A combined experimental and modeling approach for the design of high current efficiency Si electrodes

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

PI/Co-PI: X. Xiao (GM), Y. Qi (MSU), B. W. Sheldon, H. Gao (Brown), Y. Cheng (U. Kentucky)

Technical Approach:

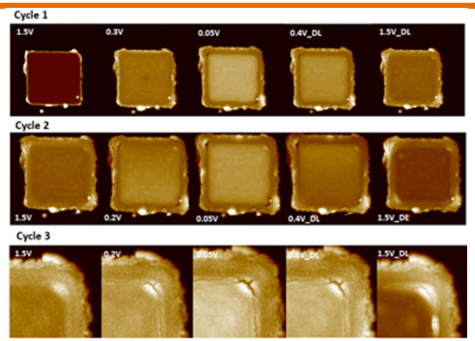
- Predict stress/strain in SEI layer and establish a correlation between the capacity loss and mechanical degradation of SEI.
- Quantify current efficiency related to artificial SEI layers using *in-situ* electrochemical experiments.
- Use modelling to optimize the coating/Si system design to mitigate mechanical degradation to both SEI and Si.

Status:

- Identified the failure mechanism of SEI during the cycling using in-situ AFM combined with continuum modeling. Demonstrated a modulus gradient coating would mitigate the mechanical degradation of Si.
- Developed a Si/graphene composite electrodes with significant improved cycle stability (>2000 cycles with 80% capacity retention)

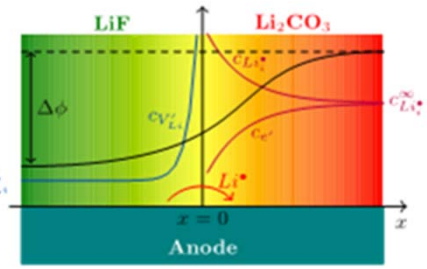
Technology:

in-situ diagnostics to probe the coupled electro-chemical-mechanic properties of SEI/Si.



Objectives:

- Combine modeling and experimental approaches to understand, design, and make stabilized nanostructured Si anode with high capacity and high coulombic efficiency.
  - Develop stabilized artificial SEI
  - Design robust Si nanostructure.



Deliverables: Approach to control SEI layer formation leading to high cycle efficiency of Si electrode. A validated model and a Si electrode with high current efficiency (>99.9%) and long cycle stability (80% capacity retention after 500 cycles).

Funding:

Duration: 4 yrs (Yr 4)
FY16 Budget: $379K (DOE)

Milestones:

- **Q1:** Identify critical mechanical and electrochemical properties of the SEI coating which can enable high current efficiency.
- **Q2:** Design a practically useful Si electrode where degradation of the SEI layer is minimized during lithiation and delithation.
- **Q3:** Construct an artificial SEI design map for Si electrodes, based on critical mechanical and transport properties of desirable SEI for a given Si architecture.
- **Q4:** Make Go/No-Go decision based on if the modelling guided electrode design can lead to high columbic efficiency >99.9%..