Tuesday Morning, October 20, 2015

IPF on Mesoscale Science and Technology of Materials and Metamaterials
Room: 210F - Session IPF+MS-TuM

Degradation Science (8:00-10:00) & Electrochemistry from Nano to Meso Scale (11:00-12:20)
Moderator: Gary Rubloff, University of Maryland, College Park, Stacey Bent, Stanford University

8:00am **IPF+MS-TuM1 Mesoscale Evolution & Temporal Analytics of Photovoltaic Energy Materials: A Degradation Science Approach**, ***Roger French***, Case Western Reserve University **INVITED**

Degradation science1 combines physical and statistical approaches to examine degradation mechanisms and pathways of a material or system in order to improve materials and reduce system failures by incorporating modeling, monitoring, and prediction of lifetime performance. Degradation of PV modules evolves over long time-frames and length scales, which is a characteristic of mesoscale science. Degradation arises due to the distinct, complex, and interactive phenomena which lead to failure. Real-world studies under diverse environmental conditions must be combined and cross-correlated with accelerated in-lab studies, using data science and analytics methodologies, so as to span the time and length scales that control the system's behavior over lifetime. Semi-supervised generalized structural equation (semi-gSEM) modeling can be used to relate physical mechanistic submodels with data-driven statistical submodels as networks of mechanisms and modes with statistically significant pathway relationships. The relationships and coupling strengths (βij) amongst variables can be rank-ordered in their contributions to the system's degradation. Temporal evolution, damage accumulation and change points among mechanisms/modes (variables) are accounted for in the semi-gSEM models. Towards these goals, a statistical methodology has been developed and applied to investigate the response of full sized PV modules to accelerated stress conditions. The results of this initial study indicate that a correlation exists between system level power loss and the buildup of acetic acid resulting from the hydrolytic degradation of EVA polymer encapsulant. To further explore this proposed mechanistic pathway, studies are underway to characterize the degradation of minimodule samples under a broader range of similar multifactor accelerated stress conditions. Sample types feature frontside silver gridlines of two different widths and exposure conditions vary in irradiance level and temperature. Samples are measured non-destructively at many points along their lifespan, using confocal Raman microscopy to capture chemical signals and various techniques to gather electrical performance information, with the goal of observing the co-evolution of EVA degradation and gridline corrosion. This represents an important first step towards exploring the often misunderstood role of EVA degradation in PV module performance loss, and building a more integrated picture of PV module degradation as a whole. Initial data analytics of six months' real-world performance data of 60 c-Si PV modules on the SDLE SunFarm shows deviation of performance ratio among modules at the same geometric location. Grouping of samples with similar performance patterns was performed with hierarchical clustering, K-means clustering was used to confirm the optimum number of clusters. A brand dependent module performance model was developed based on a subgroup of 21 modules from 7 manufactures. Over 1.5 million I-V curves measured every 5 minutes for 500 days on 10 modules with/without mirror on dual-axis trackers were analyzed use an automated analytic functions we developed. Maximum power point, open circuit voltage, short circuit current, slope of the curve near open circuit voltage, and slope of the curve near short circuit current are either directly extracted or estimated from measured I-V curves. An algorithm based on moving local regression model was developed to detect the change points on I-V curves, which caused by bypass diode turning on when I-V curve was measured under non-uniform irradiance. These examples of the use of degradation science, with its physical and statistical foundation and data analytics approach, will hopefully enable the community to address the long-term reliability uncertainty of photovoltaics as they become a major component in the world's energy systems.

1. French, Roger H., Rudolf Podgornik, Timothy J. Peshek, Laura S. Bruckman, Yifan Xu, Nicholas R. Wheeler, Abdulkerim Gok, et al., 2015, "Degradation Science: Mesoscopic Evolution and Temporal Analytics of Photovoltaic Energy Materials," Current Opinion in Solid State and Materials Science, Doi: 10.1016/j.cossms.2014.12.008

8:40am **IPF+MS-TuM3 Why Structural Failure is Mesoscale: From Dislocations to Fatigue Cracks**, ***Anthony Rollett***, Carnegie Mellon University **INVITED**

Structural failure of materials is a mesoscale problem because, for example, we lack the tools to predict when and where fatigue cracks will appear in relation to materials microstructure. Dislocations are well understood as line defects but we do not how to compute the behavior of large numbers of dislocations in relation to microstructure. Enormous strides have been made in quantifying the growth of fatigue cracks over the years and improving predictions of component lifetime but all at the microstructural scale and above. Nevertheless, it is clear that the behavior of short cracks is less well quantified, where short is relative to the length scale(s) found in materials microstructure, e.g. grain size. Short fatigue cracks in nickel-based superalloys have been characterized using conventional SEM and orientation mapping. High Energy Diffraction Microscopy (HEDM) and computed tomography (CT) was used to map out the crack positions in 3D. The main finding is that cracks develop most readily along long twin boundaries with high resolved shear stress on the slip systems parallel to the twin plane. Also, both halves of a different superalloy, fully fractured sample have been fully characterized in 3D using the same tools. The HEDM and CT were performed with high energy x-rays on beamline 1ID at the Advanced Photon Source (APS). This talk will review current dislocation modeling, empirical understanding of fatigue cracks in engineering materials and what the experimental and theoretical roadmap might be to address the problem set.

9:20am **IPF+MS-TuM5 Engineered 3D Mesoscale Battery Electrodes: Opportunities and Issues**, ***Paul Braun***, University of Illinois at Urbana-Champaign **INVITED**

Over the past decade, three-dimensional structures have been widely proposed as a path for enhanced lithium-ion batteries. While the sophistication of self and directed-assembly approaches for functional structures has increased dramatically, application of these structures has remained elusive, in part because real structures almost always contain finite defect densities, cannot be produced from materials with the appropriate electrochemical properties, and cannot be produced in sufficient volume for application. We have now made considerable strides in integration of electrically conducting and energy storage material into lithium-ion battery electrodes. We accomplish this by applying template-based and post-synthetic materials transformations, and have focused on ultra-large volume processing strategies. As the technology has approached commercialization, understanding the mechanistics of capacity fade and other electrochemical degradation pathways has become increasingly important.

11:00am **IPF+MS-TuM10 A Materials Genome Approach to Design of Novel Materials and Liquids for Energy Conversion and Storage**, ***Kristin A. Persson***, Lawrence Berkeley National Laboratory **INVITED**

The Materials Genome Initiative (MGI) aims to develop an infrastructure to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost. In this talk I will highlight the advances and development of the Materials Project (www.materialsproject.org), which is an MGI-funded effort to compute the properties of all known inorganic materials and beyond, design novel materials and offer data to the community together with online analysis and design algorithms.1 The current release contains data derived from density functional theory (DFT) calculations for over 60,000 materials, each with searchable associated properties such as relaxed structure, electronic state, energy storage capability, aqueous and solid stability, and more. The software infrastructure enables thousands of calculations per week – enabling screening and predictions - for both novel solid as well as molecular species with target properties. Current application areas include photocatalysis, thermoelectrics, beyond-Li energy storage, and alloy design.

To exemplify the approach of first-principles high-throughput materials design, we will make a deep dive into future energy storage technologies, showcasing the rapid iteration between ideas, computations, and insight as enabled by the Materials Project infrastructure and computing resources. To understand and design novel electrodes for multivalent energy storage requires efficient and robust evaluation of stability, voltage, capacity, volume change, and most importantly, active ion mobility, which is the foremost bottleneck in these systems. Understanding of the structural and chemical features – extracted from calculations and benchmarked against available experimental data - which correlate with facile, selective ion diffusion will be presented and discussed. We are also devoting a large effort to understanding, screening and designing organic liquid electrolyte systems for novel energy storage systems for which the bulk solvation structure and its impact on electrolyte performance is largely uncharted. As an example, we find that contact ion-pair interaction is prevalent in multivalent electrolytes, even at modest concentrations which influences charge transfer, conductivity and even the stability of the electrolyte.

11:40am **IPF+MS-TuM12 Electrical Double Layer Effects on Ion Transport in Thin-Layer Solid-State Electrolytes**, ***Henry White***, *J. Xiong*, *M. Edwards*, University of Utah **INVITED**

We present finite-element modeling of Li^+ transport in solid-state electrolytes, including the role of the double layer electric fields. We developed a 1-D model that describes the mass transport and electric potential, assuming that Li^+ is the predominant charge carrier. Mass transport is described by the Nernst-Planck equation and the electric potential is described by Poisson’s equation. These equations were solved in a fully coupled manner, i.e., the electric field affects the mass transport through the electromigration term in the Nernst-Planck equation, while the excess charge due to unequal ion concentrations affects the electric field as the space charge term in Poisson’s equation.

We present calculated potential and concentrations distributions, as well as the contributions of migration and diffusion to the flux of each species. We present investigations of the effect of the solid-state electrolyte thickness on mass transport, varying the thickness from 10 nm to 2000 nm. The current normalized to electrolyte thickness is shown to decreases as the thickness decreases.

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