Mechanics of Deformation, Diffusion and Failure in Lithium Ion Insertion Electrodes

Wednesday, December 4, 2013, 3:30P.M.

Carey Auditorium, Hesburgh Library

Refreshments served at 3:00 p.m. outside of Carey Auditorium

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If you are interested in meeting individually with Dr. Bower, please contact Linda at 631-5431.

The materials used in lithium ion insertion electrodes experience large changes in volume as the battery is charged or discharged and they absorb or emit lithium. For example, a graphitic electrode increases in volume by 10% when lithiated; while high-capacity materials such as Si expand by up to 300%. The stress generated by this volume expansion can lead to plastic flow and fracture, which cause batteries to lose their capacity. There is consequently great interest in designing failure resistant composite battery microstructures. Modeling deformation and failure in candidate battery materials, together with careful experimental measurements of the behavior of battery materials during lithiation will be important steps in this process. To this end, we formulate the continuum field equations and constitutive equations that govern deformation, stress, and electric current flow in a Li-ion half-cell. The model considers mass transport through the system, deformation and stress in the anode and cathode, electrostatic fields, as well as the electrochemical reactions at the electrode/electrolyte interfaces. The influence of phase transformations in the electrode material will also be discussed. Model predictions are compared with experimental measurements of stress and electric potential in thin-film electrodes that are repeatedly lithiated and de-lithiated. Calculations reveal a complex interplay between stress and chemistry in electrode materials – stresses can directly influence the electrical response of the electrode; and conversely, chemistry can have a profound influence on the stress state within the electrode, in some cases even changing the signs of the stresses.

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