Simulation of Li-ion Battery with Ceramic-Coated Separators

Introduction

Coating conventional polyolefin separators with ceramic layers is considered as one of the most effective and economic ways to enhance the safety of Li-ion batteries, as the ceramic coatings can suppress shrinkage and deformation of a polymer separator at elevated temperatures.

Here, using AutoLion-1DTM, we simulate a Li-ion battery which uses ceramic-coated separators (CCSs). The effects of key properties of the coating layer, such as thickness and porosity, on cell performance are investigated, demonstrating that AutoLion™ is a powerful tool for users who want to evaluate new materials and designs in a very short timeframe.

Problem Statement

A 10Ah Li-ion cell, with graphite as the anode material, NCM622 as cathode material, and a CCS as the separator, is simulated in this work. The CCS consists of a polyethylene membrane in the center with ceramic coatings on both sides, as sketched in Fig. 1. The ceramic coatings are introduced to enhance the thermal stability of the separator. However, this added layer is required to have minimal effects on ion transport across the separator. In this work, thickness and porosity, two key properties of the ceramic coating layers, are varied to investigate their impacts on cell performance, especially at harsh operating conditions like high C-rates and low temperatures where ion transport resistance matters most.

Setup

- The cell simulated is a 10Ah pouch cell with graphite as negative electrode and NCM622 as positive electrode. It has a dimension of 152mm x 75 mm. The positive electrode has a thickness of 40.75μm and a porosity of 0.32. The negative electrode has a thickness of 48.7μm and a porosity of 0.33. The CCS has a polyethylene membrane in the center with fixed thickness of 12μm and porosity of 0.4. Three thickness values (2μm, 5μm and 8μm) and three porosity values (0.6, 0.4 and 0.2) of the ceramic coating (single side) are investigated. The cell is discharged in 3C rate at three temperatures (25°C, 0°C and -20°C).

Results

Figure 2 studies the effects of thickness of the coated layer on the performance of the Li-ion cell at harsh operating conditions. The cells are discharged at 3C rate in different temperatures, and the discharge curves are compared. In all the cases, the porosity of the ceramic coating is the same as the membrane in the center, i.e. 0.4. Even at the condition of 3C discharge in 0°C, it can be seen from Fig. 2b that there is no big difference in discharge curves of all three coating thickness. At -20°C, however, the cell with 8μm coating has much poorer performance than the other cases, as shown in Fig. 2c, indicating that ion transfer resistance across the separator is too large at this thickness of coating.

Figures 3 & 4 investigates the effects of porosity of the coating layers on cell performance. The porosity of the coating layers varies from 0.2 to 0.6 in these cases, and the discharge curves are compared. It can be noted that cells with thinner coatings is less sensitive to the change of porosity than cells with thicker coatings. For instance, in the condition of 3C discharge at 0°C as shown in Fig. 3, the variation of coating layer porosity has no dramatic impact on the performance of the cell with 2μm thick coating (Fig. 3a), but has significant impacts on the cell with 8μm thick coating. It can be concluded from Figs. 3&4 that the thickness and porosity of the ceramic coating shall be optimized to achieve both good mechanical strength and low ion transfer resistance.

**Figure 1** Structure of a Li-ion battery with double-side ceramic coated separator.

**Technology Used**

AutoLion-1DTM Version 5.2 or AutoLion-ST™.
Figure 2 Effects of ceramic coating thickness on the performance of Li-ion cell. The cell is discharged at 3C in different temperatures. Porosity of the ceramic coatings is assumed as 0.4.

Figure 3 Effects of porosity of ceramic coating on the performance of Li-ion battery. The cell is discharged at 3C in 0°C.
Figure 4 Effects of porosity of ceramic coating on the performance of Li-ion battery. The cell is discharged at 3C in -20°C.

**Benefits**

- AutoLion-1DTM is a versatile software that enables users to easily implement new materials, design new cells, and evaluate the cell performance with minimal effort and cost.

- The effects of key properties of new battery materials and components can be easily evaluated using AutoLion-1DTM before going through tedious and expensive experimental testing.

- AutoLion-1DTM is fast. Simulation is performed in a few minutes with standard computing resources for typical performances.