Task 3.7 – First-Principles Modeling and Design of Solid-State Interfaces for the Protection and Use of Lithium-Metal Anodes

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

PI/Co-PI: G. Ceder (UC Berkeley)

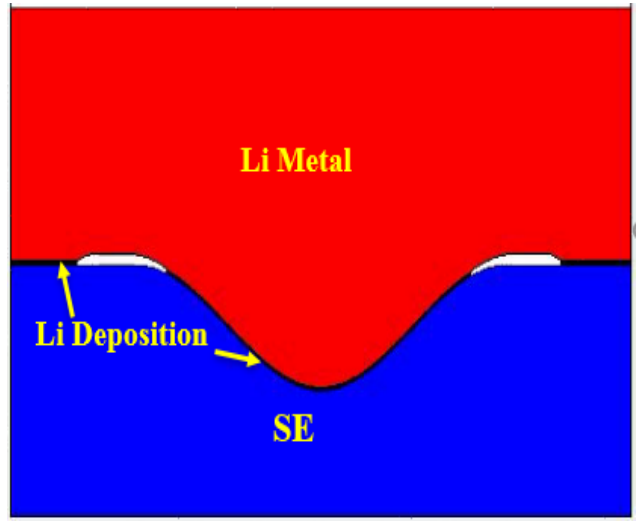
Objective:

- Determine the design principles that control the solid electrolyte/Li electrode interfaces and create more stable Li/solid-electrolyte combinations

Impact:

- Understanding of the complex evolution of Li-metal/solid electrolyte interfaces during electrochemical cycling.
- More reliable all solid-state batteries with Li metal anodes

Deposition of Li metal with surface roughness



Accomplishments:

- Developed models that integrate electrochemical transport and mechanical behavior of the electrodes
- Demonstrated that surface roughness of solid state conductor combined with plasticity of Li metal leads to growth of porosity of metallic anode

FY19 Milestones:

Q1. high-throughput framework to screen solid state electrolytes materials s.
Q2. fracture models for crack propagation in SSE: perfect crystal with cracks
Q3. fracture models for crack propagation in SSE: perfect crystal with with grain boundaries
Q4: fracture models for crack propagation in SSE as a pressed/porous electrolyte

FY19 Deliverables: Insight and design rules for Li metal anode in SSB. Papers and Presentations

Funding:

— FY19: 300K; FY18: 300K