Capacity fade of full cell considering lithium ion desolvation under pulse current charge/discharge conditions

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Rapid charge/discharge test is one of the important methods to evaluate performances of lithium ion batteries. Attempts have been made to explore the most suitable charge/discharge strategy so that batteries can maintain good electrochemical performances under rapid charging/discharging conditions. Experimental results reveal that the pulse current charge/discharge strategy is beneficial to improve the performances of batteries, especially the high rate performances[1, 2]. The pulse current charge/discharge belongs to a kind of rapid charge/discharge strategy. Some experiments have been carried out under pulse current charge/discharge conditions with various amplitudes and frequencies at different temperatures and current rates. However, few reports on the performances of full cell and the transport properties of charges and lithium ions under pulse current charge/discharge conditions have been made theoretically. To theoretically understand the capacity fade of lithium ion batteries considering lithium ion desolvation, we used the rectangular pulses with various frequencies, amplitudes, and rest time. An electrochemical model was established in this work, which combined with the growth of solid electrolyte interphase (SEI), to predict the performance of the full cell in the course of pulse current charge/discharge process. The desolvation process of lithium ions from the last solvent molecule ($\mathrm{Li(solv)^+ \rightarrow Li^+ + solv}$) in the electrode/electrolyte interface is regarded as the rate-determining step of the reactions in whole lithium ion batteries[3]. The proposed model was then solved on the software package COMSOL Multiphysics. The simulation results were validated by the experimental results. Influences of the pulse current on the desolvation/solvation process of lithium ions on the electrode/electrolyte interface during charging/discharging process were analyzed. The capacity fade and the cycle life of lithium ion batteries were compared with different kind of rapid charge/discharge strategies, such as constant current-constant voltage (CC-CV) and pulse current-constant voltage (PC-CV) with different current rates and frequencies. The results show that (1) the pulse current charge/discharge strategy has advantages that can restrain the capacity fading of batteries; (2) the pulse current charge/discharge strategies with lower amplitude and less pulse number have higher available capacities; (3) the distributions of current density and lithium ion concentrations present quite different profiles under the pulse current charge/discharge conditions. These results provide insight into alleviation of capacity fade during the rapid charge/discharge process by using the pulse current charge/discharge strategies.

References:

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