

## Abstract

As the most important component of the entire lithium-ion battery, the electrodes, their design which ultimately determines the quantity and speed of lithium storage, directly affects the capacity, power density, and energy density of the battery. The electrochemical and thermal performance of battery are analyzed using Batteries & Fuel Cells Module and Heat Transfer Module of the COMSOL Multiphysics® software. An electrochemical-thermal coupling model is established for an 18.5 Ah lithium-ion battery, and the model is validated by experiment at four discharge rates. Based on the model, the effects of the electrode design parameters (electrode thickness, volume fraction of the active material, and particle sizes) on the battery performance (electrochemical characteristics, thermal behavior, energy density and power density) are first investigated, it is found that as the electrode thickness and volume fraction of the active material increase, the polarization, heat generation rate and energy density are increased while the power density is degraded; as the particle sizes decrease, both the energy density and power density are improved, which can provide guidance for the electrode design. Afterwards, a multi-parameters (thickness of the positive and negative electrodes) and multi-objective (energy density and power density) optimization procedure is performed by means of two optimization methods, the positive electrode thickness with 55.335  $\mu\text{m}$  and negative electrode thickness with 63.188  $\mu\text{m}$  are considered as the candidate optimized parameters. As the most important component of the entire lithium-ion battery, the electrodes, their design which ultimately determines the quantity and speed of lithium storage, directly affects the capacity, power density, and energy density of the battery. The electrochemical and thermal performance of battery are analyzed using Batteries & Fuel Cells Module and Heat Transfer Module of the COMSOL Multiphysics® software. An electrochemical-thermal coupling model is established for an 18.5 Ah lithium-ion battery, and the model is validated by experiment at four discharge rates. Based on the model, the effects of the electrode design parameters (electrode thickness, volume fraction of the active material, and particle sizes) on the battery performance (electrochemical characteristics, thermal behavior, energy density and power density) are first investigated, it is found that as the electrode thickness and volume fraction of the active material increase, the polarization, heat generation rate and energy density are increased while the power density is degraded; as the particle sizes decrease, both the energy density and power density are improved, which can provide guidance for the electrode design. Afterwards, a multi-parameters (thickness of the positive and negative electrodes) and multi-objective (energy density and power density) optimization procedure is performed by means of two optimization methods, the positive electrode thickness with 55.335  $\mu\text{m}$  and negative electrode thickness with 63.188  $\mu\text{m}$  are considered as the candidate optimized parameters.

## Figures used in the abstract

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**Figure 1:** The schematic diagrams of the lithium-ion battery and the description of the P2D electrochemical model