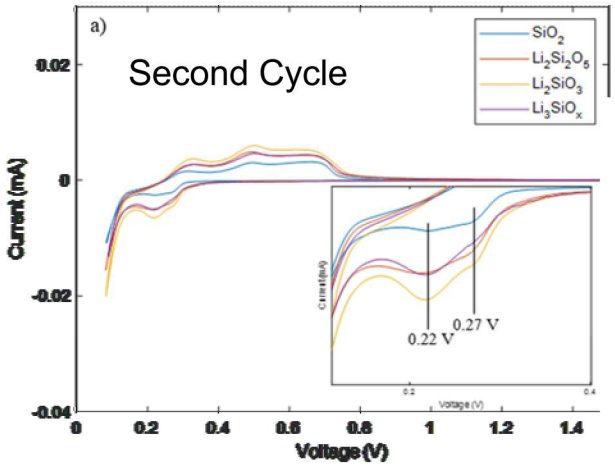
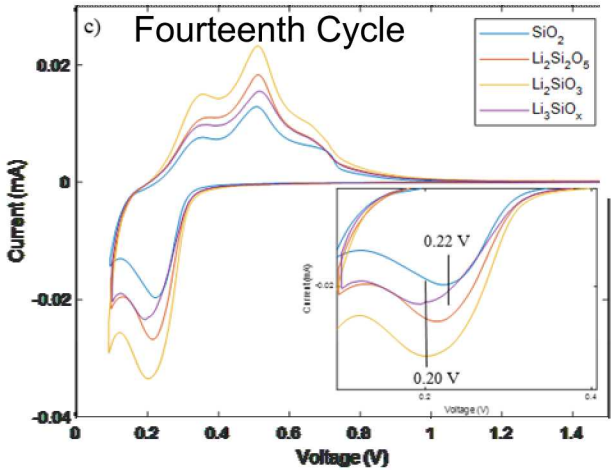
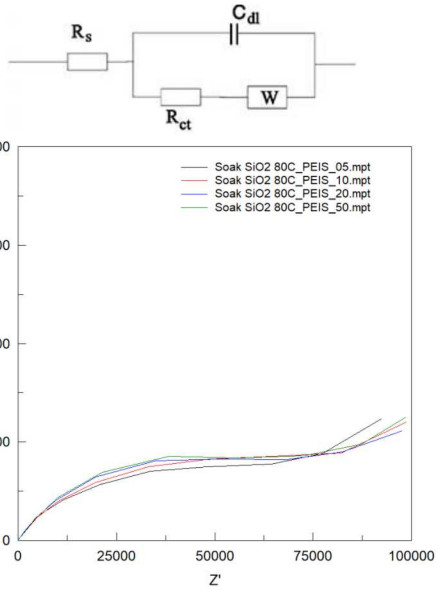
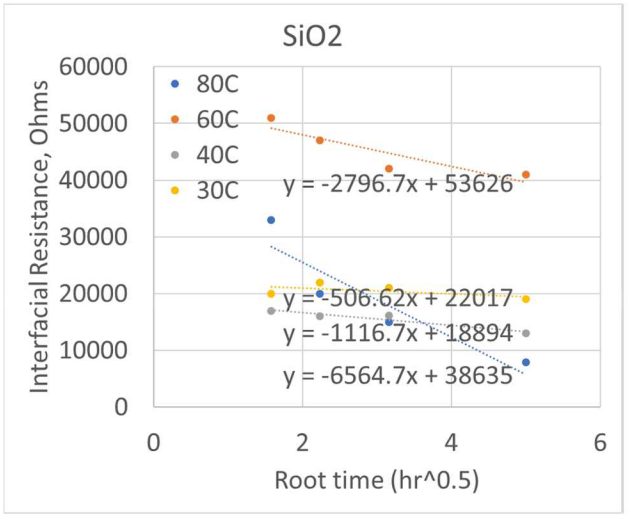
Q1: Determine the difference in the activation energy for the rate limiting step of SEI formation as a function of Li content in Li-Silicate films.

SAND2019-0439PE









Kim, S.Y. and Y. Qi, *Property Evolution of Al2O3 Coat… Prin… Elec… 137-… F3143*

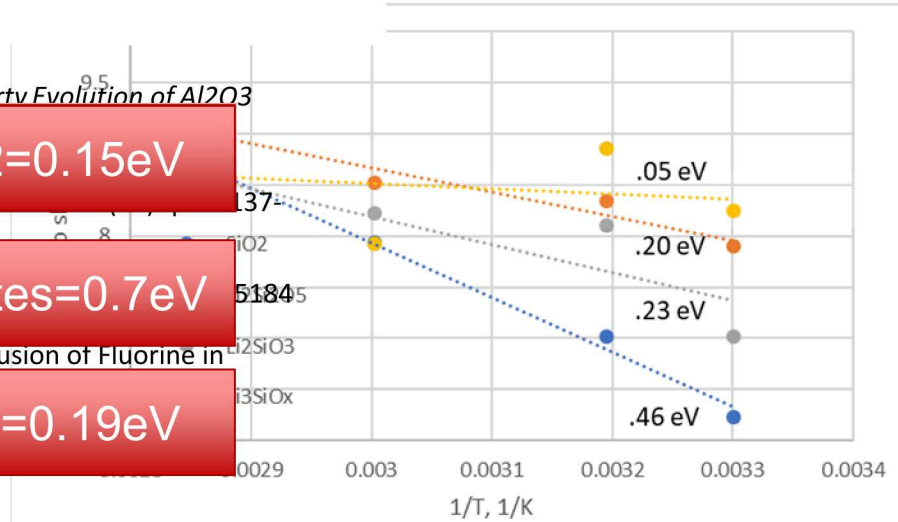
Bau… 5184

Hermann, W., et. al. "Diffusion of Fluorine in Silica… 56-5…

Li in SiO2=0.15eV

Li in Silicates=0.7eV

F in SiO2=0.19eV



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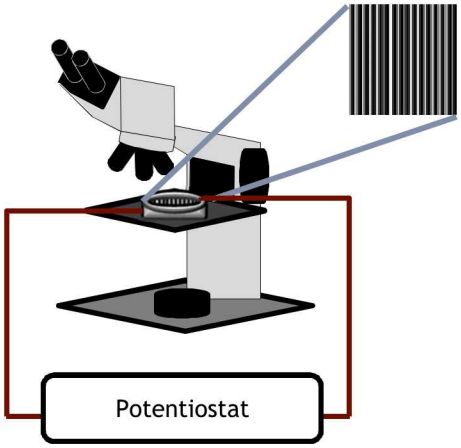
NNSA National Nuclear Security Administration

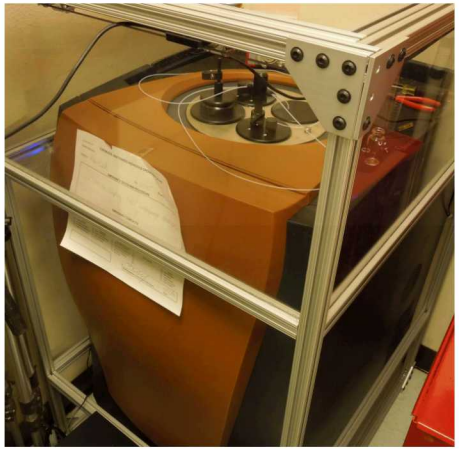
U.S. DEPARTMENT OF ENERGY

Next Steps

Q2 Milestone: Determine the extent of electrochemical conversion of versus SEI formation on silicate films through measurement of Li accumulation as a function of Li content, C rate and temperature using XPS, SIMS, ATRIR, and elastic modulus. This effort is designed to determine under what conditions surface silicates are likely to form at a Si anode under pre-alloying conditions.
Q3 Milestone: Determine how the elastic modulus of deposited amorphous SiO2 films evolves as Li enters the film as a function of temperature and C rate. Correlate these observed changes with the compositions determined in Q2 to assign mechanical evolution to the evolving chemistry.
Q4 Milestone: Determine to what extent addition of FEC to the electrolyte modifies film evolution, by monitoring impedance, elastic modulus, and composition over the previous milestones. Correlate excess fluorine content within the electrolyte with the extent of lithium and fluorine insertion into amorphous SiO2 and the composition of this film.



In situ Moiré Interferometry combined with GITT to measure stress in the SEI

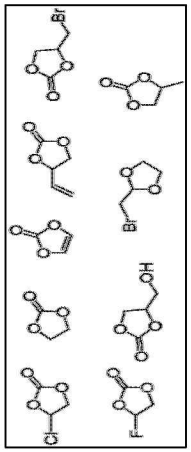


Microcalorimetry combined with electrochemical cycling to determine conversion vs. growth

Q2

EC-AFM combined with electrochemical cycling measure elastic modulus changes as Li inserts, and determine heterogeneity of films

Q3



Chemical properties determined using DFT, related to electrochemical performance of additives

Q4