Next-Generation Materials Modeling and Failure Prediction

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

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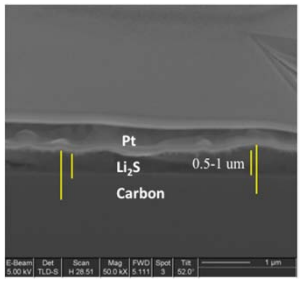
Technical Approach:

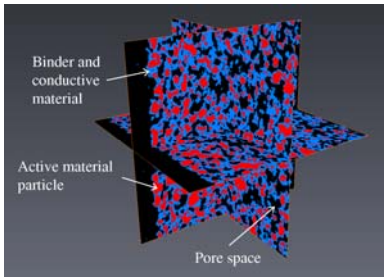
- Develop a mathematical model for a Li-S cell
- Develop a more robust description of the microstructure in porous battery electrodes to enable accurate mathematical model predictions

Status:

- Constructed electrochemical simulation of Li-ion cell using electrode microstructure from X-ray tomography; compared microscale and macroscale simulation results and modified macroscale simulation to incorporate some microscale information.
- Developed a mathematical model of lithium-sulfur batteries.
- Quantified layer thickness of Li_2S deposited on glassy carbon samples.



FIB-SEM of Li_2S deposited on glassy carbon



X-ray tomography of porous battery layered cathode

Technology:

- High capacity, long life Li-S cells enabled by understanding capacity limitations and impact of dissolution/precipitation reactions.

Objectives:

- Use continuum-level mathematical models along with controlled experiments to understand the impact of polysulfide precipitation on the capacity limitation in Li-S cells. Use models to set targets for materials (solubility of electrolytes, conductivity of passive layers).
- Perform thermodynamic, transport, and kinetic measurements to measure relevant properties.
- Develop a synchrotron x-ray technique, coupled with supercomputing simulations, to quantify microstructure-related phenomena in battery materials, including conduction in pores, and precipitation of layers.

Deliverables: Deliver a mathematical model for a Li-S cell with relevant properties that will help design new materials.

Funding:

Duration: 4 yrs (Yr 4)
FY15 Budget: $489K (DOE)

Milestones:

- **Q1:** Replace parameters (porosity gradient and tortuosity) in macroscale NMC model with corresponding values or functions obtained from tomography data
- **Q2:** Measure the relationship of film growth to electrochemical response and develop a model to interpret the relationship
- **Q3:** Go/No-Go**:** Measure transport properties of polysulfide solutions using electrochemical methods. If unsuccessful at obtaining concentration-dependent diffusion coefficient, use fixed diffusion coefficient value in upcoming
- **Q4:** Incorporate measured properties into porous-electrode model of a Li-S cell and compare to data