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Study on short circuits in power lithiumion batteries based on the radius of lithium branches

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ABSTRACT. *The growth of lithium crystal is one of the important causes of short circuit in the power lithium-ion battery, which can cause the battery heat to lose control. In this paper, the short circuit that caused by the growth of lithium branches in lithium-ion battery, was studied by using the method of finite element numerical simulation. The characteristics of battery response under the radius of different lithium branches were compared and analyzed. The results show that the inner short circuit will cause the local region to heat up rapidly, and the maximum temperature will have a certain downward trend with time; and with the increase of the radius of lithium branches, the maximum temperature of the battery and the local load value of the negative region will increase, and the local load value of the negative region will be concentrated between 0.6-0.7.*

KEYWORDS: *lithium crystal; inner short circuit; multiphysics; lithium-ion battery; thermal conduction*

1. Foreword

With the increasingly prominent environmental pollution and energy problems, the development of new energy vehicles has received more and more attention. Among them, pure electric vehicles are considered to be one of the most promising solutions of the future.[1] As the "heart" of pure electric vehicles, power batteries play an important role in their development. Currently, and lithium-ion batteries are used by most pure electric vehicles as a source of energy.[2] Lithium-ion batteries have the advantages of high energy ratio, long service life and high rated voltage, but they also have some disadvantages, such as poor safety, poor heating that is prone to thermal failure and so on. In the thermal failure problem caused by the power lithium-ion battery, the internal short circuit is one of the important causes. Generally speaking, the inner short circuit refers to the phenomenon of discharge and accompanying heat generation due to the difference in potential of the battery when the positive and negative materials are directly directed.

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In the power lithium-ion battery, the causes of internal short circuit are mechanical extrusion, lithium salt deposition, etc. Lithium crystals produced by lithium salt deposits continue to grow, will consume electrolytes and lead to irreversible deposition of lithium metal, resulting in the lithium-ion battery during the cycle electrode and electrolyte interface instability, and eventually puncture the diaphragm leading to the lithium-ion battery internal short connection, resulting in the battery's thermal loss-of-control caused combustion explosion. [3]

Steiger J and other [4] research shows that when the branch crystal grows, the lithium atom will be inserted into the lattice point at the branch defect, especially at the interface, the growth of the lithium branch crystal is not limited to the root, in the late growth of the lithium branch crystal, it is shrub-like growth, the process is affected by the SEI membrane. Golodnitsky D and so on [5] narrate the effect of the crystal boundary on the overall impedance of SEI membrane, during the lithium deposition and dissolution, the SEI membrane formed by the lithium surface is easy to break, leading to the formation of the branch crystal, while the surface reaction and the repair of the surface film, will also lead to the loss of some lithium and electrolyte. Rosso M and so on [6] found that electrolytic deposits of copper from $CuSO_4$ solution in a high electric field will produce branched deposits , the analysis suggests that the growth of the branches will prevent the arbitrary increase of the space charge , and the growth rate of the branches will increase to balance the drift speed of the anions in the body solution electric field , the system will reach a stable . Under constant current conditions, a direct insitant observation of the dendrite-like electrical deposition of lithium in the lithium battery is made, and a model for explaining the deposition of the filithons is proposed: it is assumed that the uniform deposition occurs in one-dimensional space, including the spatial charge and electric field formed in the area near the positive pole, where the growth of the sedimentary branch is essentially driven by the space charge formed when the hoclatic-ions near the positive pole are consumed.[7]

Previous studies have shown that the reaction mechanism of lithium metal electrodes is more complex, and the growth of branches in the process of lithium deposition has a great impact on the performance of battery circulation, which can also lead to serious safety problems. Based on the multiphysics software COMSOL Multiphysics, the paper uses numerical simulation to simulate the short-circuit process in lithium-ion battery by coupling the battery and the solid heat transfer interface under the fuel cell module, to study the effect of lithium-ion wafer radius on the short-circuit process in lithium-ion battery.

2. Model building

In this paper, a two-dimensional electrochemical-thermal coupling model is established. The model geometry simulates a multi-layer disc in two-dimensional axis symmetry mode, where the lithium branch crystal is placed at r-0 at the same height as the diaphragm, while assuming that the battery cross-sectional area is much larger than the disc. The specific model is shown in Figure 1, using five-layer electrode single element, and from bottom to top each rectangular layer represents

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the negative-pole set fluid, negative porous electric stage, diaphragm, positive porous electrode and positive set fluid, the disc-shaped object in the center of the disc is lithium crystal.

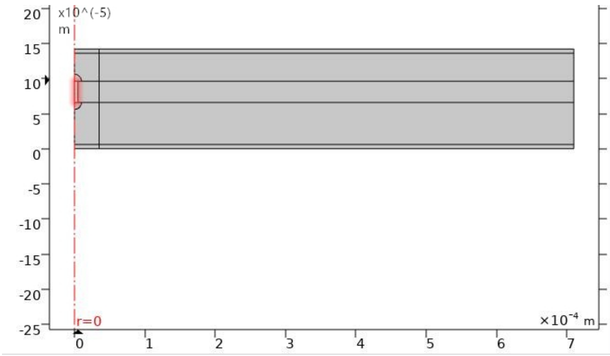

Fig.1 Simulate geometry

Model Physics couples to the "lithium-ion battery" interface of the Heat Transfer interface. The main components of the battery include the 50μm thick graphite negatives, the 40μm thick NMC positive, and the3:7EC: EMC solvent liPF thickness of 30μm of $LiPF_6$ electrolytes, etc. The battery negative and positive are used in a copper and aluminum set fluid of 6sm, respectively.

In the model, the parameter values are derived from the COMSOL material library or self-test, and all control equations are numerically solved using COMSOL Multiphysics 5.4. The model introduces a short circuit in the lithium crystal using a smooth step function, which increases the conductivity of the lithium crystal from a very small value to its original value within 1ms after the calculation has started, making the model more easily convergent. It should be noted that the battery voltage is reduced, due to a short circuit in the battery caused by lithium crystals, but in this model, the discharge time is short and the total circuit current(<10mA) is smaller, than the battery capacity (>1Ah).So we can assume that the battery voltage is constant. Therefore, the calculation time in the study is 0. 2s, and the positive boundary voltage is set to constant at 0.2 s' calculation time.

3. Simulation results and discussions

This study mainly explores the local load state and battery temperature corresponding to the radius of lithium crystal 1μm, 5μm, and 10μm respectively, and thus explores the response of the lithium branch crystal radius change to the short circuit in the lithium-ion battery.

Figure 2 shows the local state of the thermal power of the lithium branches at the t=0.2s at different radii. As can be seen from the figure, the battery discharges the battery outside the area near the lithium branch crystal, and its main heat source is

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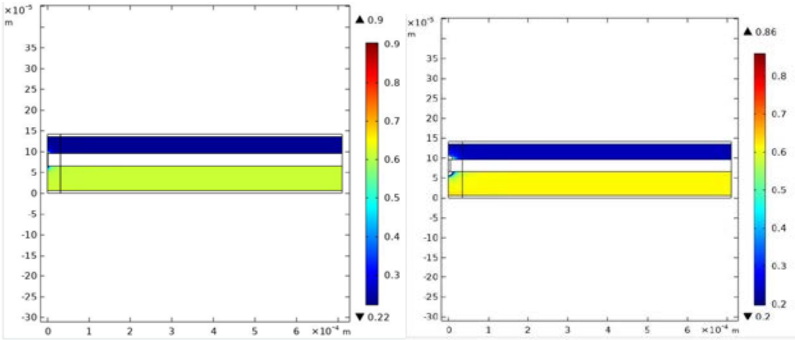
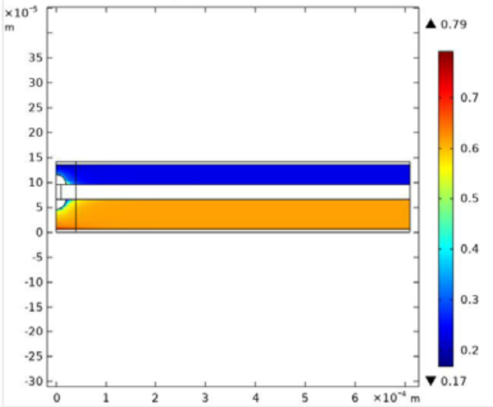
the omron heat in the lithium crystal and its nearby electrode, so the thermal phenomenon caused by the short circuit is sufficient according to the secondary current distribution. Compared to the graph, with the increase of the radius of lithium branches, the local load value of the negative area of the battery increases, and the local load value is higher than the positive local load value, and is concentrated at 0.6-0.7. In the event of a short circuit caused by a lithium crystal, the negative region has more remaining power than the positive pole in the local area, because the reaction rate of the negative pole is lower than positive under short-circuit conditions.



(a) Lithium branch crystal radius of 1μm (b) lithium branch crystal radius of 5μm,



(c) Lithium branch crystal radius of 10μm

Fig.2 The local charge state of the battery corresponding to the radius of the three lithium dendrites at 0.2 s

Figure 3 shows the three types of lithium crystal radius of the battery at t=0.2s at the three-dimensional temperature distribution. It can be concluded that the maximum temperature appears near the lithium branch crystal (specifically the

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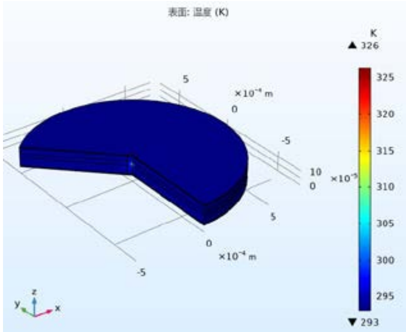
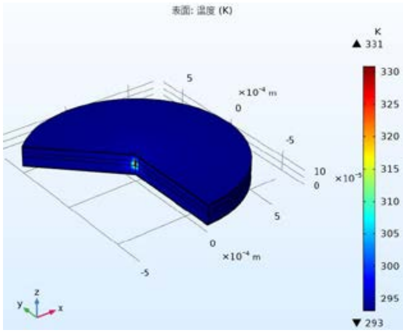
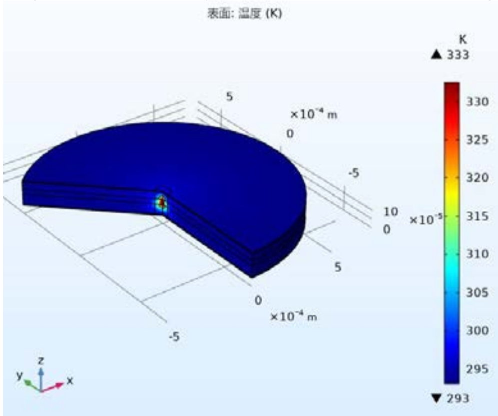
negative surface near the lithium branch crystal),and the temperature change is limited to a small space near the lithium branch crystal. In the figure, the temperature-up range of the negative material is larger than the region corresponding to the positive material, because the ratio of the negative to the thermal capacity is less than the positive pole.



(a) Lithium branch crystal radius of 1μm



(b) lithium branch crystal radius of 5 μm



(c) Lithium branch crystal radius of 10 μm

Fig.3 Temperature diagram of 3D Celsius scale corresponding to three lithium dendrite radii of the battery at 0. 2 s

Figure 4 compares further the maximum temperature of the batteries with a radius of the three lithium branches at 0.2s, the larger the radius, the higher the maximum temperature, and the increase in the heat produced by the lithium-ion battery with the increase in temperature. This is related to the cross-sectional area of lithium branches, the material and height of the case, the larger the cross-cut area, the smaller the resistance of the lithium branch crystal, the greater the total current generated, thus causing the temperature to rise. Figure 4(b) figure further shows the X-axis log chart at the highest temperature in the battery corresponding to the three lithium crystal radii, it can be seen more clearly that after the in-short circuit began,

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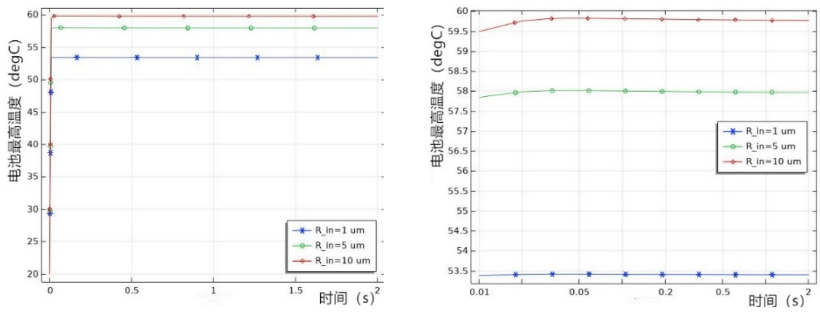
the highest temperature in the three operating conditions has a certain downward trend over time, due to the internal short circuit after the start of a large number of electrons into the positive pole, consuming lithium ions in the electrolyte near the positive pole.[8] Although there is a lithium-ion supplementary lithium source from the negative pole, its diffusion speed is much smaller than the consumption speed of lithium ions in the electrolyte near the positive pole, and the final lithium ion concentration becomes smaller, which will result in a smaller ion conductivity of the electrolyte and a smaller switching current density, so theshort-circuit current is reduced and its temperature is reduced. At the same time, it can be seen that with the increase of the radius of lithium crystal, the downward trend is more obvious.



(a)X-Y (b)X

Fig.4 The maximum temperature in the battery corresponding to the radius of the three lithium dendrites at 0. 2 s

Figure 5 shows the temperature of the battery along the diaphragm-positive boundary for the three lithium crystal at t=0.2s, and through this graph, we can more intuitively understand the temperature change selectrically with the lithium branch radius and r coordinates during the internal short circuit, which is important for promoting the upgrade of the battery management system and inhibiting the growth of the lithium crystal.

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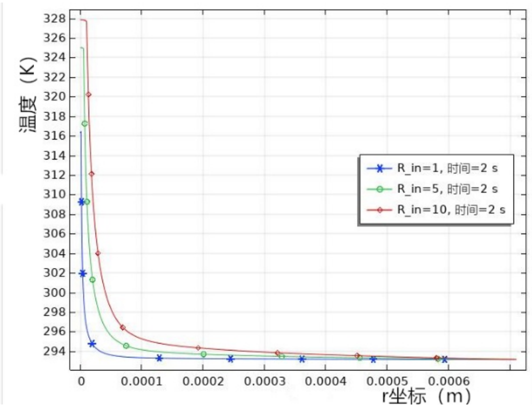

Fig.5 Temperature of the three lithium dendrite radii corresponding to the battery along the positive boundary of the diaphragm at 0.2 s

4. Conclusions

In this paper, using COMSOL multiphysics software, the Newman model simulates the phenomenon of internal short circuit caused by lithium crystal. In the model, the lithium branch crystal is only connected to the positive and negative poles, the local short circuit will not have a significant interference with the working voltage of the battery. We draw the following conclusion: the internal short circuit caused the local current increase, will cause the local area to heat up rapidly, and the maximum temperature over time will have a certain degree of downward trend; local load SOC value in negative polar region sit between 0.6-0.7.

In life, the short-circuit lithium-ion thermal loss of control is a potential risk of lithium-ion power battery. As the temperature continues to rise, the battery will produce more heat reaction, when the temperature reaches a certain stage, or even cause a fire or explosion. In the battery management system, by monitoring a series of responses caused by lithium crystal, it can effectively avoid the production of battery accidents, and also provide an important reference for the study of inhibiting the growth of lithium crystals.

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