Simulation on Li-ion Cells by Dualfoil Model under Constant-Resistance Load Operations

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In this paper Dualfoil model developed by Newman et al. [1-2] is used to simulate the electrochemical performance and temperature rise for $LiCoO_2$/MCMB Li-ion cells discharging under constant-resistance load operations.

From the simulation results, the evolution of cell potential, current density, total cell resistance, and cell temperature rise during the different discharge processes are presented and analyzed in detail. Electrolyte and solid surface concentration profiles of Li^+ ion across the anode-separator-cathode in various time scales are simulated and analyzed to explain the Li^+ ion transporting limitations.

Sensitivity tests are conducted by changing the values of different parameters, such as film resistance, solid lithium diffusion coefficient, heat transfer coefficient, and the initial Li^+ ion concentration of electrode material to examine their effects on electrochemical performance and temperature rise. The cell thermal behaviors are compared for various constant-resistance load operations and suggestions for preventing thermal runaway under different conditions are proposed.

Introduction

In recent years, Li-ion batteries have more application in mobile technologies for its high energy and power density. Li-ion battery has been used in Boeing 787 aircraft as its main battery. However, a fire incident happened to one of its batteries indicating there was an overheating issue that needs to be understood. As is known that Li-ion battery can only perform well in a short temperature range (about 20-50°C).[3-4] Various exothermic side reactions are initiated in sequence when temperature rises, resulting in internal cell resistance rising, capacity fading of battery temperature rise, and thermal runaway.[5] Battery can be safe under moderate operating condition (e.g. low current) but will be more likely to experience thermal runaway under severe operations. In the following simulation of $LiCoO_2$/MCMB cells, different temperature rise/profiles for the same cell under different resistance load mode will be presented. By looking at very high currents (approaching a short-circuit condition), we hope to learn more about parameters which can contribute to excessive overheating in batteries.

Dualfoil5.2 simulating model and program

Dualfoil model is a powerful macro homogeneous battery model that can be used to treat the coupled phenomenon in a porous electrode battery system (including Ni-H and Li-ion battery).[1-2] Dualfoil program based on Fortran programming language was originally developed by Marc Doyle and John Newman in 1992 and now has its 5.2 version as Dualfoil5.2. Dualfoil5.2. can be used to simulate the electrochemical and thermal phenomena under various operating conditions for Li-ion battery and can help researchers understand deeply battery performance and design better batteries.

Model parameters

The simulation parameters can be divided into two categories. One category includes design-adjustable parameters such as electrode thickness and volume fractions, particle sizes, separator thickness, and initial salt concentration. The other includes the intrinsic parameters of material (e.g. lithium diffusion coefficient, material density, and heat capacity) and some thermodynamic and kinetic data for the electrochemical reactions. The parameter values used in this model will be listed and explained how to get them.

References

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