The Impact of Lithium Diffusivity in the Active Electrode Material on the Power and Energy Density of Lithium-Ion Cells

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The lithium-ion (Li-ion) cell is a high capacity electrical energy storage device with applications in portable electronics and growing applications in the military and transportation market spaces. To expand the current market of this energy storage device, future work should aim to improve its power and energy densities. At present, commercialized materials are being altered or doped to enhance certain physical and chemical properties – such as diffusivity, electrical conductivity and reaction rates – to improve the cell performance. Alternatively, performance gains can be streamlined through increased understanding of the electrodes physical and chemical properties effects. Identifying the effect of electrode properties might enable the assembly of a cell with better electrode performance, tailored for the discharge rate of a specific application.

Computer simulation of Li-ion cells is an efficient tool for guiding material development and pinpointing areas of future improvement and optimizing cell performance. In this paper, the impact of lithium diffusivity in the active electrode materials on Li-ion cell performance has been studied through computer simulation. To achieve generalized results, this study is conducted for multiple cell design cases including the cells with various electrode thicknesses, volume fractions of active material, and initial salt concentrations in liquid electrolyte. A quasi-two-dimensional model is considered for computer simulation of the Li-ion cell. This model is based on the mathematical model developed by Newman's group [1]. In this model, it is assumed that both negative and positive electrodes of the cell are made of uniform-sized solid spherical particles. These particles are the active material of the electrodes. The size of these particles is assumed to be unchanged during the cell charging and discharging processes. Both electrodes contain uniform composition of binder, conductive additive and liquid electrolyte. For the computer simulation, one-dimensional mass and charge transports in both electrodes and electrolyte in the cell thickness direction and two-dimensional lithium diffusion in electrode particles at particle radius and cell thickness directions were taken into account. This simulation was accomplished by COMSOL Multiphysics Ver. 4.2.

The results of this study revealed that the lithium diffusivity in the active material of both electrodes plays an important role to improve the cell performance; and a special attention should be paid to select, altered or doped active materials for both electrodes, especially for negative-electrodes. The impact of the lithium diffusivity in active electrode materials on the cell performance is quantified in this paper.

References

[1] T.F. Fuller, M. Doyle, and J. Newman, "Simulation and optimization of the dual lithium ion insertion cell," *Journal of The Electrochemical Society*. 1994;141(1):1–9.