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A theory and a simulation capability for the growth of a solid electrolyte interphase layer at anode particles in lithium ion batteries

Rejovitzky, Elisha, lish@mit.edu; Di Leo, Claudio; Anand, Lallit, MIT, United States

ABSTRACT

A major mechanism for electrochemical aging of Li-ion batteries is the formation of a solid electrolyte interphase (SEI) layer, which results in an impedance rise at the anode and also leads to capacity fade. The formation of an SEI layer consumes Li-ions and competes with the desired Li intercalation. Often, the cyclic volume changes – or "breathing" – of an anode particle during Li-ion intercalation and deintercalation can cause the SEI layer to delaminate from the surface of the particle, which causes new SEI to be formed on the newly exposed particle surface and this accelerates capacity fade. We have formulated a continuum theory for the formation and growth of an SEI layer, and the theory has been numerically implemented in a finite-element program. This simulation capability for SEI growth is coupled with our earlier published chemomechanical simulation capability for intercalation of Li-ions in electrode particles. Using this new combined capability we have simulated the formation and growth of an SEI layer during cyclic lithiation and delithiation of an anode particle and predicted the evolution of the growth stresses in the SEI layer. The evolution of the stress state at the SEI–particle interface for spheroidal-shaped particles is studied, and this gives us a good indicator for the propensity of potential delamination of the SEI layer from the anode particle.