Applied Surface Science Division
Room A211 - Session AS-ThA

Role of Surfaces and Interfaces in Energy Material and Industrial Problems

Moderators: David M. Carr, Physical Electronics, Alan Spool, Western Digital Corporation

2:20pm **AS-ThA1 Characterization of Glass and Durable Optical Surfaces and Their Modes of Failure**, ***Albert Fahey***, *D. Baker, T. Dimond,* Corning Inc. **INVITED**

Glass has become the all-important interface between human users and information and communications in our daily lives. People not only want to look at bright, high-definition information-displays but also want to interact with and touch the displays. This has placed new requirements on the performance and durability of the surfaces we interact with.

Just below the outer boundaries of glass, the composition makes a transition from the surface that we interact with, defining the spatial limits of the solid, to the "bulk"-material that exhibits most of the macroscopic properties we experience that allow us to use it as building materials to construct displays, hand-held devices, smart-watches, etc.

The composition of the near-surface region, from a few nanometers to several micrometers generally governs the appearance and durability of these surfaces. It also is a critical component in the adhesion of thin films deposited to improve scratch resistance, cleanability, and optical performance.

We will review some compositional profiles of glass, thin films and other materials to understand how some of these surfaces appear, compositionally, and how this can inform us of chemistries and mechanical properties. I will review Secondary Ion Mass Spectrometry (SIMS) depth-profile data and its combination with data acquired by other methods that give us a more complete understanding of the optical surfaces we interact with.

3:00pm **AS-ThA3 Determination of Liquid Laundry Additives Across Fabric Surfaces**, ***Michael Clark, Jr.***, *A. Peera, S. Donovan, R. Pulukkody,* The Dow Chemical Company

Products that offer sensorial benefits in addition to cleaning are increasingly popular among consumers in the fabric care market. Such sensorial attributes are typically related to touch and smell and help provide a more enjoyable experience to the consumer both during and after the laundering process. This presentation will focus on the XPS and SIMS characterization of fabrics before and after washing with different liquid laundry formulations to determine the amount and distribution of different components on the fabric's surface.

3:20pm **AS-ThA4 Depth Profiling of Silicones with GCIB, Do They Behave like Organic or Inorganic Molecules?**, ***Michaeleen Pacholski***, *M.B. Clark, Jr., P.R. Vlasak, C. McMillan,* The Dow Chemical Company

Surface analysts have a love-hate relationship with silicones. Silicones are widely used industrially for lowering surface energy, improving slip, coefficient of friction, mar and many other surface lubricity properties. Due to their low surface energies, and sometimes low viscosity or molecular weight, there is a tendency for them to spread over surfaces or be present as surface contaminants. In these cases a surface analyst may wish to remove them using a gas cluster ion beam source (GCIB). In other instances it may be desirable to understand the chemistry of a silicone coating as a function of depth. Unfortunately, GCIB profiling of silicones is not as straightforward as it is with other organic polymers.

Examples of depth profiles under different GCIB conditions from some reference silicones and silicone-containing coatings will be discussed in this presentation.

4:00pm **AS-ThA6 Active Control of Interfacial Chemistry for Thin Film Solar Cells**, ***Alexandra Koziel***, *K.A. Montiel, L.G. Wilson, J.L.W. Carter, I.T. Martin,* Case Western Reserve University

Global energy demand requires the development of efficient and reliable thin film photovoltaics with inexpensive processing. As the efficiency of hybrid perovskite solar cells has skyrocketed, practical constraints of the technology have put the scalability and durability into scientific focus. The development of inorganic interfacial layers, such as metal oxides, is a potential pathway to overcoming the stability and cost limitations associated with organic interlayers in perovskite solar cells. Thin films are sensitive to both the growth conditions, and the composition and morphology of the previously deposited layer. Interfacial engineering of metal oxides using molecular modifiers provides a powerful tool to tune interlayer properties, which can result in improved performance and stability.

This work details the effect of underlying layers on the growth of $CsGeI_3$, a novel all-inorganic perovskite absorber. The hole-transport layer (HTL) and the underlying substrate were systematically varied. Surface and bulk properties of the film stack were characterized at every growth step. The choice of HTL affects the absorber film morphology, and resulting device efficiency. Further, this approach reveals that the choice of substrate can affect the properties of layers through the entire device.

Two common HTLs, PEDOT:PSS and MoO_3, were deposited on substrates with differing surfaces. Glass, ITO (indium tin oxide, a common thin film solar cell transparent electrode), and Si substrates were selected to explore how a range of surface structures, from amorphous to polycrystalline to crystalline, affects the subsequent layers. The vapor-deposited MoO_3 was further modified with gas-phase treatments (UV-ozone and O_2 plasma exposure) and small molecules (silanization). Specifically, an IPTMS ((3-iodopropyl) trimethoxysilane) silanization procedure was developed to produce an iodine-terminated surface, for improved adhesion of the $CsGeI_3$ absorber layer. A suite of materials characterization methods were applied to the samples after each step of device fabrication to assess the evolution of morphology and composition. Bulk, surface, and interface characteristics were probed using UV-Vis absorption measurements, X-ray photoelectron spectroscopy, scanning electron microscopy, optical profilometry, and spectroscopic ellipsometry. Notably, the absorber film morphology and ultimately the stability of the film stack is sensitive to not only the HTL, but the nature of the material under the HTL (ITO vs. glass), demonstrating the influence of surface/interface properties across multiple layers in a device.

4:20pm **AS-ThA7 Solar Energy From a Big-Picture Perspective to Nanoscale Insights via TOF-SIMS**, ***Steven Harvey***, National Renewable Energy Laboratory **INVITED**

We have used time-of-flight secondary-ion mass spectrometry (TOF-SIMS) at the National Renewable Energy Laboratory to investigate the performance and reliability of solar cell materials and devices, and we will present some recent work that highlights the versatility of TOF-SIMS. This work includes: 1) Multi-scale, multi-technique investigations of photovoltaic module failure including TOF-SIMS to enable insights into the root-cause mechanisms of module degradation at the nanoscale that are observed at the length scale of meters; 2) Investigations into the performance and stability of hybrid perovskite solar cell devices and 3) Using a combination of 1-D profiling and 3-D tomography to elucidate the fundamentals of incorporating dopants in CdTe solar cells.

5:00pm **AS-ThA9 Investigation of Surface and Bulk Properties of Extended Surface PtNi and PtNiCo Catalysts**, ***Sarah Zaccarine***, Colorado School of Mines*; W.W. McNeary,* CU Boulder*; S. Shulda, S.A. Mauger, K. Hurst,* National Renewable Energy Laboratory*; A.W. Weimer,* CU Boulder*; S.M. Alia, B.S. Pivovar,* National Renewable Energy Laboratory*; S. Pylypenko,* Colorado School of Mines

Polymer electrolyte membrane fuel cells (PEMFCs) produce electricity with only heat and water as byproducts, but sluggish kinetics of the oxygen reduction reaction (ORR) at the cathode restrict widespread commercialization, motivating development of advanced catalysts such as the extended surface platinum nickel (PtNi) and platinum nickel cobalt (PtNiCo) nanowires investigated in this work.

These catalysts were synthesized using atomic layer deposition (ALD), a scalable route that allows controlled deposition of Pt on Ni or Co nanowires. Surface and bulk composition and structure of the PtNi and PtNiCo nanowires was investigated as a function of synthesis conditions and a series of post-synthesis modifications. A variety of characterization techniques was used to gain a comprehensive understanding of structure-property-performance relationships. The catalyst was first studied using a combination of x-ray absorption near-edge structure (XANES) spectroscopy, extended x-ray absorption fine structure (EXAFS) spectroscopy, x-ray photoelectron spectroscopy (XPS), and scanning transmission electron microscopy (STEM) coupled with energy dispersive x-ray spectroscopy (EDS) hypermapping to obtain detailed complementary information about speciation and distribution of Pt and Ni, distinguishing differences between surface and bulk. Rotating disk electrode (RDE) testing was conducted to assess activity and stability of the catalysts. Differences between ALD-derived PtNi and PtNiCo samples will be discussed and compared to previously reported catalysts synthesized via spontaneous

galvanic displacement (SGD). Catalysts were then integrated into membrane electrode assemblies (MEAs) and properties of the fabricated catalyst layers were investigated using STEM/EDS and transmission x-ray microscopy (TXM) to better understand the interfaces between catalyst and ionomer, with and without addition of carbon into the structure of the electrode. Our results demonstrate important advances in the performance of this class of materials achieved through optimization of surfaces and interfaces of the catalyst and catalyst layer.

5:20pm **AS-ThA10 Interfaces in Electrodeposited Li-Ion Battery Electrodes**, ***Paul Braun***, University of Illinois at Urbana-Champaign **INVITED**

Electrodeposition of electrode materials has the potential to enhance secondary battery performance and broaden the scope of available electrode form factors. For example, as we have shown, electrodeposited electrodes provide energy densities not achievable via conventional slurry-cast electrode processing methodologies. I will present our work on the electrodeposition of high performance silicon and tin-based Na and Li-ion anodes and $LiCoO_2$, $NaCoO_2$, $LiMn_2O_4$, and related Na and Li-ion cathodes. The electrolytically active materials were formed either as solid films, or where significant volume changes upon cycling are present, as a 3D mesostructured film. The capacities are near-theoretical, and in the case of the electroplated oxides, the crystallinities and electrochemical capacities are comparable to powders synthesized at much higher temperatures. What we have found, is that the interfaces, and interphases that may form during cycling, have significant impacts on the properties of the resulting electrodes. Understanding the properties of these interfaces/interphases is critical to understanding, and ultimately improving, overall cell performance.

Author Index

Bold page numbers indicate presenter

— A —
Alia, S.M.: AS-ThA9, 1
— B —
Baker, D.: AS-ThA1, 1
Braun, P.: AS-ThA10, **2**
— C —
Carter, J.L.W.: AS-ThA6, 1
Clark, Jr., M.B.: AS-ThA3, **1**; AS-ThA4, 1
— D —
Dimond, T.: AS-ThA1, 1
Donovan, S.: AS-ThA3, 1
— F —
Fahey, A.J.: AS-ThA1, **1**
— H —
Harvey, S.: AS-ThA7, **1**
Hurst, K.: AS-ThA9, 1
— K —
Koziel, A.C.: AS-ThA6, **1**
— M —
Martin, I.T.: AS-ThA6, 1
Mauger, S.A.: AS-ThA9, 1
McMillan, C.: AS-ThA4, 1
McNeary, W.W.: AS-ThA9, 1
Montiel, K.A.: AS-ThA6, 1
— P —
Pacholski, M.L.: AS-ThA4, **1**
Peera, A.: AS-ThA3, 1
Pivovar, B.S.: AS-ThA9, 1
Pulukkody, R.: AS-ThA3, 1
Pylypenko, S.: AS-ThA9, 1
— S —
Shulda, S.: AS-ThA9, 1
— V —
Vlasak, P.R.: AS-ThA4, 1
— W —
Weimer, A.W.: AS-ThA9, 1
Wilson, L.G.: AS-ThA6, 1
— Z —
Zaccarine, S.F.: AS-ThA9, **1**