Electrode Materials Design and Failure Prediction

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

PI/Co-PI: Venkat Srinivasan (Argonne National Laboratory)

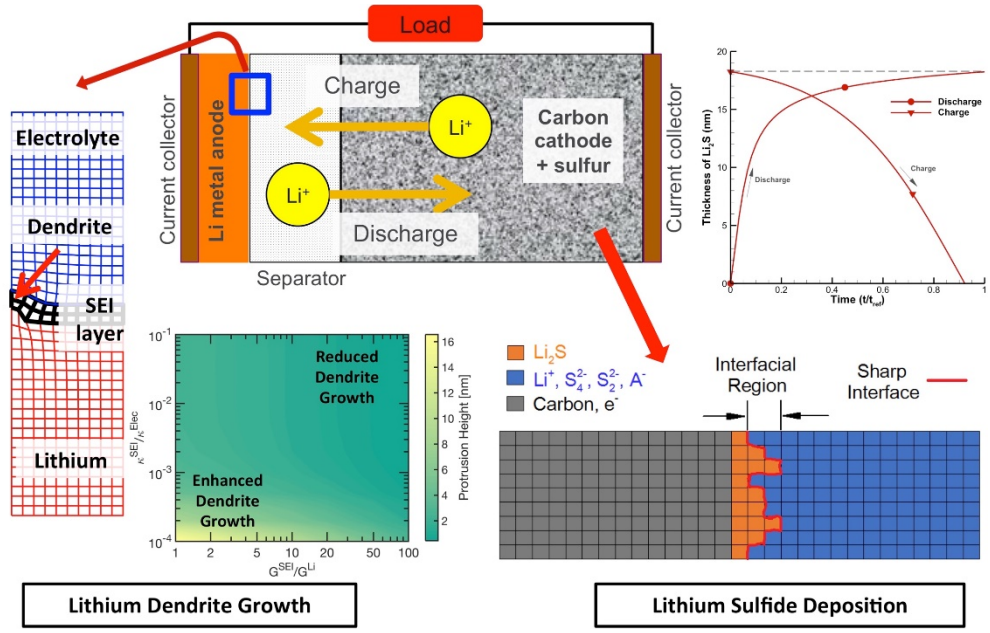
Objective:

Develop computational models for understanding the various degradation mechanisms for next generation lithium ion batteries. In FY19, majority of the focus will be devoted to understanding the cathode solid-state-electrolyte interface.

Impact:

- Findings from this research will give a better understanding of the factors limiting the cycle life of solid state electrolyte lithium ion batteries on the cathode side.
- These results will enable the incorporation of cathode particles within solid state electrolytes.

Deposition Induced Degradation in Lithium Batteries.



Accomplishments:

- Developed a computational model incorporating elastic-plastic deformation of lithium and electrolyte, which also solves for potential and concentration distribution.
- Increasing the yield strength and elastic modulus of polymer electrolytes can prevent growth of dendrites.
- Presence of inhomogeneity and mechanical stiffness of the solid-electrolyte-interphase layer, can have a significant impact on the growth of dendritic protrusions.
- Simulation of the Li_2S precipitation process reveals that, operation at high C-rates can lead to Li_2S accumulation, because its precipitation is faster than dissolution.

FY19 Milestones:

- Analyze the effect of delamination at the cathode/solid-state-electrolyte interface as a mode of degradation. (Q2)
- **Go/No-go:** Estimate SOC dependent impedance at cathode solid-state-electrolyte interface. If not possible, proceed with the impedance measured at fixed SOC. (Q4)

FY19 Deliverables:

Computational framework to estimate delamination and impedance at cathode/solid-state-electrolyte interface.

Funding:

— FY19: $450k, FY18: $450k, FY17: $450k