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High temperature record for lithium-ion battery with PCM: design and simulation validation

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Abstract. Under abuse conditions, the temperature of lithium-ion battery increases rapidly and brings high safety risk. To monitor the high temperature incident of battery with a simple and reliable method, a novel design scheme was presented and validated by thermal numerical calculation, in which phase change material (PCM) block is bonded with the battery shell and gets melt down when the battery temperature exceeds its phase-transition point. The melting process is irrecoverable and can be perceived by easy visual observation. Computation results show that the temperature rising of the PCM block gets slower when it meets the melting point, but it generally increases synchronously with the shell of the battery and can be used to reflect the temperature rising of the inner cell. Thus the design scheme is valid, and may possess a good applied perspective in the after-sales maintenance and second-hand transactions of lithium-ion battery.

1. Introduction

Lithium-ion batteries are widely used in electric vehicles, electric tools, electronic products and other fields for energy storage. Due to the high chemical activity of electrode materials, the safe operation and storage of lithium-ion batteries requires appropriate temperature environment^[1]. Generally, 25°C to 35°C is the best working range of lithium-ion batteries. When the lithium-ion battery experiences high temperature, the electrode materials and electrolyte inside the lithium-ion battery are easily affected by high temperature, which leads to the decrease of its safety and stability^[2, 3]. When the temperature is very high, it will lead to irreversible safety hazards of lithium-ion batteries.

In the current well-known technical solutions, the temperature sensor is usually used to collect the surface temperature of the lithium-ion battery shell, and the collected data is stored and statistically analyzed, so as to monitor the thermal condition of the lithium-ion battery, and give identification or alarm when the temperature of the lithium-ion battery is too high. This method depends on the temperature sensor and related acquisition, storage, communication and calculation components, and external power supply is needed for the temperature acquisition device. Therefore the monitor and record system is complex with limited reliability.

Phase change material (PCM) is widely concerned by researchers in the area of battery thermal management system (BTMS)^[4, 5], because its capability of storing and releasing a lot of energy, especially around the phase-transition (melting and solidifying) temperature^[6]. But at the moment, PCM is seldom used in industry for its high cost and low heat conductivity. Considering its phase change around the phase-transition temperature, PCM is introduced in this work for the high temperature record of lithium-ion battery. The design scheme was described at first, and then numerical calculation was

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made to valid the design. In the end, the application value of PCM for the high temperature record of lithium-ion battery was discussed.

2. Design scheme

A commercial lithium-ion battery was chosen as the research object, and its three dimensional appearance picture was shown in figure 1. The main parameters of the lithium-ion battery were listed in table 1.



Figure 1. 3D structure of the battery.

Table 1. Main parameters of the battery.		
Parameter	Value	
Nominal capacity	25Ah	
Nominal Voltage	3.7V	
Maximum discharge rate	20C	
Maximum charge rate	8C	
Three dimensional size	120 mm×80 mm×30mm	
Shell thickness	2mm	

In figure 1, a Cartesian coordinate system was added, and the Y-axis points to the thickness direction of the battery. There is a cylinder located in the middle and upper part of the outer shell of the battery, which is made of PCM and bonded with the shell. Paraffin wax was chosen as the PCM in this design. It keeps in solid state under the melting point, and it is highly chemical stable. However, when the battery temperature rises above the melting point of paraffin due to abuse conditions, such as overheating, overcharge, inner or external short-circuit and so on, the paraffin melts immediately and changes into liquid state. As the liquid paraffin is flowable, the PCM cylinder can no long hold its original shape with the act of gravity, so it can be easily observed that the PCM cylinder collapses, which means the battery temperature exceeds the melting points of the paraffin.

What's more, the melted PCM cylinder can not return its original shape when the battery cools down, so the high temperature occurrence of the battery is recorded. If needed, several PCM cylinders with different melting points can be bonded to the battery shell, according to the monitor and record requirement of the battery.

3. Simulation model

To valid the above design scheme, numerical thermal analysis was applied with commercial computation code ANSYS Workbench^[7]. Based on the 3D structure of the battery shown in figure 1, the battery was meshed with hex-dominated element, as shown in figure 2. There are totally 1,296,085 nodes and

291,893 hexahedral elements, and the average mesh quality is above 0.9. The properties for each kind of material were listed in table 2.



Figure 2. Mesh of the battery. Table 2. Material properties for battery.

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Matarial	Conductivity	Density	Specific heat capacity		
Material	(W/(m·K))	(kg/m^3)	(J/(kg·K))		
NCM	1.58	3054	1270		
Graphite	1.04	1347	1437		
Separator	0.33	1009	1978		
Copper	401	8933	385		
Aluminum	238	2702	903		
Stainless steel	16	8030	502		
PTFE	0.26	1500	2000		

There are several kinds of paraffins with different phase-transition temperature. In this work, the paraffin with the melting point as 56°C was chosen for study, for which the number of carbon atoms of one molecule is 26. The material properties for the paraffin were listed in table 3.

Table 3. Material properties for paraffin.						
Thermal	Density	Specific heat	Transformation	Phase-transition		
conductivity	(kg/m^3)	capacity	latent heat	temperature		
(W/(m·K))		$(J/(kg \cdot K))$	(J/kg)	(°C)		
15.1	780	2.12	256000	56		

Thermal source as high as 50,000 W/m³ was evenly loaded in the inner cell volume to simulate the heat generation caused by thermal abuse. The heat gets dissipated mainly in the way of heat convection. The ambient temperature was set to be 35°C and the heat transfer convection coefficient between surfaces of the battery and ambient was 3 J/(m²·K), which means poor thermal management ability. Transient calculation was made with initial temperature of the whole battery as 35°C, and the total calculation time for the heat transfer process was 1200 seconds. During the calculation process, a fixed time step size value Δt =10s was given, so there were totally 120 time steps for the computation and the iterative residual for each time step was set to be 0.001.

4. Results and discussion

Three points including the center of the PCM cylinder surface, the center of the inner cell and the center of the shell surface were monitored to obtain their temperature variations, and their temperature versus time were drawn in figure 3. It shows that the temperature increases lineally at the center of the inner cell, and its temperature exceeds 65° C at the time *t*=1200s. At the same time, the temperature at the center of the shell surface also increases lineally but with a litter lower slope. However, the variation of

temperature at the center of the PCM cylinder surface keeps similar with that at the center of the shell surface until it meets the paraffin melting point, which is 56°C. There is a slower rising process when the paraffin begin to melt (at t=800s), and the slope of the temperature variation curve returns to the original value when the paraffin gets fully melted.





To further obtain the heat transfer phenomena of the batter, the temperature contour distribution of the battery shell at t=800s and t=1200s were shown in figure 4(a) and figure 4(b), respectively. The temperature pattern tendency are almost the same between t=800s and t=1200s, but the temperature of the paraffin cylinder is obviously lower than its surrounding area under the influence of paraffin melting. Similarly, the temperature contour distribution on the middle section plane of the battery was shown in figure 5. It shows a continuous symmetrical temperature gradient, and the maximum temperature locates at the center of the battery. The maximum temperature difference of the whole battery is about 6°C.



(b) Figure 4. Temperature distribution contour of the shell: (a) t=800s; (b) t=1200s.



Figure 5. Temperature distribution contour of the inner cell: (a) t=800s; (b) t=1200s.

It can be known that the temporal and spatial temperature variation of the whole area of the battery are both continuous and uniform from the computation results. Although there is a slower temperature rising process for the paraffin cylinder when it exceeds the phase-transition point, it can still be used as a temperature monitor method for the battery because it basically reflects the inner temperature incensement of the battery. Once the temperature gets above the melting point of paraffin, the paraffin cylinder melts down and can not remain its original shape, which can be easily observed. When the shell temperature of the lithium-ion battery is higher than the melting point of the PCM block, the phase change material block melts and has irrecoverable deformation. In this case, the user can quickly judge whether the lithium-ion battery has experienced the temperature higher than the melting point of the phase change material block by visually observing the shape of the phase change material block. This kind of lithium ion battery with high temperature recording function does not need temperature sensor and its attached transmission and storage elements, but it has high temperature recording and indicating function with good pertinence and stability.

More importantly, the shape change process of the paraffin cylinder is irreversible, thus the high temperature of the battery can be recorded. What needs to be pointed out is that the paraffin block bonded with the batter shell can be made into other shapes with different molds. And the manufacturers can even add some anti-fake label on the surface of paraffin block, so the battery with potential security issue can be identified, which is high difficult of fake and can be used in the fields of after-sales maintenance and second-hand transactions of lithium-ion battery.

What should be noted is that, although the PCM block bonded can not be replaced or returned by ordinal users, it can be conveniently replaced by the manufacturers and the PCM material can be recycled for further use, which fits the ecologist requirements.

5. Conclusion

A novel design of lithium-ion battery with PCM for the high temperature recording was introduced in the present work, and thermal numerical calculation shows that the design scheme is valid. It has the advantages of low cost, simple operation, convenient manufacture and high anti-counterfeiting ability, so it has great application prospect in the fields of after-sales maintenance and second-hand transactions of lithium-ion battery, and some main conclusions can be drawn as follows:

(1) Computation results shows that the inner heat caused by thermal abuse of the lithium-ion battery can be well conducted to the shell and finally make the temperature increment of the PCM block

bonded with the shell, thus using PCM for the high temperature indicating and recording function of lithium-ion battery is reasonable and practicable.

(2) There is a delay period for the temperature rising process of the PCM block compared with that of the battery shell, which is more obvious when the PCM block begins to melt. And this defect may be improved by adding some high conductivity material into the PCM block to increase its thermal conductivity.

In further research, some physical prototypes needs to be made and finally tested by experiment to demonstrative the validity of high temperature record ability of PCM blocked bonded with lithium-ion battery shell.

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