Research on Optimization Application Strategies of Phase Change Materials in Lithium Battery Thermal Management Systems

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Abstract: With the development of the new energy industry, lithium batteries are prone to performance degradation and thermal runaway risks due to heat accumulation exceeding the optimal operating range (25-40°C) during the charging and discharging process, and traditional thermal management methods have limitations. Although Phase Change Materials (PCM) have advantages such as high heat storage density, they still face problems such as low thermal conductivity and easy leakage. This paper first explains on the heat generation mechanism of lithium batteries and the core characteristics of PCM, then proposes optimization strategies of PCM itself from four aspects: improving thermal conductivity, suppressing leakage, regulating phase change characteristics, and enhancing cycling performance, and further presents collaborative optimization schemes (structure, packaging, layout, maintenance) corresponding to design and thermal management systems. Finally, evaluation indicators such as temperature control effect and evaluation methods combining experiments and simulations are clarified. The research provides theoretical support for the design of lithium battery thermal management systems and contributes to the safe and stable development of the new energy industry.

1. Introduction

1.1. Research Background

With the rapid development of the new energy industry, lithium batteries have been widely applied in the fields of new energy vehicles, energy storage systems, portable electronic devices, etc., and their performance and safety directly determine the reliability of terminal products. During the charging and discharging process, lithium batteries continuously generate heat, mainly including Joule heat generated by current passing through electrodes and electrolytes, polarization heat caused by electrode reaction polarization, and reaction heat of the electrochemical reaction itself. When the accumulated heat cannot be dissipated in time, the battery temperature is likely to exceed the optimal operating range of 25-40°C, which will not only accelerate capacity degradation and shorten service life, but may also cause thermal runaway, threatening the safety of equipment and personnel.

Traditional thermal management methods such as air cooling and liquid cooling have problems such as limited heat dissipation efficiency and complex structure in the compact space of battery modules. Phase Change Materials (PCM), with advantages of high heat storage density, good temperature stability, and passive temperature control without additional energy consumption, have become an important technical direction of lithium battery thermal management [1]. However, current phase change materials still face problems such as low thermal conductivity, easy leakage during phase change, and insufficient matching degree of phase change characteristics with battery demands, which urgently need targeted optimization to meet the thermal management requirements of lithium batteries in different scenarios.

1.2. Research Significance

From the perspective of practical application, the study of optimization application strategies of

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phase change materials in lithium battery thermal management can effectively compensate for the limitations of traditional thermal management methods. By improving the thermal conductivity of phase change materials, suppressing leakage, and regulating phase change characteristics, the core problems in practical application can be solved, making phase change materials more compatible with the heat generation law of lithium batteries, thereby more stably controlling battery temperature within the safe range, reducing thermal runaway risks, and extending battery service life, which has important practical significance for ensuring the driving safety of new energy vehicles and the stable operation of energy storage systems.

From the perspective of technological development, this study can provide theoretical support and directional guidance for the design and optimization of lithium battery thermal management systems. At present, the application of phase change materials mostly focuses on single performance improvement, lacking collaborative design with thermal management systems. This study, by sorting out the correlation between the optimization of phase change materials themselves and system collaborative optimization, can promote the deep integration of phase change materials and lithium battery thermal management systems, and promote the iterative upgrading of related technologies. The research results can also provide reference for the development of new phase change materials, help reduce the cost and energy consumption of lithium battery thermal management systems, and further promote the green and sustainable development of the new energy industry.

2. Basic Theory of Lithium Battery Thermal Management and Phase Change Materials

2.1. Heat Generation Mechanism of Lithium Batteries

The heat generation of lithium batteries during the charging and discharging process mainly originates from three types of core heat sources. The first is Joule heat which occurs heat generated when current passes through components such as electrodes and electrolytes, due to the resistance of the materials. Its magnitude is positively correlated with the square of current, resistance, and working time, and the higher the charge-discharge rate, the more significant the Joule heat. The second is polarization heat. Because the electrochemical reaction on the electrode surface cannot instantly reach equilibrium, phenomena such as activation polarization and concentration polarization exist, leading to additional heat generation in the reaction process. At the end of charging and discharging, the degree of polarization increases, and the proportion of polarization heat rises. The third is reaction heat, which refers to the heat absorption/release accompanied by the redox reaction of the positive and negative electrodes inside the lithium battery, and the reaction heat differs greatly among different battery systems (such as ternary lithium, lithium iron phosphate).

Excessively low ambient temperature will increase the internal resistance of the battery, indirectly aggravating heat generation; after battery aging, the structural changes of electrodes will also lead to decreased heat generation efficiency and uneven heat distribution, while overheating will further accelerate battery capacity degradation and even trigger thermal runaway.

2.2. Core Characteristics of Phase Change Materials

The core characteristics of Phase Change Materials (PCM) revolve around their temperature control function, with five key indicators. The first is phase change temperature, which needs to accurately match the optimal operating range of lithium batteries (25-40°C). Too low a temperature will easily solidify and fail in low-temperature environments, while too high a temperature will not be able to absorb battery heat in time. The second is phase change latent heat, which refers to the heat absorbed/released when PCM undergoes solid-liquid or solid-solid phase change. The higher the latent heat, the stronger the heat storage capacity of PCM per unit mass, and the longer the temperature control duration.

The third is thermal conductivity. Traditional PCM (such as paraffin) has a thermal conductivity of only 0.2-0.5 W/(m·K), with low heat transfer efficiency, requiring optimization improvement to quickly respond to battery heat generation. The fourth is stability, including chemical stability (not reacting with battery electrodes and electrolytes) and cycle stability (no significant attenuation of latent heat and phase change temperature after multiple phase changes). The fifth is leakage characteristics. PCM tends to flow and leak when changing from solid to liquid, which will destroy the insulation of the battery [2]. Therefore, suppressing leakage is an important prerequisite for its application.

2.3. Working Principle of Phase Change Materials in Lithium Battery Thermal Management

The working logic of phase change materials in lithium battery thermal management is passive temperature control, without additional energy consumption. When the lithium battery generates heat during operation and the temperature rises to the phase change temperature of PCM, PCM will absorb heat and undergo phase change (mostly solid-liquid phase change) [3]. During this process, the temperature of PCM remains basically stable, thereby “anchoring” the battery temperature within the safe range and avoiding sudden temperature rise. The heat transfer path is: battery internal heat generation→heat transfer through contact interface to PCM → PCM absorbs heat, phase change stores heat; when the heat generation of the battery decreases and the temperature drops, PCM will release the stored heat, preventing the battery temperature from being too low and affecting performance.

The contact mode between PCM and lithium batteries will affect the temperature control effect-direct contact can reduce contact thermal resistance, making temperature control more efficient; indirect contact (through metal partitions) can avoid the leakage risk of PCM, but the heat transfer efficiency will be slightly reduced.

3. Optimization Strategies of Phase Change Materials Themselves

3.1. Optimization of Improving the Thermal Conductivity of Phase Change Materials

Traditional phase change materials (such as paraffin and fatty acids) typically have relatively low thermal conductivity (0.2 to 0.5 W/(m·K)), resulting in poor heat transfer efficiency and difficulty in quickly responding to the heat generation demands of lithium batteries. Therefore, improving thermal conductivity is one of the core optimization directions. Optimization can be achieved by adding high thermal conductivity fillers, commonly used fillers include metal powders (copper powder, aluminum powder, with an addition ratio usually 5% to 20%) and carbon materials (graphene, carbon nanotubes, with an addition ratio of 1% to 5%). However, the dispersion uniformity of fillers needs to be controlled; if dispersion is uneven, agglomeration may occur, instead increasing thermal resistance, which can be improved by ultrasonic dispersion or adding dispersants.

Constructing continuous thermal conduction networks can further improve efficiency. For example, by magnetic field induction or directional freezing process, fillers are arranged along the heat transfer direction, forming through thermal conduction channels and reducing “bottlenecks” in the heat transfer process [4]. Optimization of preparation process is also the key point. When using the melt blending method, controlling stirring temperature and speed (such as 80 to 100℃, 300 to 500 r/min), or combining in-situ polymerization method to make fillers more closely bonded with PCM matrix, can reduce interfacial thermal resistance. Finally, the thermal conductivity of composite PCM can be improved to 1 to 5 W/(m·K), meeting the rapid heat dissipation demand of lithium batteries.

3.2. Optimization of Suppressing the Leakage of Phase Change Materials

Phase change materials are prone to transition from solid to liquid and cause flow leakage during the solid-liquid phase change process, which not only reduces heat storage capacity but may also destroy the insulation of lithium batteries. Therefore, suppressing leakage is an important link to ensure application safety. The first optimization method is microcapsule encapsulation technology. Polymer shell materials with good temperature resistance and strong sealing properties (such as urea-formaldehyde resin, melamine-formaldehyde resin) are selected, and liquid PCM is encapsulated into microcapsules with particle size of 5 to 50 μm through in-situ polymerization method. The shell thickness is controlled at 1 to 5 μm (too thin shells are easy to rupture, too thick shells affect thermal conductivity). After encapsulation, PCM leakage rate can be reduced to less than 5%.

The second method is porous medium adsorption, using the porous structure of materials such as expanded graphite (porosity 80% to 90%) and porous ceramics to adsorb liquid PCM in pores, restricting PCM flow through capillary force and surface tension. For example, mixing paraffin and expanded graphite at a mass ratio of 7:3, after adsorption there is no obvious leakage even at high temperature of 80°C. The third method is structural modification, by adding 0.5% to 2% of thickeners (such as fumed silica) or gelling agents (such as polyacrylamide) into PCM, to improve the viscosity of liquid PCM, making it form a semi-solid gel state, reducing flow leakage, and not significantly affecting phase change latent heat.

3.3. Optimization of Regulating the Phase Change Characteristics of Phase Change Materials

The phase change temperature and latent heat of phase change materials need to accurately match the optimal operating range of lithium batteries (25 to 40°C). If the phase change temperature is too high, it cannot control the temperature in time; if too low, it easily solidifies in low-temperature environments. Therefore, regulating phase change characteristics is the key to improving adaptability. It can be achieved by composite ratio adjustment, mixing two or more PCMs with different phase change temperatures [5]. For example, mixing paraffin with a phase change temperature of 32°C and stearic acid with a phase change temperature of 40°C at a mass ratio of 1:1, can obtain composite PCM with phase change temperature of 35 to 37°C, precisely covering the optimal operating range of the battery, and the latent heat retention rate after mixing can reach more than 85%.

Screening high latent heat materials is the core to improving heat storage capacity. The first choice is Paraffin-based (latent heat 200 to 250 J/g), fatty acid-based (latent heat 180 to 220 J/g) PCMs or latent heat can be improved by doping nanoparticles (such as Al_2O_3, TiO_2)—for example, adding 5% Al_2O_3 nanoparticles can increase the latent heat of paraffin by 10% to 15%. Functional additives can also be added to adjust the phase change temperature. For example, adding 1% to 3% cetyl alcohol into paraffin can reduce the phase change temperature by 2 to 3°C; adding 2% to 5% octadecane can increase the phase change temperature by 1 to 2°C, realizing fine adjustment of phase change temperature, to adapt to the heat generation demand of lithium batteries in different scenarios.

3.4. Optimization of Improving the Cycling Performance of Phase Change Materials

After multiple phase changes (usually requiring more than 1000 times), phase change materials are prone to problems such as latent heat attenuation, phase change temperature shift, and structural damage, affecting long-term temperature control effect. Therefore, improving cycling performance is the key to ensuring durability. The first optimization method is adding stabilizers. By adding 0.1% to 0.5% antioxidants (such as dibutylhydroxytoluene, vitamin E) into PCM, the oxidative degradation of PCM during high-temperature phase change process can be inhibited, reducing latent heat attenuation; by adding 1% to 3% anti-settling agents (such as organic bentonite, fumed silica), sedimentation and agglomeration of high thermal conductivity fillers during cycling process can be prevented, maintaining stable thermal conductivity (for example, after adding 0.3% dibutylhydroxytoluene, the latent heat attenuation rate of PCM after 1000 cycles can be reduced from 20% to less than 5%).

The second method is to improve preparation process, using vacuum drying process (vacuum degree 0.095 MPa, temperature 60 to 80°C) to remove bubbles inside PCM, reducing structural damage caused by bubble rupture during cycling; using ultrasonic-assisted melt blending process (ultrasonic power 300 to 500 W, time 10 to 20 min) to enhance the interfacial bonding force between PCM matrix and fillers, reducing interfacial separation risk during cycling. The third method is optimizing matrix materials, selecting aging-resistant polymer matrices (such as polyethylene, polyethylene glycol) to replace traditional low molecular PCMs, or coating a layer of aging-resistant film (such as polytetrafluoroethylene film) on PCM surface, reducing the erosion of PCM by environmental factors (such as high temperature, humidity), and extending cycling service life.

4. Collaborative Optimization Strategies of Phase Change Materials and Lithium Battery Thermal Management System

4.1. System Structure Design Matching Thermal Conductivity Optimization

For the high thermal conductivity phase change materials (such as composite PCM with added metal/carbon fillers and constructed thermal conduction networks) improved in Chapter 3, system structure design needs to focus on reducing thermal resistance and strengthening heat transfer paths, so as to fully exert their thermal conductivity advantages. To enhance battery performance, it is crucial to optimize the contact structure between the battery and PCM by adopting customized fitting designs (such as processing PCM into arc-shaped or sheet-like forms matching the battery cell) and applying thermal interface materials (such as thermal grease with a thermal conductivity of 1 to 5 W/(m·K)) on the contact surface. This approach can reduce contact thermal resistance by more than 30%, ensuring that the battery heat is quickly transferred to the PCM.

Secondly, researchers should combine high thermal conductivity phase change materials (PCM) to design composite structures of PCM and heat dissipation components. They can embed heat pipes or metal fins (such as aluminum fins with a spacing of 5 to 10 mm) in the PCM filling layer, utilizing the synergistic effect of PCM heat absorption and component heat conduction to form an efficient path of heat absorption–transfer–dissipation, which is especially suitable for high-rate charge/discharge scenarios. In addition, based on the heat generation distribution of the battery module (with the central region being hotter than the edges), designers should arrange composite PCM with higher thermal conductivity (for example, PCM with 20% copper powder added, reaching 3 to 4 W/(m·K)) in high heat generation areas, while placing conventional high thermal conductivity PCM in the edge areas to achieve uniform heat transfer through structural partitioning and avoid local overheating [6].

4.2. System Packaging Design Suitable for Leakage Suppression

For phase change materials that achieve leakage prevention through microcapsule encapsulation, porous medium adsorption, and structural modification as introduced in Chapter 3, system packaging design needs to focus on matching PCM characteristics and blocking leakage risks to ensure battery safety. For microcapsule PCM (particle size: 5 to 50 μm), they should design sealed cavity packaging structures, with the cavity material selected as temperature-resistant and insulated engineering plastics (such as PA66, which is resistant to temperatures above 150℃). The cavity size is determined based on the bulk density of the microcapsule PCM (typically 0.8 to 1.0 g/cm^3), ensuring that no voids remain after filling. At the same time, ultrasonic welding is used to seal the cavity edges, and the sealing width is not less than 2 mm, which prevents leakage after microcapsule rupture.

For porous medium adsorption type PCM (such as expanded graphite adsorbed paraffin), it is recommended to add an external protective film layer (such as PTFE film, thickness 0.1 to 0.2 mm) in the PCM filling area to avoid PCM seepage caused by vibration or aging-induced damage of the porous material; it is also advisable to reserve a 0.5 mm buffer gap between the protective film and the battery to prevent PCM phase change expansion from squeezing the battery. In addition, for all leakage-proof PCM, it is important to use sealing glue (such as silicone sealant, resistant from -60 to 200℃) to fill the gap between the PCM module and the housing during system assembly, forming a secondary sealing barrier and controlling the leakage rate below 0.1%, thereby eliminating the risk of liquid PCM contacting battery electrodes and causing short circuits.

4.3. System Layout Optimization Matching Phase Change Characteristics Regulation

For PCMs optimized by composition adjustment and high latent heat selection in Chapter 3 (such as composite PCM with phase change temperature of 35 to 37°C and latent heat above 200 J/g), system layout design needs to follow the principle of demand-based distribution and precise temperature control, so that PCM phase change characteristics highly match battery heat generation needs. First, the reseachers should adopt a zoning layout strategy: in high-temperature areas of the lithium battery module (such as near charging interfaces and central cells), arrange PCM with lower phase change temperatures (such as 32 to 34℃), to preferentially absorb heat and prevent rapid temperature rise; in low-temperature areas (such as module edges and near heat dissipation outlets), they arrange PCM with higher phase change temperatures (such as 38 to 40℃), to avoid premature solidification of PCM and loss of heat storage capacity [8]. By zoning temperature, the temperature difference within the module can be controlled within 5°C.

Secondly, it is necessary to calculate PCM dosage according to the maximum heat generation of the battery (such as about 5 to 10 W per cell during 1C charge/discharge), ensuring that the total heat storage of PCM (mass × latent heat) is no less than the maximum heat generation of the battery within 1 hour. For example, each single cell with 20 g of PCM (latent heat 200 J/g, total storage 4000 J) can meet the 40-minute temperature control demand under 10 W heat generation, avoiding temperature runaway caused by PCM exhaustion. In addition, it is suggested to adopt a fitting layout, processing PCM into ring-shaped or block-shaped structures fully matching the battery module, covering more than 90% of the battery surface area, maximizing PCM-battery contact area, improving phase change temperature control response speed, and shortening the time from heat absorption start to phase equilibrium to within 5 minutes [9].

4.4. System Maintenance Design Coordinated with Cycle Performance Optimization

For PCMs with improved cycle performance through stabilizer addition and process improvement in Chapter 3 (such as latent heat decay rate below 5% after 1000 cycles), system maintenance design needs to focus on extending PCM service life and reducing maintenance cost, ensuring long-term stable operation of the thermal management system. First, the researchers designed detachable PCM modules, which are connected to the system housing through snap-fit structures, allowing for quick PCM replacement without disassembling the battery. When PCM shows cycle performance degradation (latent heat decline above 10%) after long-term use (such as 3 to 5 years), the module can be replaced within 30 minutes, avoiding system scrap caused by PCM failure [10].

Secondly, they embed monitoring components inside PCM modules, including temperature sensors (accuracy ±0.5°C) and humidity sensors (to detect PCM leakage). Sensor data is transmitted in real time to the Battery Management System (BMS). When abnormal PCM temperature (such as phase change temperature deviation exceeding 2°C) or increased humidity (indicating leakage) is detected, the BMS issues a warning in time for early maintenance [11]. In addition, it is suggested to optimize environmental adaptability design of the system, add an insulation layer (such as polyurethane foam, thermal conductivity 0.03 W/(m·K)) outside the PCM module to avoid accelerated aging caused by repeated solidification-melting under low-temperature environments; under high-temperature environments, it is essential to use built-in small fans (wind speed 1 to 2 m/s) to assist PCM heat dissipation, which reduces cycle performance degradation caused by long-term high temperature exposure. The actual PCM service life is extended to more than 5 years.

5. Performance Evaluation and Future Prospect of Optimized Application of Phase Change Materials

5.1. Performance Evaluation Indicators

The performance evaluation after the optimized application of phase change materials needs to set key indicators around the core requirements of lithium battery thermal management, and ensure that the indicators are quantifiable and fit actual application scenarios. First is temperature control effect, the core is to judge whether the battery is stable in the optimal working range of 25–40°C, and under extreme conditions (such as 3C high-rate charge and discharge), the maximum battery temperature needs to be lower than 60°C, to avoid triggering thermal runaway risks. Second is temperature uniformity, the maximum temperature difference at different positions inside the battery module should be less than 5°C, to prevent capacity degradation differences caused by local overheating. Third is response speed, the time from PCM sensing battery heat generation to entering stable phase change temperature control needs to be less than 10 minutes, to ensure quick response to sudden heat accumulation. Fourth is long-term stability, after more than 1000 charge and discharge cycles, the temperature control effect attenuation rate of PCM needs to be lower than 10%, and there should be no obvious leakage or structural damage, to ensure long-term reliability.

5.2. Performance Evaluation Methods

Performance evaluation needs to combine experimental testing and simulation analysis, to ensure results are comprehensive and accurate. In terms of experimental testing, a lithium battery charge and discharge experimental platform is built, the optimized PCM is assembled with the battery module, and high-precision temperature sensors (such as PT100, accuracy ±0.1°C) are arranged on the battery surface and key positions inside the module, to record temperature changes in real time under different charge and discharge rates (0.5C, 1C, 2C, 3C), and calculate temperature control effect, uniformity, and response speed. At the same time, long-term cycle experiments are conducted, monitoring PCM phase change latent heat and leakage after 1000 cycles, to evaluate stability. In terms of simulation analysis, finite element analysis software (such as ANSYS, COMSOL) is used to establish PCM-lithium battery thermal management system models, optimized PCM parameters such as thermal conductivity and phase change temperature are input, and temperature field distributions under different ambient temperatures (-20°C, 25°C, 45°C) are simulated, to verify the rationality of experimental results and to predict system performance under extreme conditions, reducing experimental cost.

5.3. Future Prospect

The optimized application of phase change materials in lithium battery thermal management can develop in the direction of higher efficiency, intelligence, and environmental protection in the future. First is research and development of new phase change materials, focusing on breakthroughs in nano-composite PCM (such as graphene-based PCM) and intelligent responsive PCM (temperature-triggered adjustment of phase change characteristics), to further improve thermal conductivity and temperature control accuracy. Second is multi-technology integration, combining optimized PCM with air cooling and liquid cooling, to form hybrid thermal management systems of passive temperature control and active heat dissipation, which meet the demand of high-rate and large-capacity lithium batteries. Third is intelligent management, combining sensors and AI control algorithms, to monitor battery heat generation and PCM status in real time, dynamically adjust PCM working modes (such as auxiliary heat dissipation starting time), and realize on-demand temperature control. Fourth is environmental protection and low cost, developing recyclable bio-based PCM (such as plant waxes), optimizing preparation processes to reduce production costs, promoting large-scale application of the technology, and supporting the green development of the new energy industry.

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