Thin Films
Room 206 B W - Session TF1-MoA
Thin Films for Energy I

Moderators: Blake Nuwayhid, Naval Research Laboratory, **Matthias Young**, University of Missouri

1:30pm **TF1-MoA-1 Enabling Scalable Sustainable Energy Devices via Spatial Atomic Layer Deposition*, Paul Poodt,*** SparkNano and Eindhoven University of Technology, Netherlands **INVITED**

Atomic Layer Deposition is a key enabler for next-generation energy storage and conversion technologies, offering unmatched control over film thickness and composition with excellent conformality on complex and porous surfaces. However, many applications—such as electrolysis and batteries—require high-throughput, low-cost processing, making Spatial ALD (sALD) an attractive solution.

We present recent advances in sALD for two key applications: electrocatalyst coatings for proton exchange membrane water electrolysis (PEMWE) and LiF passivation layers for Li-ion battery electrodes.

PEMWE is a leading method for green hydrogen production. Current systems rely on Ir- and Pt-based electrocatalysts, but the high cost and scarcity of these materials pose scalability challenges. ALD enables ultrathin, conformal catalyst layers with atomic-level control, allowing significant reductions in noble metal usage. We demonstrate sALD of Ir- and Pt-based materials at full PEM stack scale. These coatings achieve 10–100× lower Ir loadings than current standards while maintaining excellent stability under accelerated stress tests.

In Li-ion batteries, LiF has emerged as a promising solid-electrolyte interphase (SEI) component due to its chemical robustness and wide electrochemical stability window. Conventional ALD of LiF often requires high temperatures and undesirable sources of fluorine. We introduce a plasma-enhanced sALD process using a new lithium precursor to deposit pure, crystalline LiF at 100–200°C—compatible with Li-metal anodes and other sensitive substrates. The films exhibit high growth rates, excellent conformality, and are free of oxygen and carbon. Examples of significant improvements in capacity retention will be shown.

Finally, we address the critical role of precursor utilization efficiency in sALD. Through combined experiments and modeling, we show how process parameters—such as surface area, aspect ratio, throughput, temperature, and pressure—can be tuned to minimize precursor waste. Efficient precursor use is essential for the cost-effective and sustainable scaling of ALD in electrochemical device manufacturing.

2:00pm **TF1-MoA-3 Vapor Phase Methods for Tailoring Electrode−Electrolyte Interfaces in Lithium-Ion Batteries*, Reeja Jayan,*** Carnegie Mellon University **INVITED**

Interfaces between battery electrodes and electrolytes play a critical role in determining how fast a battery can charge, how long it lasts, and how safe it is under heat. Designing stable interfaces that support rapid movement of ions is essential for advancing next-generation lithium-ion batteries. We investigated how different nanoscale coatings—applied using a vapor-phase technique—can influence ion transport at these interfaces. One particular formulation enabled fast charging by balancing low ion-binding energy with ample ion-anchoring sites. Real-time X-ray measurements revealed that this coating also improved how evenly current was distributed across the electrode during battery operation. Additionally, it created strong chemical interactions with the electrode material, helping prevent metal loss and electrolyte breakdown. As a result, the battery's cycle life improved by over 10X with this coating. These findings help define key design principles for using vapor phase methods to enhance electrode–electrolyte interfaces in advanced batteries.

2:30pm **TF1-MoA-5 Manufacturing-Scale Powder Atomic Layer Deposition for Battery Applications*, Arrelaine Dameron,*** Forge Nano Inc **INVITED**

Historically Atomic layer deposition (ALD) has been regarded as a lab-only process, disregarded as too expensive and an unrealistic process for commercial adoption outside of semiconductor manufacturing. However, several methods for high volume manufacturing have been developed over the last decade, making ALD on powders affordable as a material-upgrading technique. Forge Nano has patented, constructed, and demonstrated the highest throughput ALD capability in the world, unlocking new potential for lower cost integration of ALD into products. ALD is a well utilized platform technology for powders, porous particles, and high-surface area objects that has been widely demonstrated throughout the literature. Fundamentally, ALD on powders or any high surface area surface is the same as on flat surfaces -- if the chemistry is self-limiting, the precursors can be kept separate and supplied at a concentration to saturate the available surface area, the thin film growth will be controlled and uniform. In practice, the very high surface area, long diffusion pathways, and complexities of gas solids mixing bring a few additional challenges not usually encountered during lab-scale ALD.

Commercial adoption of EVs requires that we overcome consumer angst around battery range by enabling fast charge and increasing specific capacity, while also significantly decreasing cost ($/kWh). Achieving these objectives requires higher energy density and higher charge rate operation of high-capacity cathodes and anodes. It also requires that we standup a robust supply chain for battery materials and implement process intensification to minimize manufacturing costs. The major challenge of high-capacity cathode materials paired with low-cost graphite or Si/graphite anodes is their propensity for transition metal dissolution and crossover, and gas generation, which stems from electrochemical decomposition of the electrolyte solvent at electrode-electrolyte interfaces. These degrade battery performance and increase safety risk.FN has developed ALD coatings that can improve anode and cathode materials.

This talk will highlight the benefits of nano-engineering the surface of anode and cathode materials for lithium-ion battery cell development and manufacturing considerations when scaling those solutions for battery production.

3:00pm **TF1-MoA-7 Thin Film Solid-State Electrodes for Electrochemical-Mechanical Coupling Experiments*, M. Florencia Petracci,*** *Bhuvsmita Bhargava, Yueming Song, David Stewart, Taeho Jung,* University of Maryland, College Park*; Alec Talin,* Sandia National Laboratories*; Gary Rubloff, Paul Albertus,* University of Maryland, College Park

Measuring and studying the coupling between mechanical stresses and electrochemical responses in solid state batteries can be challenging due to the presence of several irregular interfaces, and to the non-uniform stress distributions present at them. It is essential to understand this coupling since these mechanical stresses and strains, resulting from fabrication, volume changes from ion insertion and extraction and applied operating pressures, can affect the thermodynamics, kinetics and transport mechanisms in batteries and thus impact their performance.

Our platform, which consists of thin-film electrode samples with mechanically planar interfaces in lateral configurations, and the use of a flat platen connected to a Nanoindenter, allows us to apply controlled uniaxial forces to single electrode interfaces [1]. This platform is used to directly measure the effect that applied stresses have on interfacial equilibrium potentials.

In this presentation we will introduce our platform, including the fabrication of our thin-film V_2O_5 cathodes through reactive sputtering [2] on LATP solid electrolyte substrates with a Lithium metal anode, our testing and characterization protocols, as well as our results showing clear coupling between applied mechanical loads and open-circuit voltage. This coupling varies with lithiation state of the sample due to changes in the partial molar volume of Lithium in the V_2O_5. The partial molar volume of Lithium in V_2O_5 obtained from this platform falls into the range between 2.5 to 5 cm^3/mol, which is consistent with what has been observed for other intercalation materials[3].

References:

[1] Song, Y., Bhargava, B., Stewart, D. M., Talin, A. A., Rubloff, G. W., & Albertus, P. (2023). Electrochemical-mechanical coupling measurements. *Joule*, 7(4), 652-674.

[2] Warecki, Z., Ferrari, V. C., Robinson, D. A., Sugar, J. D., Lee, J., Ievlev, A. V., ... & Talin, A. A. (2024).Simultaneous Solid Electrolyte Deposition and Cathode Lithiation for Thin Film Batteries and Lithium Iontronic Devices. *ACS Energy Letters*, 9(5), 2065-2074

[3] Koerver, R., Zhang, W., De Biasi, L., Schweidler, S., Kondrakov, A. O., Kolling, S., ... & Janek, J. (2018). Chemo-mechanical expansion of lithium electrode materials–on the route to mechanically optimized all-solid-state batteries. *Energy & Environmental Science*, 11(8), 2142-2158

3:15pm **TF1-MoA-8 Mapping Lithium Diffusion in Thin-Film V_2O_5 Using Raman Spectroscopy*, Daniel MacAyeal,*** University of Vermont*; Leopoldo Jose Tapia-Aracayo,* University of Maryland, College Park*; Spencer Caverly,* University of Maryland*; David Stewart, Gary Rubloff,* University of Maryland, College Park*; Alexander Kozen,* University of Vermont

Understanding the lateral diffusion of lithium in thin-film solid state battery (SSB) materials is critical to improving SSB performance, stability, lifespan, and architecture. Using model test structures of sputtered annealed- and unannealed-V_2O_5/LiPON, we use Raman spectroscopy peak shifts to map Lithium concentration in V_2O_5/VO_x. We evaluate the diffusion of lithium from LiPON layers into thin-film Vanadium Oxide, measure the impact of different sputter deposition process conditions on lateral lithium diffusion into crystalline and amorphous metal oxide films. We confirm experimental results with simulations, exploring both potential-driven diffusion and Fickian diffusion as possible mechanisms for Lithium transport. Lastly, we will discuss the important implications of the lateral spacing limitations of clustered SSB devices due to lateral diffusion and propose architectural design rules based on this diffusion behavior for optimized device performance.

3:30pm **TF1-MoA-9 High-Voltage Interdigitated Micro-Supercapacitor Utilizing Bimetallic Nitrides for Miniaturized Energy Storage Applications*, sheetal Issar***, *Ramesh Chandra,* Indian Institute of Technology Roorkee, India

High voltage microsupercapacitors (MSCs) along with energy harvesters can be used to integrate miniaturized self-powered system in many microelectronic devices. On-chip MSCs are considered as one of the promising energy storage devices due to their high energy density, long cycle life, and fast charging-discharging rate. In this regard, transition metal nitrides (TMNs) based nanostructured are considered as an effective electrode material for fabrication of high performance on-chip MSCs due to their high electrical conductivity. We report fabrication of highly stable interdigitated micro patterns of titanium vanadium nitride (TiVN) and titanium chromium nitride (TiCrN) over SiO_2-coated Si substrate by using single-step magnetron sputtering technique. Generally, the low voltage window of on-chip MSCs is a bottleneck in designing miniature power sources in microelectronic devices. One of the most technical challenges with the on-chip MSCs is to enhance cell voltage without compromising its tiny size. The electrochemical voltage window of the MSCs is greatly dependent over the electrolyte itself. In the present work ionic liquid incorporated polymer gel electrolyte are utilized to check the electrochemical performance of TMN-based MSCs. An exceptionally high voltage window of more than 3 V is achieved in TiVN and TiCrN-based MSCs with $TEABF_4$/ethylene carbonate/propylene carbonate ionic liquid entrapped in the polyvinylidene fluoride (PVDF) polymergel electrolyte. The on-chip MSC exhibits an optimum capacitance of ~500 $\mu F.cm^{-2}$ at a current density of 0.07 $mA.cm^{-2}$ with an energy density of ~ 0.7 $\mu Wh.cm^{-2}$and a power density of 169.02 $\mu W.cm^{-2}$. This study provides new opportunities to integrate nanocomposite-based microelectrodes directly for on-chip MSCs for utilization as high voltage miniaturized power sources.

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