Simulation of Heat Generation in a Reconstructed $LiCoO_2$ Cathode during Galvanostatic Discharge

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Abstract

A three dimensional numerical framework with finite volume method was employed to simulate heat generation of a semi lithium ion battery (LIB) cell during isothermal galvanostatic discharge processes. The microstructure of the LIB cathode electrode was experimentally determined using X-ray nano computed tomography technology. Heat generation in the semi LIB cell during galvanostatic discharge processes from different mechanisms, such as electronic resistive heat, ionic resistive heat, contact resistive heat, reaction heat, entropic heat and heat of mixing, was investigated. The spatial distribution of heat generation rates from different mechanisms was also studied. The simulation results demonstrate that the magnitude of heat generation rates spans a wide range in the electrode due to structural inhomogeneity. The simulation results of heat generation from the three dimensional model and the porous-electrode theory model were compared in this study. It is found that the typical Bruggeman coefficient, 1.5, underestimated ionic resistance in the electrolyte and overestimated electronic resistance in the cathode particles. In general, the three dimensional model predicted more heat generation than the porous-electrode theory model at large discharge rates due to the wider distribution of physical and electrochemical properties.

Keywords: lithium ion battery, heat generation, X-ray computed tomography, galvanostatic discharge, structure inhomogeneity