Research on Influence of Temperature on Capacity Fade of Lithium Ion Battery

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Abstract. In this paper, the research object is the ternary lithium battery with the NCA as positive material and graphite as negative material. The model of one-dimensional capacity fade is established by COMSOL. At different simulated temperatures, the changes of the SOC and the voltage drop of the SEI film on the positive surface were analyzed. The results show that the SOC of average on the positive surface of the battery decreases with the increase of temperature and increase of the battery impedance.

1. Introduce

Ternary lithium battery is widely used in the field of new energy vehicles due to high energy density, also impeded by its poor high-temperature performance. By studying the thermal runaway of ternary square shell lithium-ion battery cells and modules, the temperature difference between the surface and the inside of the battery can reach 403 °C when the thermal runaway occurs, and it is accompanied by the concentration change of chemical materials \cite{1}. The ambient temperature will affect the NCM power system. When the ambient temperature is lower, the discharge capacity of the battery is lower \cite{2}. The lower the temperature is, the smaller the cell voltage is, and the faster the discharge energy and efficiency decrease \cite{3}. As for the lithium-ion battery, the discharge ratio has no effect on the voltage drop and discharge capacity of at room temperature. The effect of the double discharge in the low temperature region on the temperature rise of the battery is obvious \cite{4}, but the effect of rate discharge on the performance of the battery at different temperatures has not been studied.

In this paper, a model of one-dimensional ternary lithium-ion battery is built by COMSOL. In the simulation, the average variation of the SOC on the positive surface of ternary lithium-ion battery was studied at -60 °C, -50°C, -40 °C, -30°C, -20 °C, -10°C, 0 °C, 10°C and 25 °C. At -60 °C, 0 °C and 25 °C, the change of resistance was obtained by analyzing the change of the SEI film.

2 Simulation and analysis

2.1 Modeling

The ternary lithium battery model was built by COMSOL Multiphysics 5.4. In Figure 1, the main steps of this model, such as, importing parameters, selecting materials, setting environment and boundary conditions. In Figure 2, the simulation operation steps of the battery, such as, the model starts to run after charging, mainly including constant current charging, constant voltage charging, standing, constant
current discharging and standing. The model has 4000 charge discharge cycles at different temperatures, and the convergence accuracy is $10^{-4}$.

![Figure 1. Model building steps](image1)

![Figure 2. Battery charging and discharging steps](image2)

The model adopts one-dimensional structure and is divided into three parts, such as, positive electrode, electrolyte and negative electrode. In the battery, the NCA material is used as the positive electrode, LiPF6 as electrolyte and graphite as the negative electrode. Some parameters of the model are shown in Table 1.

| Name       | Expression                          | Value       | Describe              |
|------------|-------------------------------------|-------------|-----------------------|
| E_max      | $3.7\text{V}$                       | $3.7\text{V}$ | Maximum cell voltage  |
| E_min      | $2.5\text{V}$                       | $2.5\text{V}$ | Minimum cell voltage  |
| no_cycles  | 4000                                | 4000        | Number of cycles      |
| T          | $-10\text{degC}$                    | 263.15 K    | Cell temperature      |
| Q0         | $\text{cs}_{\text{pos}}\text{max}*(1-0.25)*\text{epss}_{\text{pos}}\text{L}_{\text{pos}}\text{F}_{\text{const}}$ | 58354 C/m$^2$ | Initial Capacity      |

2.2 Analysis and Discussion

In Figure 3, by simulating the charge and discharge cycles of ternary lithium battery at different temperatures, the change of battery SOC is judged. The average change of SOC on the positive surface at low temperature was obtained by simulation, such as, a (−60 ℃), b (−50 ℃), c (−40 ℃), d (−30 ℃), e (−20 ℃), f (−10 ℃), g (0 ℃), h (10 ℃), i (25 ℃). It is found that when the ambient temperature is −60 ℃, after 4000 charge discharge cycles, the SOC is about 91.8%, but when the ambient temperature is 25 ℃, SOC is about 86%. At room temperature, with the increase of temperature, the SOC of lithium battery decreases gradually. Through research and analysis, low temperature will affect the activity of internal chemical materials of lithium-ion battery, which is not conducive to the normal charge and discharge.
Figure 3. SOC of positive electrode surface at different temperatures

In Figure 4, the potential drop of the negative SEI film was changed at three temperatures, such as, a (-60 °C), b (0 °C), c (25 °C). When the simulation temperature is -60 °C, the potential drop at the negative collector is about 0.5, but the potential drop at 0 °C and 25 °C is 0.4, which indicates that low temperature will effect the voltage change at the negative collector. The potential drop at negative diaphragm is about -18V at -60 °C, and -30V at 0 °C and 25 °C. The simulation results show that when the temperature increases, the voltage drop at the negative diaphragm will be enhanced, while the voltage drop at the negative collector will be more stable.
3. Conclusion

In this paper, the charge and discharge simulation experiment of ternary lithium-ion battery is carried out. The capacity change of ternary lithium battery at different temperatures was analyzed. The simulation results show that the SOC on the positive surface of the battery is about 86% after 4000 times of charge and discharge at room temperature. When the temperature increases from -60 °C to 25 °C, the SOC on the positive surface of the battery decreases gradually. With the increase of temperature, the potential of negative the SEI film decreases, which affects the change of the SOC on the positive surface of the battery. Therefore, it is of great significance to study the capacity degradation of ternary lithium-ion battery in the field of temperature.

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