The interconnection between modeling and experiments toward understanding Li-ion battery failures

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ABSTRACT
The durability of lithium-ion batteries is controlled by many coupled chemical and mechanical degradation mechanisms. Although empirical models have been trying to include more degradation mechanisms in order to predict battery life, they generally lack of proper input materials’ properties and direct experimental supports. To address this issue, we investigated both mechanical and chemical degradation via combined and interconnected first principles calculations, continuum modeling and experiments. Toward the understanding of mechanical degradation, we predicted that graphite anode modulus is tripled during Li insertion from first principles calculations. It is important to include this effect in diffusion induced stress modeling when compared with in-situ measurements of microstructural strain in a commercial graphite anode. Toward the understanding of chemical degradation, we focused on Li+ transport through the solid electrolyte interphase (SEI). Based on the insights from experiments and first principle calculations, meso-scale diffusion equations were then formulated upon a new two-layer/two-mechanism model: pore diffusion in the porous organic layer and knock-off diffusion in the dense inorganic layer of SEI. This diffusion model not only predicted the unusual isotope ratio profile measured by Time-of-flight secondary ion mass spectrometer, but also suggested that Li transport in SEI is voltage dependent. Overall, our results underscore the importance of integrating state of charge (SOC) dependent material properties into Li-ion battery performance and failure modeling.