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

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The durability of lithium-ion batteries, especially the new large format cells and packs developed for transportation applications 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). Using first principles calculations, we found that diffusion of excess interstitial Li⁺ proceeds via repetitive knock-off of Li⁺ at lattice sites in crystalline Li₂CO₃ (one of the main components of the SEI). Time-of-flight secondary ion mass spectrometry experiments on SEI films provide compelling evidence for the knock-off mechanism. Our results underscore the importance of integrating state of charge (SOC) dependent material properties into Li-ion battery failure modeling.

Short Bio: Dr. Yue Qi is a Staff Research Scientist working on computational materials sciences at Chemical Sciences and Materials Systems Lab, General Motors R&D Center. She completed her B.S. degrees on Materials Science and Computer Science at Tsinghua University in 1996. She received her PhD in Materials Science from California Institute of Technology in 2001 and joined GM R&D in the same year. In GM R&D, she has been using multi-scale modeling approach to solve problems related to energy materials for batteries and fuel cells, forming and machining of light weight alloys. Her recent research topic is on “integration of material properties into Li-ion battery failure modeling”. She received GM Campbell awards (on research) for “Multi-scale Modeling of High-temperature Deformation in Aluminum” (2009), “Fundamentals of Interfacial Tribology”(2009), and “Advances in Nano-scale Plasticity” (2006). She was also the coreipient of 1999 Feynman Prize in Nanotechnology for Theoretical Work with Dr. T. Cagin and Prof. W. A. Goddard III (PhD advisor).

All students, faculty, and public are welcome.