-1 The Physics of Low Symmetry Metal Oxides with Special Attention to Phonons, Plasmons and Excitons***, Alyssa Mock,* Linköping University, Sweden **INVITED**

We discuss the analysis of the dielectric function tensor for monoclinic metal oxides. We investigate the potential high-power device material gallium oxide and derive dispersions of transverse, longitudinal and plasmon coupled modes [M. Schubert *et al*., Phys. Rev. B 93, 125209 (1-18) (2016); Editors' Suggestion], the band-to-band transitions and excitons and their eigenvectors [A. Mock *et al*., Phys. Rev. B 96, 245205 (1-12) (2017)], the effective electron mass tensor using optical Hall effect measurements [S. Knight, A. Mock *et al*., Appl. Phys. Lett. 112, 012103 (2018); Editors' Pick], and the temperature dependence of band-to-band transitions energies [A. Mock *et al*., Appl. Phys. Lett. 112, 041905 (2018)]. We present the Lyddane-Sachs-Teller relation for monoclinic and triclinic semiconductors [M. Schubert, Phys. Rev. Lett. 117, 215502 (2016)]. We also discuss the identification of transverse and longitudinal phonons in scintillator material cadmium tungstate [A. Mock *et al*., Phys. Rev. B 95, 165202 (1-15) (2017)], and the dielectric and inverse dielectric tensor analysis method for transverse and longitudinal phonon mode dispersion characterization in high-power laser material yttrium orthosilicate [A. Mock *et al*., Phys. Rev. B, 97 165203 (1-17) (2018)]. Additionally, we discuss the application of these analysis techniques to triclinic single crystalline oligoclase. Further, we apply our methods to epilayers of beta-phase gallium oxide and discuss strain induced effects.

2:40pm **C2-WeA-3 Materials Interfaces for β-Ga_2O_3 Power Devices***, Rebecca L. Peterson,* University of Michigan, USA **INVITED**

Beta-phase gallium oxide (β-Ga_2O_3) is an ultra-wide bandgap semiconductor that holds great promise for future power electronics due to its ease of bulk crystal growth and facile ability to extrinsically dope *n*-type over a wide range of dopant concentrations. Power devices often operate at elevated temperature with large surge currents and high blocking voltages. Reliable operation under these aggressive conditions requires that the metal and dielectric interfaces, as well as the doping profiles within the device, be highly stable under thermal and electrical stress, including thermal cycling. Obtaining stable materials interfaces is a particular challenge for oxide semiconductors, due to the ready supply of oxygen within the bulk, and to thermodynamic competition amongst adjacent metal atoms to oxidize or reduce. This property has been exploited in other oxide devices, for instance in oxygen-vacancy based resistive memory (ReRAM). However such behavior must be strictly avoided in power devices to ensure reliable and stable operation.

In this talk, I will present our experimental investigations on the stability of dielectric and contact electrode interfaces to beta-phase gallium oxide, using comprehensive materials characterization and electrical measurements. We study novel dielectrics that can be used as gate insulators in field-effect transistors, and for field plates and passivation layers. We also investigate metal contacts to bulk Ga_2O_3 with a variety of dopants and doping levels, to determine pathways to form low-resistance and stable ohmic contacts. The experimental results will be compared to thermodynamic predictions based on Gibbs' free energies of reactions. Using these results, we will identify and discuss strategies for designing stable dielectric and contact interfaces in order to enable high-performance Ga_2O_3 power electronics.

3:20pm **C2-WeA-5 Phase Selectivity in Heteroepitaxial Ga_2O_3 Thin Films***, Virginia Wheeler, N Nepal,* U.S. Naval Research Laboratory, USA*; L Nyakiti,* Texas A&M University at Galveston, USA*; D Boris, S Walton, D Meyer, B Downey, C Eddy Jr.,* U.S. Naval Research Laboratory, USA **INVITED**

Ga_2O_3 has emerged as a promising material for next generation power electronics and UV photodetectors applications due to its large bandgap (4.9 eV) and the availability of affordable native substrates from melt-grown bulk crystals. While β-Ga_2O_3 (monoclinic) is the most stable and studied of five Ga_2O_3 polymorphs, the slightly less energetically favorable α- and ε-Ga_2O_3 phases have unique characteristics that can be exploited. The α -Ga_2O_3 (rhombohedral corundum) has the largest bandgap of 5.3 eV and can be alloyed with α-Al_2O_3 and α-In_2O_3 for bandgap engineering. T he ε-Ga_2O_3 phase (hexagonal wurtzite) is a polar phase, with a calculated polarization strength that is 10 and 3 times larger than that of GaN and AlN, respectively. Like the III-N system, polarization induced charges can lead to higher charge densities and mobilities in two-dimensional electron gases formed at heterojunctions, which would improve the viability of Ga_2O_3 electronic devices. In this work, we use atomic layer epitaxy (ALEp) to produce high-quality heteroepitaxial Ga_2O_3 films and investigate phase selectivity as a function of substrate type and orientation, growth temperature (T_g), plasma gas phase chemistry and gas pressure.

All ALE Ga_2O_3 films were deposited in a Veeco Fiji G2 reactor equipped with a load lock and turbo pump using trimethygallium and O_2 plasma precursors. Initial studies on c-plane sapphire substrates showed that decreasing chamber pressure an order of magnitude during the plasma step resulted in a shift from mostly ε-Ga_2O_3 to pure α-Ga_2O_3. Additionally, at 350°C and 8 mTorr, the phase could be altered by a varying the O_2 plasma flow from 5-100 sccm. Optical emission spectroscopy indicate that the ratio of O*/O2 is critical for phase selectivity while the high ion flux to the surface can contribute to the crystallinity at low T_g. By varying T_g from 300 to 500°C at 8 mTorr, films went from mixed β/ε phase at <350°C, to pure α-Ga_2O_3 at 350°C, to pure β-Ga_2O_3 at 500°C. Using the optimum growth conditions for α-Ga_2O_3 on c-sapphire, the influence of substrate was explored using a variety of substrates including AlN, GaN (bulk and epilayers), SiC, diamond, and Si. Deposition on III-N and β-Ga_2O_3 substrates all resulted in crystalline β- Ga_2O_3 films, while amorphous films were deposited on both SiC and Si. This suggests that a clean crystalline substrate interface is critical to obtaining high quality films and promoting metastable phases is more dependent on growth parameters than underlying crystal symmetry. Finally, we will discuss simple electrical properties of optimum films of each phase to validate feasibility of the process in device applications.

4:00pm **C2-WeA-7 Exfoliated β-Ga_2O_3 Nano-layer based (Opto)electronic Devices***, J Kim,* ***Sooyeoun Oh,*** Korea University, Republic of Korea **INVITED**

β-Ga_2O_3, which is a ultra-wide band-gap semiconductor (>4.8 eV at room temperature), is an attractive material for next-generation power electronics devices and solar-blind photodetectors. Owing to its ultra-high (theoretical) critical field strength of ~8 MV/cm, Baliga's figure of merit of β-Ga_2O_3 (at 3214) outperforms other wide bandgap semiconductors including SiC (at 317) and GaN (at 846), indicating that β-Ga_2O_3 offers a superior power switching capability. In β-Ga_2O_3 electronic devices, high breakdown voltage by using field plate structures has been demonstrated. In addition, a hetero-junction field-effect transistor by the integration with p-type semiconductor was reported. In β-Ga_2O_3 optoelectronic devices, various types of solar-blind (deep-UV) photodetectors have been demonstrated, including photoconductive-type, MSM-type, and Schottky barrier-type photodetectors. The details of the results will be presented at the ICMCTF2019.

4:40pm **C2-WeA-9 Towards Controlled Exfoliation of β-Ga_2O_3 through Ion Implantation***, Michael E. Liao, T Bai, Y Wang, M Goorsky,* UCLA, USA

β-Ga_2O_3 is a wide bandgap semiconductor that has the potential for high-power device applications. While heterostructures of thin film β-Ga_2O_3 grown on various materials such as GaN[1,2] and sapphire[3,4] have been reported, the understanding of direct wafer bonding β-Ga_2O_3 to form heterostructures is still limited. The benefits of wafer bonding β-Ga_2O_3 would be two-fold: (1) enables even more novel materials combinations to be realized and (2) other unprecedented orientations of β-Ga_2O_3 could be integrated with various materials. This last point is important for β-Ga_2O_3 due to its anisotropic properties especially since β-Ga_2O_3 exhibits the low-symmetry monoclinic crystal structure.

Currently there are reports of mechanically exfoliating β-Ga_2O_3 along cleavage planes parallel to the (100) and (001) planes.[5,6] However, this approach will be challenging to integrate in large-scale processing. Demonstrated with Si,[7,8] III-V's,[9-12] and CdZnTe,[13] the "SMART-Cut" method[14] is more compatible with large-scale processing. In this approach, ions are implanted in a handle substrate and subsequently annealed. Under the appropriate processing conditions, the implanted ions diffuse and agglomerate into bubbles during annealing and surface blistering, accompanied by exfoliation, can occur. In this work, (010) β-Ga_2O_3 substrates are implanted with hydrogen ions and subsequently annealed. Both high-resolution X-ray diffraction (XRD) measurements and transmission electron microscopy (TEM) images were employed to monitor the structural evolution with annealing. Symmetric ω:2θ XRD scans showed

that annealing at 150 °C and 300 °C did not change the implantation-induced strain appreciably; while annealing at 500 °C for 1 hour was sufficient in removing this strain. Additionally, TEM images showed subsurface hydrogen bubble formation. Despite implanting along a non-cleavage plane, ion implantation for exfoliation provides a promising pathway for obtaining thin layers of β-Ga_2O_3 with orientations other than (100) and (001).

References

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5:20pm **C2-WeA-11 Investigation on Microstructure and Piezoelectric Property of High Orientation Y-doped ZnO Thin Films via RF Magnetron Sputtering**, ***Li-Cheng Cheng***, *C Liu, J Huang,* National Cheng Kung University, Taiwan

In this study, we focused on the piezoelectric coefficients (d_{33}) depended on doping rare earth element, yttrium (Y), into ZnO thin films. Pure ZnO and Y doped ZnO (Y:ZnO) thin films with different yttrium contents were synthesized on p-type Si (111) substrates via RF magnetron sputtering, and the thickness of these thin films were fixed at 650 nm. In X-ray diffraction (XRD) patterns, Y:ZnO films with low yttrium contents (<3 at%) showed preferential orientation of (002) plane and still maintained columnar wurtzite structures. The positions of diffraction peaks shifted to lower angle as the concentration of yttrium increased due to the substitution of smaller host ions (Zn^{2+}: 0.74Å) by larger dopant ions (Y^{3+}: 1.04Å). When the concentration of yttrium is over 3 at%, the drastic transformation of morphology was observed in scanning electron microscopy (SEM) images, which consisted with the results of XRD analysis. This phenomenon caused by the lattice distortion, owing to the larger radii of Y^{3+} ions. The piezoelectric coefficients of pure ZnO and Y:ZnO thin films were measured by piezoresponse force microscopy (PFM) as well. The piezoelectric coefficients had achieved higher values (d_{33} ~ 86.8 pm/V) when the contents of yttrium was 3 at%, which compared to the theoretical values of pure ZnO thin films (d_{33} = 12.4 pm/V). Therefore, Y doped ZnO thin film was regarded as the promising candidate for piezoelectric nanogenerators (NGs).

Fundamentals and Technology of Multifunctional Materials and Devices

Room Pacific Salon 3 - Session C3+C2+C1-ThM

Thin Films for Energy-related Applications II/Novel Oxide Films for Active Devices/Optical Metrology in Design, Optimization, and Production of Multifunctional Materials

Moderators: Per Eklund, Linköpings Universitet, **Tushar Shimpi**, Colorado State University, USA

8:40am **C3+C2+C1-ThM-3 Nanoflaky Titanium Dioxide Grown on Titanium Foil for Capacitive Deionization Purpose**, ***Jung-Ta Huang***, *P Hsieh, J He,* Feng Chia University, Taiwan

Capacitive deionization (CDI) is considered to be one of the most promising technologies for many water treatment and purification applications. To meet the demand for pursuing high efficiency of desalination, the key component, CDI electrode, requires high chemical stability, high specific surface area, high water wetting ability, and suitable porous structure for ion electrosorption. In this study, a facile approach involving alkali treatment followed by post-annealing was utilized to develop nanoflaky titanium dioxide (TiO_2) structure on titanium (Ti) foil. Furthermore, the feasibility of using nanoflaky TiO_2 grown Ti as electrode for CDI application was evaluated.

The results showed that the grown TiO_2 possessed a porous nanoflaky structure with a mixed-phase of anatase and rutile; in addition, the porous size is in the range of 30 ~ 100 nm. Such microstructure characteristics implies a high specific surface area. Superhydrophilic surface property was also obtained for this nanoflaky TiO_2 structure. According to the cyclic voltammetry results, the nanoflaky TiO_2 grown Ti electrode exhibited electrosorption/electrodesorption ability in 1 M sodium chloride solution, indicating the stability and regeneration. Finally, the deionization performance of flow-through CDI device using nanoflaky TiO_2 grown Ti electrode was demonstrated.

9:00am **C3+C2+C1-ThM-4 Mixed-oxide Coated Ni Foam for High Performance Supercapacitor**, ***Kuang-Cheng Lin***, National Cheng Kung University, Taiwan

Supercapacitors have become a popular energy storage device in the past ten years, owing to its excellent properties in many aspects, like electrical conductivity, cycle stability, and higher power density than lithium battery. However, the biggest challenge for supercapacitors to compete with the Li battery is energy density, i.e., its discharging time is still insufficient to satisfy for many desired applications. Therefore, we have studied a novel supercapacitor electrode made out of a mixed transition metal oxide grown on Ni foam to combat this problem. The mixed transition metal oxide is MnCo2O4 was synthesized using a one-pot synthesis involving hydrothermal treatment. We show that simply varying the precursor concentration would lead to the formation of MnCo2O4 nanostructures having different morphologies. The resulting MnCo2O4 provides more oxidation states that can participate in the electron transfer than monoxide. Several material characterizations and electrochemical tests were performed. Moreover, we demonstrate that the novel electrode gives very excellent specific capacitance of 1,740 F/g and stability after 5,000 cycles. Effect of the material characteristics on the electrochemical performance is discussed.

9:20am **C3+C2+C1-ThM-5 Wavefront Shaping: A New Tool in Optics**, ***Moussa N'Gom***, University of Michigan, USA **INVITED**

The newly emerging field of optical wavefront shaping involves the ability to manipulate light fields both spatially and temporally. It has largely been enabled by the availability of spatial light modulators (SLM). SLMs are used to create arbitrarily complex light fields that are now powerful elements of the optics toolbox. An SLM provides means to manipulate the fundamental constituents of classical light or single photons, which obey the laws of quantum physics. These new tools open up novel ways to address topics where conventional optical techniques are hard to apply, such as the control of light propagation in biological tissues, complex photonic structures, plasmonic systems, and multimode fibers. In this talk, I outline how I exploit the versatility of wavefront shaping to focus through and beyond highly scattering media. I will show its potential to manipulate entangled structured light fields to address coherence degradation in optical communication transmission channels and to address challenges in biomedical imaging.

10:00am **C3+C2+C1-ThM-7 Optical Optimisation of Semi-transparent a-Si:H Solar Cells for Photobioreactor Application**, ***Agathe Brodu***, *C Ducros,* Univ. Grenoble Alpes, CEA, France*; C Dublanche-Tixier,* Univ. Limoges, France*; C Seydoux, G Finazzi,* Univ. Grenoble Alpes, CNRS, CEA, France

One of the main limitations of microalgae culture in a photobioreactor is the low efficiency of sunlight conversion. To improve the overall photoconversion efficiency and provide energy support, a photobioreactor (PBR) and photovoltaic technology (PV) coupled system can be developed.

Semi-transparent thin film solar cells based on hydrogenated amorphous silicon technology could be directly placed on the PBR's surface. PV cells absorb a part of the incident light to produce electricity while being transparent in the specific photosynthesis wavelength range. To reach this objective, very thin solar cells must be produced. Decreasing the active layer thickness (intrinsic a-Si:H layer) of solar cells induces a better transparency but also a lower efficiency. As a consequence, we worked on the compensation of efficiency losses of thin solar cells by improving optical properties of substrate surfaces. Texturing process using reactive ion etching was applied on glass substrate to obtain a light scattering property on its back side and an antireflective property on the upper side. We studied the influence of those both textured surfaces on a-Si:H solar cells properties.

First, by texturing the back side of the substrate, the influence of light scattering was investigated. That should improve the light absorption in PV solar cells. The best result shows a raise of the short circuit current (Jsc) of the thin solar cells from 8.5 to 10 mA/cm^2, while the other parameters (the open circuit voltage (Voc) and the fill factor (FF)) remained the same. Thus the efficiency increased from 3.7 to 4.5 %.

In a second step, the influence of an antireflective texture of the substrate upper side was studied. The antireflection texture with light scattering effect gives the best results on PV cells. Short circuit current of this thin solar cell goes to 11.2 mA/cm^2 and its efficiency increased to 5.2 %.

The influence of these solar cells, used as optical filter, on the microalgae production rate was investigated. The photosynthesis peaks of microalgae correspond to wavelengths [400 - 500 nm] and [550 – 700 nm]. The first peak of photosynthesis is absorbed by the solar cell. Furthermore, an important diffusion of light in the solar cells also induces losses of transmitted light to microalgae for the second peak of photosynthesis. Finally growing test of *Phaeodactylum Tricornutum* shows that PV optical filtering does not have influence on growth rate. Optical modifications of substrate applied to very thin solar cells allowed to keep a high PV efficiency while maintaining the growing rate of microalgae.

10:20am **C3+C2+C1-ThM-8 Properties of Highly Transparent AlN/SiOx Multilayer Systems**, ***Chelsea Appleget***, *A Sáenz-Trevizo, A Hodge,* University of Southern California, USA

The new generation of engineered materials is required to perform under extreme conditions of stress, temperature and irradiation, among others. Nano multilayer (NM) materials have been shown to be promising candidates to overcome current structural and functional limitations. To date, most of the studied NM systems are comprised of metal/metal layers, where the optical properties do not represent an area of interest. Therefore, in this work we extended the structural potential of metal/metal NM configurations to ceramic/ceramic NMs which display a broad range of properties but in particular, they offer the possibility to modulate the optical properties depending on their morphology, grain size, layer thickness, and composition. Three different systems composed of alternated layers of AlN and SiO_xwere studied. For each sample, the number of layers and the individual thicknesses were varied until a total thickness of 1 µm was reached. The optical properties of the multilayers were determined using UV-Vis-NIR spectroscopy, revealing the formation of uniform and smooth interfaces with an average optical transparency above 80% that extends through the entire region. Furthermore, the microstructure and plastic behavior were also studied and correlated with the multilayer configuration of the synthesized systems.

10:40am **C3+C2+C1-ThM-9 Tailoring the Optical Properties of Highly Porous Superlattice-type Si-Au Slanted Columnar Heterostructure Thin Films**, *U Kilic,* University of Nebraska-Lincoln, USA*; A Mock,* Linköping University, Sweden*; R Feder,* The Fraunhofer Institute for Microstructure of Materials and Systems (IMWS), Germany*; D Sekora, M Hilfiker, R Korlacki,* ***Eva Schubert***, *C Argyropoulos, M Schubert,* University of Nebraska Lincoln, USA

The subwavelength scale periodic arrangement of nanostructures, so-called artificially engineered nano-structures exhibit distinct optical,

mechanical, and magnetic properties when they are compared with their bulk counterparts which has recently gained a growing interest due to its potential applications in various optical and optoelectronic systems such as lenses, solar cells, photodetectors, and sensors [1-3]. Tailoring aforementioned inherent properties cannot merely possible with the material choices (ie. elemental composition), but also the size and shape of these artificial structures play a significant role. Unraveling the mechanisms that influence and control the optical properties of highly-porous, periodic, and three dimensional arrangements of nanoplasmonic structures can offer new approaches for the development of next generation sensors. Particularly, both glancing angle deposition and atomic layer deposition can be used to create periodic nanostructures with multiple constituent materials, so-called heterostructured metamaterials.[4]

In this study, we employ a two-source (ie. Au and Si) electron-beam-evaporated, ultra-high-vacuum glancing angle deposition which allows for the fabrication of highly-ordered and spatially-coherent super-lattice type Au-Si slanted columnar heterostructured thin films. We perform a combinatorial spectroscopic generalized ellipsometry and finite-element method calculation analysis to determine anisotropic optical properties. We observe the occurrence of a strong locally enhanced dark quadrupole plasmonic resonance mode (bow-tie mode) in the vicinity of the gold junctions, with a tunable and geometry dependent frequency in the near-infrared spectral range. In addition, inter-band transition-like modes are observed in the visible to ultra-violet spectral regions. Using finite element method, we demonstrate that changes in the index of refraction due to the concentration variation of a chemical substance environment (gaseous or liquid) within a porous nanoplasmonic structure can be detected by transmitted intensity alterations down to 1 ppm sensitivity.

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11:00am **C3+C2+C1-ThM-10 Microstructures and Optoelectronic Properties of Cu_3N Thin Films and its Diode Rectification Characteristics**, ***Yin-Hung Chen***, *S Chen, S Sakalley, S Huang, A Paliwal,* Ming Chi University of Technology, Taiwan*; M Liao,* National Taiwan University, Taiwan*; H Sun,* Shandong University at Weihai, China*; S Biring,* Ming Chi University of Technology, Taiwan

Rapidly growing applications of p-type Copper nitride (Cu_3N) films in optical storage media, photovoltaics etc. has motivated us to study Cu_3N thin films which were deposited on glass and silicon substrates by reactive magnetron sputtering at 150˚C from a metallic copper target. Until now, few researchers have studied the p-type conductivity of Cu_3N films which is low compared to the result obtained in our experiment. In this work, we discuss the effects of working pressure on the microstructures, electrical, and optical properties of the Cu_3N films. The working pressures were varied from 5 mtorr to 23 mtorr while gas flow rate was kept constant at $N_2/(Ar+N_2)$%=40%. When the working pressure increases, the Cu_3N (111) peak intensity decreases as evident from XRD studies. Meanwhile, conduction type changes from n-type to p-type. When working pressure is increased to 15 mtorr, the resistivity is 1.575 Ω•cm and the sample shows p-type conduction. This is possibly due to the formation of many copper vacancies (i.e. vacancies at Cu cation sites) in the films. When the working pressure is 5 mtorr, a Cu (111) pattern was observed from selected area electron diffraction (SAED) by TEM analysis. It disappears upon increasing the working pressure to 15 mtorr. It was also found that the ratio of Cu^{2+}/Cu^{+} increases from 0.39 to 0.93 when the working pressure is raised from 5 mtorr to 20 mtorr. More substitution of Cu^{2+} for Cu^{+} results in the formation of more Cu vacancies, which leads to the transition in conduction from n-type to p-type. Finally, n-type Cu_3N/p-type Cu_3N homojunctions and n-type ZnO/p-type Cu_3N heterojunctions diodes were fabricated. It was found that homojunction devices Al/n-type Cu_3N/p-type Cu_3N do not show significant rectification effects. As we observed, at ±3Volts, the I_{on}/I_{off} was only 0.24. Whereas, in heterojunction devices Al/n-type ZnO/p-type Cu_3N, a higher I_{on}/I_{off} of 3118 can be achieved. Heterojunction devices outperform the homojunction devices instead of interfacial issues indicating the superior electrical properties which are explained considering the mismatch in the built-in potentials of the p-n junctions.

11:20am **C3+C2+C1-ThM-11 Effects of the Frequency of Pulsed DC Sputtering Power on Amorphous Carbon Film used for Metallic Bipolar Plates in Proton Exchange Membrane Fuel Cells**, ***Xiaobo Li***, *P Yi, L Peng, X Lai,* Shanghai Jiaotong University, China

Amorphous carbon (a-C) film is a promising material serving as a protective film for metallic bipolar plates in proton exchange member fuel cells (PEMFCs) due to its high electrical conductivity and corrosion resistance. However, the performance of a-C needs to be further improved to meet the commercial requirements of PEMFCs. During the process of preparing a-C film by magnetron sputtering, the sputtering power supply has significant influences on the structure and performance of the film. In this paper, the influence of the frequency of pulsed DC sputtering power supply are investigated to further improve the performance of a-C. The corrosion and interfacial contact resistance (ICR) test results show that the film prepared at 200 kHz exhibits excellent performance. The compactness of the films can be enhanced by the bombardment of high-energy sputtering particles produced by pulsed DC sputtering power. In addition, the proper frequency is beneficial to the formation of graphite nanocrytalline, which is embedded into a-C and improve the sp2 fraction of the film and decrease the ICR synchronously. Furthermore, the a-C containing graphite nanocrytalline exhibits better stability in simulated acid environment of PEMFCs. This study provides a new direction for further improving the performance of a-C films on bipolar plates in PEMFCs.

11:40am **C3+C2+C1-ThM-12 On the Mechanisms of Halloysite Nanotubes Incorporation in the Surface Layer of Forsterite Grown by Plasma Electrolytic Oxidation**, *B Mingo, Y Guo, A Němcova, A Gholinia, A Matthews,* ***Aleksey Yerokhin,*** The University of Manchester, UK

Increasing demand for high-performance lightweight metallic materials underlies the interest to Plasma Electrolytic Oxidation (PEO) as one of the most promising techniques for surface engineering of Mg alloys. In order to enable smart and multifunctional performance, it can be beneficial to incorporate into ceramic PEO coatings nanocontainers to carry appropriate active and functionalising agents. In situ incorporation of nanocontainers is challenging since their integrity may be compromised by plasma discharge assisting coating formation. We studied incorporation of halloysite nanotubes (HNTs) as potential nanocontainers into forsterite, Mg_2SiO_4, formed during PEO processing of AM50 Mg alloy. Detailed analysis of the coating microstructure, chemical and phase composition carried out by Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy, Transmission Kikuchi Diffraction and X-ray Diffraction enabled evaluation of a pattern of surface temperature evolution during current pulses underpinning the PEO process. Consequent thermal transient analysis revealed that at pulses longer than 10^{-4} s, the surface heating becomes affected by the metal substrate acting as a heat sink. As the pulse duration approaches 10^{-3} s, raising surface temperature and increasing thermal gradients across the coating cause crystallisation of forsterite and grain growth towards the surface; this triggers thermally induced degradation and decomposition of HNTs adsorbed on the surface. In contrast, at short pulse durations (2´ 10^{-5} s), the energy released is insufficient to induce forsterite crystallisation and incorporated HNTs are retained in their original tubular structure. Due to the fine porosity and good structural integrity, such coatings show the highest corrosion resistance in saline solution. Strong correlations between surface thermodynamic conditions and evolution of coating microstructure disambiguate the fundamental mechanisms underlying incorporation of nanoparticles into growing PEO coatings, thus creating the basis for efficient design of PEO processes and development of novel smart and multifunctional coatings with potential applications in many industrial sectors.

12:00pm **C3+C2+C1-ThM-13 Inorganic-Organic Perovskites: Handle with Care, Properties May Depend on It**, ***Nikolas Podraza***, *B Subedi, M Junda, K Ghimire,* University of Toledo, USA

Inorganic-organic lead halide based perovskites (ABX3) have been applied as the absorbing, current-generating layer in thin film photovoltaics over the last decade. In that time, device efficiency has increased from virtually nothing to 22.7% at the time of writing this abstract (that number is likely now higher at the time you are reading it). In spite of the ability to manipulate band gap to absorb different parts of the solar irradiance spectrum, the low deficit between the open circuit voltage and band gap, and the overall high electronic quality of the material based on fill factor and device efficiency, these perovskites still pose challenges—namely related to instability in atmosphere and under external heat, moisture, and electric field driven stimuli. Some instability is mitigated when layers are within solar cell devices, as the perovskites are over-coated with other layers and do not share an interface with the ambient. The susceptibility of

thin films to atmosphere leads to a disconnect between measured properties for films and what those properties of similarly prepared materials are in the final device structure. Spectroscopic ellipsometry over the near infrared to ultraviolet is applied for perovskite (A: MA, FA, Cs; B: Pb, Sn; X: I, Br, Cl) thin films and layers in solar cells to deduce structure in the form of thickness and surface roughness as well as complex optical response in the form of the complex index of refraction and complex dielectric function spectra. Photothermal deflection spectroscopy probes the optical response in the vicinity of the band gap for improved sensitivity to low values of the absorption coefficient resulting from Urbach tails and other sub-band gap absorption. For both techniques, measurements are performed for films with no exposure to atmospheric ambient and those exposed for controlled amounts of time. From these comparisons, changes appear in the complex optical response both above and below the band gap, including higher energy electronic transitions, Urbach energies, and other sub-gap absorption features. Understanding the origin of differences due to sample handling allows for more realistic comparison of samples and results in literature. Expectedly, upon continued atmospheric exposure Urbach energies increase and very prominent sub-gap absorption features develop. Samples characterized without atmospheric exposure have comparable properties to layers of the same composition in device structures, and correlations between Urbach energies and photovoltaic device performance parameters are identified.

Fundamentals and Technology of Multifunctional Materials and Devices

Room Pacific Salon 3 - Session C4-ThA

Fundamentals of Metallurgy in Thin Films and Coatings

Moderators: Karsten Woll, Karlsruhe Institute of Technology (KIT), **Ibrahim Gunduz**, Purdue University, USA

1:40pm **C4-ThA-2 Analytical Modelling of Propagation Velocity in Electron Transparent Nanolaminates*, Michael Abere,*** Sandia National Laboratories, USA*; G Egan,* Lawrence Livermore National Laboratory, USA*; D Adams,* Sandia National Laboratories, USA

The ignition of sputter deposited bimetallic nanolaminate films results in rapid, self-propagating reactions. Analytical models of the measured propagation velocities have been typically performed using a framework developed by Mann et al. (J. Appl. Phys. 1997). This work seeks to expand upon this model to handle electron transparent Co/Al samples for experiments in dynamic TEM. This work utilizes a three resistor thermal circuit model to account for thermal conductivity in the intermixed zone that is an order of magnitude less than that predicted by rule of mixtures. Also, this work utilizes cross-sectional scanning transmission electron microscope energy-dispersive X-ray spectroscopy data to calculate the Fourier coefficients in the Mann et al. model from the physical composition profile in the intermixed region. The effect of radiation loss for 150 nm thick foils is calculated as a perturbation to the difference in the heat of reaction measured in calorimetry and the adiabatic heat of product formation. Finally, the model considers two independent activation energies for when the reaction proceeds via co-melted reactants versus solid Co dissolution into molten Al.

This work was supported by the Sandia National Laboratory Directed Research and Development

(LDRD) program. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-NA0003525. This work describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S.

Department of Energy or the U.S. Government.

2:40pm **C4-ThA-5 Twin-Wire Arc Coatings for Repair of Structural Components*, C Jasien, Nicole Wagner,*** Cal Poly Pomona, USA

There has been a growing interest in additive manufacturing technologies for the repair of metallic structural components. Among the proposed techniques, twin-wire arc plasma spraying offers the advantage of providing high deposition and growth rate capabilities, coupled with process robustness and versatility, which are always desirable in real-life applications. In addition to these considerations, the fundamental materials science of these plasma-sprayed coatings is surprisingly still under-explored. Nanostructured depositions and coatings should be achievable with this additive technique given its high temperature and fast quenching rate. Motivated by these considerations, we have performed a study on the deposition of metallic coatings on steel substrates using an Oerlikon Metco FlexiArc 300 twin-wire arc plasma spraying system. We used 1.6mm diameter stainless steel wires and compressed air as a carrier gas. The process conditions that were varied include power, standoff distance and coating thickness. Dense coatings, approximately 150 micrometers thick, were achievable at the highest electrical input power of 10 kW within a few seconds of deposition time. Structural and morphological characterization has been performed using scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS). We have found that substrate temperature has a significant influence on the adhesion layer between the substrate and the coating.

3:00pm **C4-ThA-6 Unstable Propagating Reactions in Sputter-Deposited Nanolaminates*, David Adams, M Abere,*** Sandia National Laboratories, USA

Reactive metal multilayers are a form of energetic material that continue to attract attention for various applications. Generally composed of two layered reactants, these heterogeneous solids can be stimulated at a point or in bulk to initiate internal, self-sustained chemical reactions that give off heat and light. Their reactions are characterized by propagating high temperature wavefronts, little or no gas emission, and rapid local heating rates of ~106 K/s. Reactions often propagate in a stable manner characterized by a uniform propagation speed and smooth wavefront morphology. Other less reactive forms exhibit unstable reactions characterized by stalled wavefronts, spatially non-uniform temperatures, and variable propagation speeds. Unfortunately, unstable reaction modes are poorly understood, thus limiting the use of reactive multilayers in emerging applications. In order to better understand the various behaviors of reactive multilayers, we have investigated how surrounding gaseous environment affects wavefront stability. Rare-earth / transition metal multilayers (e.g., Sc/Ag) of different periodicity were deposited by DC magnetron sputtering and tested as freestanding foils in different environments. Their reaction in 1e-3 Torr vacuum demonstrates inherent unstable intermetallic reaction fronts. Reactions in air are complicated by oxidation of the rare earth metal species which produces metal oxide and residual elemental metal. A separate oxidation wavefront trails the intermetallic reaction wavefront when reacted in air. In some cases, oxidation occurs long after the passage of the intermetallic reaction and there is little effect on the intermetallic reaction dynamics. However, large-period (low speed) multilayers show evidence for interference between intermetallic and trailing oxidation reaction waves. Prompt oxidation after the passage of the slow intermetallic reaction wave leads to a complex oscillatory behavior. The high exothermicity oxidation reaction repeatedly transitions the intermetallic front from an unstable mode to a stable form, while boosting its net velocity.

This work was supported by a Sandia Laboratory Directed Research and Development (LDRD) program. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

3:20pm **C4-ThA-7 Synthesis of Reactive Ni-Al Composites Using High Pressure Torsion*, O Renk,*** Austrian Academy of Sciences, Austria*; M Tkadletz, N Kostoglou,* Montanuniversität Leoben, Austria*; I Gunduz,* Naval Postgraduate School, USA*; C Doumanidis,* Nazarbayev University, Astana, Kazakhstan*; R Pippan,* Austrian Academy of Sciences, Austria*; C Mitterer,* Montanuniversität Leoben, Austria*; **Claus Rebholz**,* University of Cyprus, Cyprus

Mechanical mixing methods provide a bottom-up scalable route for fabricating nanostructured bulk materials. These include high energy ball milling (HEBM) used in metal-based reactive systems such as Nickel-Aluminum that can yield high performance NiAl and Ni_3Al intermetallic alloys upon combustion synthesis or used for in-situ welding with the heat generated from the exothermic reactions. The drawback of HEBM is the final product form, which consists of fine hardened powders that need to be processed further to form a dense part. This study investigates an alternative route, high pressure torsion (HPT), which applies a combination of large normal and shear stresses to a powder mixture in a die to yield nanostructured materials. HPT was used for fabricating consolidated reactive pellets of Ni-Al with microstructures comparable to HEBM and magnetron sputtering. The results show that materials undergoing HPT beyond 5 full rotations at processing temperatures of up to 473 K are highly reactive and can be ignited below the Al melting point, yielding a product phase of NiAl with residual Ni_2Al_3 and Ni_3Al, while reaching very high reaction temperatures near 1900 K.

Fundamentals and Technology of Multifunctional Materials and Devices
Room Grand Hall - Session CP-ThP
Fundamentals and Technology of Multifunctional Materials and Devices (Symposium C) Poster Session

CP-ThP-1 Comparison of SiC_xN_y Barriers using Different Precursors Deposited on Porous Low-Dielectric-constant SiCOH Dielectric Films, *Y Cheng, Y Lin,* ***Chih-Yen Lee,*** National Chi-Nan University, Taiwan

In this study, two different SiC_xN_y films using different deposition precursors were deposited onto the porous SiOCH low-*k* films. Their impacts on the electrical characteristics and reliability of a $SiCOH/SiC_xN_y$ dielectric stack were compared. A lower plasma damage on the SiOCH low-*k* film was made as SiC_xN_y film was deposited onto the SiOCH low-*k* film using single-source precursor compared to that using the conventional multi-source precursors. This results in a lower capacitance of $SiCOH/SiC_xN_y$ dielectric stack. Moreover, better TDDB reliability and comparable Cu barrier performance were detected. As a result, the SiC_xN_y layer deposited using a single precursor is a promising method to serve as a capping barrier for porous low-*k* dielectrics.

CP-ThP-2 Stretchable Ultrasonic Transducer Arrays for Three-Dimensional Imaging on Complex Surfaces, ***Hongjie Hu****, X Zhu, C Wang, L Zhang, S Xu,* University of California, San Diego, USA

Ultrasonic imaging has been implemented as a powerful tool for noninvasive subsurface inspections of both structural and biological media. Current ultrasound probes are rigid and bulky and cannot readily image through nonplanar three-dimensional (3D) surfaces. However, imaging through these complicated surfaces is vital because stress concentrations at geometrical discontinuities render these surfaces highly prone to defects. This study reports a stretchable ultrasound probe that can conform to and detect nonplanar complex surfaces. The probe consists of a 10 × 10 array of piezoelectric transducers that exploit an "island-bridge" layout with multilayer electrodes, encapsulated by thin and compliant silicone elastomers. The stretchable probe shows excellent electromechanical coupling, minimal cross-talk, and more than 50% stretchability. Its performance is demonstrated by reconstructing defects in 3D space with high spatial resolution through flat, concave, and convex surfaces. The results hold great implications for applications of ultrasound that require imaging through complex surfaces.

CP-ThP-6 Fabrication and Characterization of Ni-coated Ag Nanowire Electrodes with Bubble-like Random Meshes, ***Jong-Seol Park****, R Yoo, T Park, J Park,* Hanyang University, Republic of Korea

Recently, as the applications of flexible electronic devices have been expanded, transparent electrode materials are required to be flexible and stretchable in addition to having excellent electrical and optical properties. Examples of such materials include carbon nanotubes, metal meshes, metal nanowires, and graphene. Among them, metal nanowires along with metal meshes, are evaluated to be advantageous in terms of commercialization because they have a low electrical sheet resistance and a high visible light transmittance. In particular, compared to other materials, metal nanowires are the most advantageous in terms of flexibility and have the advantage of being able to fabricate electrodes using simple and relatively inexpensive solution-based methods. However, metal nanowires have a relatively high reflectance, high haze, and high contact resistance between their wires. They also have oxidation problems when exposed to the atmosphere. As an example of inhibiting the oxidation of metal nanowires, studies have been introduced to coat the nanowires with oxidation resistant materials. Also, in the case of the widely adopted grid-type electrode, there is another disadvantage in that it is difficult to secure high visibility due to the diffraction of light or the moiré phenomenon due to a regularly repeated lattice structure. To solve this problem, studies on the fabrication of random-type electrodes using the irregular patterns of crack, leaf, spider web, and bubble have been reported.

In this study, embedded-type nickel (Ni)-coated silver nanowire (AgNW) transparent electrodes with random-mesh patterns were fabricated via solution processes. The major manufacturing processes of the Ni-coated AgNW random mesh electrodes are summarized as follows. The AgNW bubble solution was prepared by mixing a surfactant with the AgNW solution and agitating it. The surface modification of polyethylene terephthalate (PET) substrate was performed using corona plasma. Using a spin-coating method, the AgNW bubble solution was deposited on the PET substrate with various surface energies. Then, the bubble solution was evaporated through the baking process to form a bubble-like random pattern. This was transferred to polydimethylsiloxane (PDMS) and coated with Ni by electroplating. The line width and line-to-line spacing of the fabricated electrodes were estimated according to the number of corona treatments and baking temperature on the PET substrate. For the electrodes fabricated, we have measured and characterized their morphology, transmittance and reflectance at visible light region, electrical sheet resistance, flexibility, stretchability, and oxidation-stability.

CP-ThP-13 Study of Stress-electrical Properties of ITO Film Deposited on Stretchable Substrate, ***Pierre-Olivier Renault****,* Université de Poitiers, France*; C Grossias, P Goudeau, P Godard, F Paumier, S Hurand,* University of Poitiers, France*; D Thiaudière,* SOLEIL Synchrotron, France*; P Guerin,* University of Poitiers, France

Indium Tin Oxide (ITO) is one of the most widely used material with the unusual property of being transparent and conductor. The fabrication and characterization of these materials, called transparent conductive oxides (TCO), is a very active field of research motivated by their potential applications in optical and optoelectronic devices. ITO is almost always used as a thin film in a more or less complex stacking deposited on substrates. The mechano-electro-optical properties of transparent conductive oxide thin films deposited onto substrates depend on many elaboration parameters as well as their piezoresistive response.

In the present work, 400 nm thick ITO films have been prepared by ion beam sputtering controlling the oxygen partial pressure. Each thin film has been deposited on a polyimide stretchable substrate. The deformations are applied thanks to a biaxial tensile tester in situ during x-ray diffraction measurements at the french synchrotron SOLEIL. Thus, x-ray stress or x-ray strain (measured by x-ray diffraction technique), true strain (measured by digital image correlation technique) and electrical resistivity (Van der Pauw method) measurements are performed during in situ biaxial straining. The first results obtained on x-ray stress- true strain – electrical conductivity relation are reported. A negative gauge factor is observed for all thin films. The influence of oxygen residual pressure does not seem to have a large effect on gauge factor contrary to the mechanical behavior.

CP-ThP-18 Dual Box Model based *In situ* Ellipsometry Growth Characterization: Oxygen Plasma Enhanced Atomic Layer Deposition of Metal Oxide Ultra-thin Films, *U Kilic,* University of Nebraska-Lincoln, USA*; A Mock,* Linköping University, Sweden*; D Sekora, N Ianno,* ***Eva Schubert****, M Schubert,* University of Nebraska Lincoln, USA

Atomic Layer Deposition (ALD) of conformal ultra-thin films has been shown to have potential for applications in microelectronics, photovoltaics, photoluminescence and fuel cells [1]. The integration of spectroscopic ellipsometry (SE), an optical, contactless, and non-invasive technique, into the ALD instrumentation has been a powerful and widely-used process monitoring method[2] which paves the way to unravel the surface roughness and thickness evolution during the ALD process.

In this study, we successfully optimized the oxygen plasma enhanced ALD recipes for two different metal-oxides: WO_3 and TiO_2, in which employs $(tBuN)_2(Me_2N)_2W$ and $Ti(OC_3H_7)_4$ organometallic precursors, respectively. Multi-sample analysis method is employed in order to obtain both thickness and optical constants from SE data analysis[3]. Thus, three films are deposited by using 75, 100, and 150 ALD cycles under the same conditions and *ex-situ* SE data is collected in the spectral range from 0.7-6.5~eV.

The as-grown WO_3 and TiO_2 dielectric functions are determined along with the respective film thicknesses. With this information, the *in-situ* SE data is retroactively analyzed to attain inherent layer-by-layer deposition parameters. We employed the dual-box model in order to obtain sub-angstrom scale in-cycle resolution time evolution of thin film thickness and effective surface roughness layer thickness parameters during the growth process. Our model analysis permits determination of growth rate and identification of cyclic surface modifications during exposure to individual cycle steps. Further implementation of this method allows for precise control and real-time optimization of deposition parameters ultimately providing us with the ability to develop ALD recipes *in-situ*.

References:

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[2]: Leick, N., et al. Journal of Physics D: Applied Physics 49.11 (2016): 115504.

[3]: Kilic, U., et al., Journal of Applied Physics:*1805.04171* (2018).

CP-ThP-19 Controlled Release of Encapsulated Agents Deposited on Plasma Electrolytic Oxidation (PEO) Coatings for Corrosion Resistance and Biomedical Applications*, Y Guo, B Mingo, A Matthews,* ***Aleksey Yerokhin,*** The University of Manchester, UK

A number of surface treatment methods has been developed in order to increase the protective and functional properties of magnesium alloys. Plasma Electrolytic Oxidation (PEO) is an environmentally friendly treatment resulting in ceramic coatings with high hardness, excellent adhesion to the substrate and good wear and corrosion resistance. However, the passive corrosion protection provided by PEO coatings can be undermined if the coating is worn off or damaged.

Therefore, the aim of this work is to investigate a possibility functionalisation of PEO coating surfaces in order to achieve: i) sustained release of corrosion inhibitors encapsulated by halloysite nanotubes (HNT) for non – biological applications of magnesium alloys, in order to achieve self-healing effect; and ii) sustained release of encapsulated drugs for biological applications of degradable magnesium alloys, in order to develop the next generation of 'smart' biomedical implants materials.

Halloysite nanotubes (HNT) represent a type of bio-compatible naturally occurring clay with the walls consisting of two layered aluminosilicates. The hollow tubular structure of HNT allows different agents to be loaded by vacuum-induced capillarity. The release of the agents can be triggered by e.g. changes in the pH of environment, on mechanical impact or simply by osmotic pressure. The corrosion inhibitors in this study (vanadate, molybdate and 8-hydroxyquinoline) consist both negatively charged particles and electrically neutral molecules. For biological applications, the drugs are mostly electrically neutral molecules, and in this study is penicillin.

The main challenge of this work is ensure the adequateness of the deposited agents. The incorporation of encapsulated agents onto PEO coatings can be achieved by two approaches: hybrid and sequential. The hybrid approach is to incorporate the particles as the same time as the coating synthesis whereas the sequential approach is by post-treatment. In this work, post-treatment will be discussed. There are two post-treatment methods: electrophoretic deposition (EPD) and immersion. Both of the post-treatment methods require aqueous suspension of loaded HNT. So, the release kinetics of the loaded agents is of great importance since there are possibility of release during the deposition process. Ultraviolet-visible (UV-VIS) spectroscopy is employed for the release kinetics.

Successfully encapsulated and deposited corrosion inhibitors significantly improves the corrosion resistance of magnesium alloys. And for drugs, observation of zone of inhibition (ZOI) on Gram-positive bacteria Staphylococcus Aureus indicates the success of drug loading.

CP-ThP-21 Influence of Substrate Temperature on the Growth of Molybdenum Trioxide Thin Films*, Madhuri Venkat Kalapala,* VFSTR University, India

Molybdenum oxide is one of the most important inorganic materials which exhibit several phases such as MoO_3, MoO_2, Mo_4O_{11}, Mo_5O_{14}, etc,. Out of this molybdenum trioxide (MoO_3) can crystallize in various phases such as Orthorhombic, Monoclinic etc., which lead it to the useful for potential applications in chemical, electrical and electrochemical industry. In the present work MoO_3 thin films were prepared by pulsed laser deposition techniques at various substrate temperatures from room temperature to 400^{0}c. The films were deposited on to glass and FTO quoted substrates at a base pressure of 10^{-5}mbar. The crystal structure morphology and elemental analysis were recorded by XRD, SEM, EDS and AFM. The substrate temperature strongly influences the structure and surface topography. The films prepared at base pressures are found to be oxygen deficient and after annealing the films were found to be transparent. The presence of oxygen atmosphere at the time of deposition makes the films to show better properties.

CP-ThP-22 Evaluation of the Influence of Pre-carburisation on the In-situ Performance of Chromized 304 Stainless Steel Bipolar Plate*, Atinuke Oladoye,* University of Lagos, Nigeria*; J Carton, J Stokes,* Dublin City University, Ireland*; A Olabi,* University of the West of Scotland, UK

This paper reports preliminary attempts at improving the in-situ performance of chromised 304 stainless steel (304SS) bipolar plates via the introduction of a pre-carburisation step prior to chromising. 304 stainless steel bipolar plates with parallel flow field design were pre-carburised at 900^{o}C for 3 hours and subsequently chromised at 1040^{o}C for 3 hours. The surface modified plates were tested in a 5cm^2 active area single proton exchange membrane fuel cell at room temperature for performance and durability. Results obtained was compared to that of non-carburised chromised 304SS bipolar plate tested under identical conditions. It was found that the single fuel cell with pre-carburised chromised bipolar plates attained a peak power density of 18.20 mW/cm^2, which was a double-fold increase in that of the single fuel cell with non carburised chromised 304SS bipolar plates. The ten-hour durability test, however, indicated the need for further research efforts to enhance the stability of the pre-carburised-chromised stainless steel bipolar plates.

CP-ThP-23 Piezo- and Thermo-resistive Thin Films Integrated into a Polymer Injection Mold to Control Dynamically the Pressure and Temperature of the Injection Process*, Filipe Vaz, A Ferreira, M Barbosa,* University of Minho, Portugal*; J Larangeira,* Moldit, Portugal

The present work reports on the development of metallic piezoresistive thin films, aiming to investigate an innovative solution to control dynamically the temperature of the injection molding process of polymeric parts using technologies of thin films. The general idea was to analyse the signal response of the $Ti_{1-x}Cu_x$ and ZnO/Ag based transducers exploring the possibility to use this thin film system in force, deformation and temperature sensor devices. $Ti_{1-x}Cu_x$ and ZnO/Ag thin films were produced by the Glancing Angle Deposition technique (GLAD).

The results reveal that the zigzag microstructure has an evident influence on the overall response of the films as well as the influence of the Cu or Ag doping level. The values of temperature coefficient of resistance reach 8 .73×10^{-3} ºC^{-1} for pure copper films and 4.38 ×10^{-3} ºC^{-1} for films with an intermedium composition. The values of the gauge factor show that a longer distance between Ag particles, which varies from 0.1 to 10 nm, leads to enhanced GF, which ranges from 8 ± 1 to 120 ± 3, respectively.

In order to demonstrated the sensing capabilities of the system, a proof-of-concept experiment was carried out by integrated the thin films of $Ti_{1-x}Cu_x$ and ZnO/Ag with the best response in an injection steel mold and connected to a data acquisition system based on a homemade dedicated read circuit hardware and LabVIEW software, connected to a radio-frequency access point, plugged to a universal serial bus (USB) port. The most challenging part in this work is to quantify the results obtained from this experiment which has not been done in literature yet.

CP-ThP-25 Investigation of Sb_2Se_3 Ultra-thin Hole-transporting Material for Perovskite/ Sb_2Se_3 Heterojunction Solar Cells*, Gwomei Wu,* Chang Gung University, Chang Gung Memorial Hospital, Taiwan

Sb_2Se_3 thin film photovoltaic has a low energy band gap for effective and wide solar-spectrum utilization. This report presents a new solar cell architecture with ultra-thin Sb_2Se_3 hole-transporting material (HTM) layer (<300 nm) in between bi-layer Mo metal-electrode layer and $CH_3NH_3PbI_3$ ($MAPbI_3$) perovskite active absorber layer. The solar cell nano-structures were prepared as Mo/ Sb_2Se_3/perovskite/ ZnS/Ag multi-layers on FTO (fluorine-doped tin oxide) glass substrates. The hole-transporting layer, active absorber layer, electron-transporting buffer layer, and top metal-electrode contact layer, were made of Sb_2Se_3, perovskite, zinc-sulfide, and silver, respectively. The ultra-thin Sb_2Se_3 HTM layers were annealed at temperature of 400, 500, and 600℃. The nano-crystal grain size, revealed by scanning electron microscopy, was enhanced with the increaing annealing temperature. T he advantages of using Sb_2Se_3 HTM on perovskite photovoltaics included better device performance, reduced HTM film thickness, and diminished HTM film cost. The Sb_2Se_3 HTM has acted to maintain perovskite absorber layer's optical-current and stability. The device photo power-conversion efficiency can reached about 14.4%, and the related photo-electronic characteristics will be summarized and further discussed. This work was supported in part by the Ministry of Science and Technology under research grants MOST105-2221-E182-059-MY3/BMRP246 and CGMH CMRPD3G0062.

Keywords: Sb_2Se_3, Hole-transporting material, perovskite, $MoSe_2$, ZnS,

CP-ThP-27 Fabrication of a Thermoelectric Generator Device by Suspension Plasma Spray Technique*, Fabian Ambriz-Vargas, C Moreau,* Concordia University, Canada

About seventy percent of the world energy production is lost in the form of heat dissipation which is one of the most significant contributions in the global warming. Thermoelectric generators are one of the most viable devices to recover waste heat (generated by the vehicles, factories, houses etc.) and convert it into electricity. With the rising cost of fuel and increasing demand for clean energy, solid-state thermoelectric devices are good candidates to reduce fuel consumption and CO_2 emissions. Although, they are reliable energy converters, there are several issues that have

limited their implementation into the market. These issues include toxicity of the thermoelectric materials (coatings-based lead and tellurium) and the limited ability to mass-manufacture thermoelectric materials. Recent theoretical predictions have demonstrated that titanium dioxide (TiO_2) can overcome the above issues, since they are non-toxic, relatively abundant and present excellent thermoelectric properties. However, formation of high quality TiO_2 phase is not feasible. Among the different emerging synthesis process, suspension plasma spray technique is a good candidate to synthesize TiO_2 coatings since it presents several advantages such as control over the chemical stoichiometry, industry-scalable and low-cost process. Then, this work presents the evaluation of the thermoelectric properties of TiO_2 coatings produced by suspension plasma spray technique. This research strategy involves the study of the effect of the synthesis technique parameters on the microstructural, structural and thermoelectric properties of TiO_2.

CP-ThP-31 Morphology Controlled of Silver/Silver Oxide Nanoparticles-MnO2 Nanocomposites for Supercapacitor Application, *F Sari,* ***Kuang-Cheng Lin****, J Ruan, J Huang, J Ting,* National Cheng Kung University, Taiwan

Ag nanoparticles (NPs)-MnO_2 having various morphology have been synthesized through a facile method. It was found that by controlling the amount of Ag NPs, temperature, and time of reaction lead to the formation of urchin-like structure with Ag_2O NPs on the tips of □-MnO_2 nanowires, while the addition of surfactant agent poly(vinylpyrrolidone) (PVP) leads to the formation of nanoflower-like structure with Ag NPs distribute well on the δ-MnO_2 nanosheets surface. Moreover, the formation of the Ag sub-oxides such as Ag_2O and Ag_2O_2 were also investigated. Varied dimension and different morphology resulting the different of specific surface area. Supercapacitors having the obtained Ag/Ag sub-oxides –MnO_2 nanocomposite as the electrodes were evaluated. We demonstrated the synergistic effect of high specific surface area with the Ag/Ag_2O NPs, which provide more active sites and effectively reduce the resistance. As a result, the obtained nanocomposite with optimum specific surface area of 250.9 m^2g^{-1} and low Rct of 84 ohm showing high Csp of 226 F g^{-1} at 5 mV s^{-1} which is three times compare to pure □-MnO_2. The nanocomposites also show no degradation after 1000 cycles, indicating excellent electrochemical stability.
Keywords: MnO_2, Ag nanoparticles, Ag_2O, supercapacitor

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