Mechanical Engineering Doctoral Defense

Mechanics of Silicon Electrodes in Lithium Ion Batteries

School for Engineering of Matter, Transport and Energy

Yonghao An

Advisor: Prof. Hanqing Jiang

abstract

As one of the most promising materials for high capacity electrode in next generation of lithium ion batteries, silicon has attracted great deal of attention in recent years. Advanced characterization techniques and atomic simulations helped to depict that the lithiation/delithiation of silicon electrode involves processes including huge volume change (anisotropic for the initial lithiation of crystal silicon), plastic flow or softening of material dependent on composition, electrochemically driven phase transformation between solid states, anisotropic or isotropic migration of atomic sharp interface, and mass diffusion of lithium atoms. Motivated by the promising prospect of the application and interesting physics underlying, mechanics and multi-physics coupling in silicon electrodes is studied in this dissertation. For silicon electrodes with large size, diffusion controlled kinetics is assumed, and coupled large deformation and mass transportation is studied. For crystal silicon with small size, interface controlled kinetics is assumed, and anisotropic interface reaction is studied, with a geometry design principle proposed. As a preliminary experimental validation, enhanced lithiation and fracture behavior of silicon pillars via atomic layer coatings and geometry design is studied, with results supporting the geometry design principle we proposed based on our simulation. Through the work documented in this dissertation, a consistent description and understanding of the behavior of silicon electrode is given at continuum level and some insights for the future development of the silicon electrode are provided.

March 18, 2014; 3:00 PM; ERC 490