Electrode Materials Design and Failure Prediction

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

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Objective: Develop computational models for understanding the various degradation mechanisms for next generation lithium ion batteries, such as, dendrite growth on lithium metal anodes, and deposition and microstructure evolution of lithium sulfides in lithium-sulfur batteries.

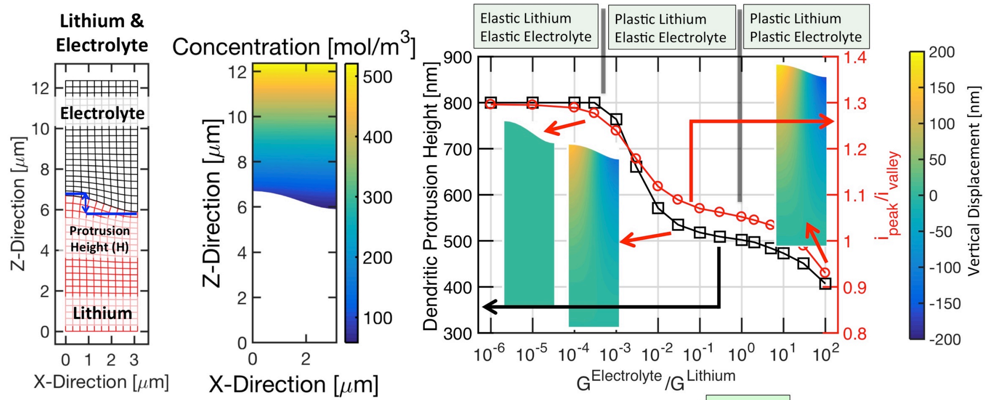
Impact:

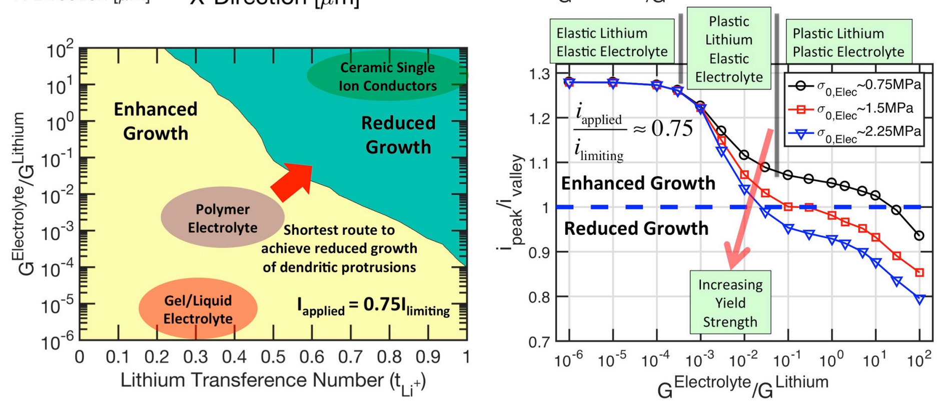
- Improve the understanding of different mechanisms responsible for degradation in next generation lithium ion batteries.
- Develop strategies to minimize the impact of different degradation mechanisms and enhance the performance and lifetime of next generation lithium ion batteries.

Accomplishments:

- Developed a computational model that can capture elastic-plastic deformation of lithium and electrolyte along with the appropriate potential and concentration distribution around dendritic protrusions.
- Simulations indicate that increasing the yield strength of present day polymer electrolytes can prevent growth of dendritic protrusions.
- Improving the shear modulus and transference number of polymers by small amount can help to stabilize the lithium deposition process.
- Externally applied pressure also helps to prevent dendrite but comes with the cost of extra overpotential.

Computational model for Lithium Dendrite Growth





FY 18 Milestones:

- Develop a mathematical model to describe surface morphology evolution in sulfur electrode
- Evaluate the impact of mechanical properties and thickness of SEI layer on propensity for dendrite growth

FY18 Deliverables:

- Mathematical model that provides guidance on the material properties needed to retard morphology change.

Funding:

- FY18: 400k, FY17: 400k, FY16: 400k