

Thermal Management Strategies for High-Energy-Density Lithium-Ion Batteries in EV system

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Abstract. Against the backdrop of the global energy structure accelerating its transition towards clean energy, the electric vehicle (EV) industry has experienced explosive growth. Lithium-ion batteries (LIBs), with their core advantages of renewability and environmental friendliness, have been widely used for EVs. To further enhance the driving range and lightweight design of EVs, nickel-cobalt-manganese ternary (NCM) batteries have been commercially adopted due to their high energy density and long cycle life. However, current research reveals constraints in NCM battery development: high cost of cobalt (accounting for 40% of battery cost) and low thermal stability of materials like $\text{Li}[\text{Ni}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}]\text{O}_2$ (NCM811), which easily triggers thermal runaway with severe consequences. This review analyzes the process and mechanism of thermal runaway in the NCM811 system. Studies indicate that the intense exothermic reactions during thermal runaway are caused by oxygen released from redox reactions of the anode and cathode at elevated temperatures. To further improve energy density and mitigate potential thermal runaway risks, this study discusses advanced anode materials and solid-state electrolyte modifications for the NCM811 system, compares the advantages and disadvantages of traditional materials, and reviews novel battery cooling systems and thermal simulation models.

Keywords: Electric vehicles, Lithium-ion batteries, NCM811, Battery thermal runaway, Battery thermal management

1. Introduction

Amidst the accelerating global energy transition towards clean energy, the electric vehicle industry is experiencing explosive growth [1]. According to official data, in 2024, the production and sales of automobiles in China reached 31.436 million and 31.282 million respectively, and the market size of power batteries exceeded 500 billion RMB [2]. Lithium-ion batteries serve as the critical component determining vehicle's driving range, safety [3]. According to the forecast of the F. Degen team, the global demand for LIB will exceed 10000GWh by 2040 [4]. The common positive electrode material for batteries in the market is lithium cobalt oxide (LiCoO_2). The constrained availability of cobalt resources presents significant cost-related challenges for its widespread adoption in electric vehicle applications [4]. The development of high-nickel NCM811 ternary materials has significantly reduced cobalt dependency, thereby lowering material costs. More importantly, the high content of nickel increases the specific capacity, making ternary materials have excellent

application prospects as positive electrodes. However, the current commercial power battery system is facing multiple technological bottlenecks: in terms of positive electrode materials, the NCM ternary system, as shown in Figure 1 [5], has a theoretical specific capacity of 270mAh/g, but its thermal decomposition temperature is below 200 °C, which seriously restricts safety; In negative electrode materials, although traditional graphite has excellent conductivity of >10 S/cm, the damage of the solid electrolyte interface (SEI) film at the graphite anode is one of the important forms of LIB accidents, and safety needs to be urgently addressed [6]. This study is based on NCM811 positive electrode material to improve the driving range. However, the cationic mixing of Li^+ and Ni^{2+} in NCM materials adversely impacts electrochemical performance, particularly compromising cycling stability. The scheme can improve energy density and achieve higher cycle life by designing the negative electrode material and electrolyte of the battery, combined with a thermal simulation model. This study investigated the issue of battery thermal runaway and conducted relevant research on high-energy lithium-ion batteries using battery thermal management methods and structural modification methods.

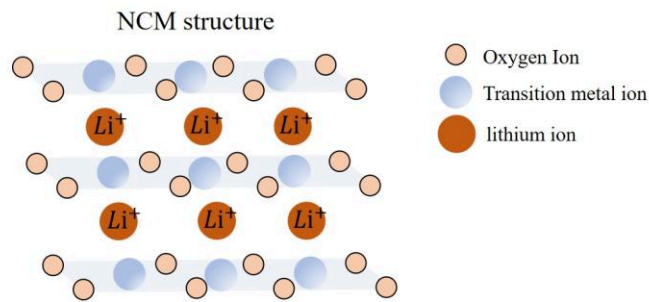


Figure 1. NCM positive electrode material structure [5]

2. Technological path for improving energy density of lithium-ion batteries

2.1. Materials innovation

This paper reviews key battery components, with particular focus on positive electrode material, anode material, and electrolyte system.

2.1.1. Positive cathode material

The positive electrode material of lithium-ion batteries is a crucial factor determining their energy density, cycle life, and safety performance. The positive electrode of traditional lithium-ion batteries uses LiCoO_2 , LiFePO_4 (LFP), and LiMn_2O_4 (LMO). For example, the LFP voltage platform is only 3.2V, and even if its capacity is comparable to NCM, its energy density will be reduced by more than 30%. This physical limitation is determined by the material crystal structure and is difficult to break through process improvements [4]. The theoretical maximum specific capacity of traditional positive electrode materials is 274mAh/g, but the actual usable capacity is only 140-160mAh/g. The high nickel ternary material NCM811, with a structure shown in Figure 2, is a representative of high-energy density batteries developed in recent years [7]. This system significantly improves the theoretical specific capacity of lithium-ion batteries by increasing the nickel content to 80%. Research has shown that NCM811 cathode material can achieve a mass energy density of 300Wh/kg, showing enormous potential for energy density improvement [8].

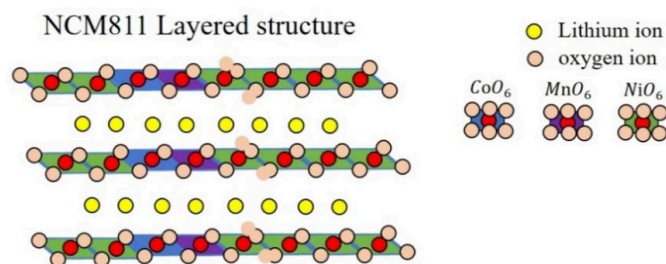


Figure 2. NCM811 high nickel ternary positive electrode material structure [7]

2.1.2. Negative electrode material

The safety limitations of conventional anode materials appear as a critical challenge in commercial lithium-ion battery development. Graphite anode SEI films significantly influence thermal runaway behavior, a primary mechanism in LIBs [6]. During the fast-charging process of lithium-ion batteries, if the rate at which Li^+ pass through the SEI film is slower than the deposition rate of lithium on the negative electrode, lithium dendrites will continue to form with charge and discharge cycles, which enlarge current and cause heat accumulation in the lithium-ion battery. Silicon anodes show superior theoretical capacity (4200mAh/g), 11-fold higher than conventional graphite anodes (372mAh/g), offering improvement in energy density despite graphite's inherent stability. However, the volume change of silicon during the lithium extraction process can cause the SEI film to repeatedly rupture and regenerate, consuming active lithium, which is the reason for the poor cycle life [9]. The silicon-based negative electrode needs to balance the advantages and disadvantages of "high capacity, high expansion". To overcome the significant volume expansion problem of silicon-based negative electrodes during charge and discharge processes, a stable electrode structure is constructed through nanostructured modification technology, effectively suppressing the damage of volume changes to the electrode material structure, thereby improving the cycling stability and service life of negative electrode materials. Research has shown that, while pursuing high energy density, the issue of lifespan can be solved through nanocomposites and pre lithiation. Considering safety and cost, graphite negative electrode is still the mainstream, and LFP batteries combined with graphite can meet the demand for a range of 600km. At present, mainstream car companies have already commercialized large-scale silicon-based negative electrodes, such as the existing Tesla 4680 battery (SiO-C silicon oxygen negative electrode), which has an energy density of up to 300Wh/kg.

2.1.3. Electrolytes system

Conventional carbonate solvents (EC/DMC, flash point $<40^\circ\text{C}$) show violent oxidative chain reactions with oxygen released from cathodes at elevated temperatures, accelerating thermal runaway propagation. Studies indicate battery temperatures exceeding 60°C trigger exponential growth in cathode lattice oxygen release rates and 3-5-fold faster Li-dendrite formation, drastically increasing short-circuit risks. Current liquid cooling systems (thermal conductivity $<0.5\text{W/m}\cdot\text{K}$) struggle to maintain thermal uniformity during $>3\text{C}$ fast-charging, frequently resulting in $>8^\circ\text{C}$ temperature gradients and localized hotspot formation.

A fluorinated high-voltage electrolyte (≥ 4.6 V) is employed, with LiFSI as the key component, enabling in situ formation of compact CEI and SEI layers on electrode surfaces. The LiFSI enhances Li^+ conductivity, facilitating fast ion intercalation/deintercalation and supporting high energy density. The CEI layer suppresses high-voltage electrolyte decomposition, while sulfur-rich SEI components (Li_2SO_x) reduce interfacial resistance, improving charge/discharge efficiency [10]. Tests confirm superior cyclability: 85% capacity retention after 1000 cycles and stable discharge capacity (230 mAh/g at C/10), validating the system's efficacy.

2.2. Security balance

LFP power batteries are considered as a safety benchmark due to their inherent high thermal stability. However, the latest research shows that hydrogen accounts for a remarkably high proportion of the released gas components during the thermal runaway process of LFP batteries, which significantly increases the actual risk of explosion compared to NCM systems [4]. Therefore, in battery design, the influence of reactive gas species evolution on thermal runaway should also be considered. It is necessary to focus on optimizing the thermal management design of high nickel systems while improving energy density.

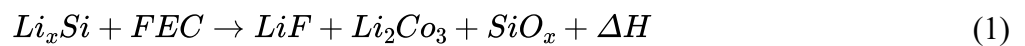
3. Lithium-ion battery thermal runaway

Experimental results reveal notable variations in thermal runaway onset temperatures among cathode materials: LFP ($\sim 180^\circ\text{C}$) > NCM523 ($\sim 143^\circ\text{C}$) > NCM811 ($\sim 136^\circ\text{C}$) > NCM90.50.5 ($\sim 131^\circ\text{C}$) [4]. This trend proves that increasing Ni content reduces lattice oxygen stability, enhancing the material's thermodynamic propensity for thermal decomposition at elevated temperatures. Consequently, higher-Ni cathodes show progressively lower thermal runaway thresholds, significantly raising battery safety risks. The thermal runaway process evolves through three distinct stages.

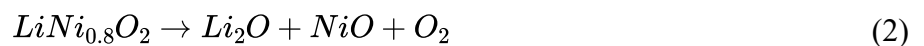
3.1. Thermal runaway process

Stage 1: Initial Heat Accumulation Period ($70\text{-}90^\circ\text{C}$)

When the battery is subjected to violent impact or external heat source, the temperature can exceed 70°C . At this temperature, the silicon based negative electrode interface will undergo progressive degradation, and the volume expansion stress of more than 300% will be generated during the lithium insertion process of Li_xSi , leading to the dynamic fracture recombination cycle of the SEI film. Irreversible reduction reaction occurs between the surface of newly formed silicon and fluorinated carbonate-based electrolyte (FEC):



At the same time, the highly oxidized Ni^{4+} on the positive electrode surface of NCM811 undergoes valence state reduction under thermal disturbance, accompanied by the formation of oxygen vacancies and the precipitation of rock salt phase (NiO):

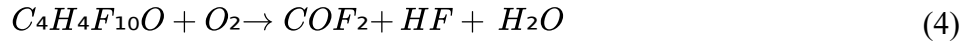


The electrolyte system undergoes hydrolysis side reaction. The heat accumulation rate during this stage shows a growth characteristic, dominated by the synergistic effect of SEI decomposition and positive electrode oxygen release [6].



Stage 2: Thermal Acceleration Period (90-260°C)

The thermal runaway process at this stage is dominated by the bulk lattice oxygen deintercalation of the NCM811 positive electrode. When the temperature rises to around 200°C, the lattice oxygen (O²⁻) in the structure of NCM811 undergoes deintercalation reaction, accompanied by a significant phase transition sequence: layered structure (R-3m) → spinel phase (Fd-3m) → rock salt phase. The released molecular oxygen reacts with FEC through gas-liquid two-phase oxidation combustion, releasing a large amount of heat. The silicon-based negative electrode undergoes nanoparticle sintering and agglomeration at high temperatures (>150°C), forming an electron conduction network that penetrates the electrode, triggering local micro short circuits and leading to rapid accumulation of Joule heating. At this stage, a significant acceleration in the temperature rise rate caused the electrolyte to boil and splash from local overheating, further worsening thermal diffusion [10].



Stage 3: Thermal runaway outbreak period (>260°C)

When the internal temperature of the battery reaches 260 °C , the system enters a strong exothermic self-sustaining state, and the thermal runaway process is irreversible and exponentially accelerated. The reaction process is shown in Figure 3. The NCM811 positive electrode undergoes deep decomposition, causing the layered structure to completely collapse and transform into a mixture of NiO, CoO, and Mn₂O₃ oxides, releasing high valence metal vapors and residual oxygen. The silicon-based negative electrode undergoes melting loss due to continuous high temperature (>800°C), and the molten silicon forms an Al-Si eutectic alloy with the aluminum current collector at the eutectic point (577 °C), resulting in a global short circuit where the positive and negative electrodes are directly conductive. At the same time, LiFSI undergoes explosive pyrolysis, releasing highly toxic gases such as HF, SO₂F₂, SOF₂ , and NSF. At this stage, the total heat released reaches 1600-1800 kJ/kg, which is more than 100% higher than the traditional graphite system. The thermal runaway propagation rate exceeds 500°C/s, accompanied by intense gas release and pressure wave effects leading to battery explosion [4,11].

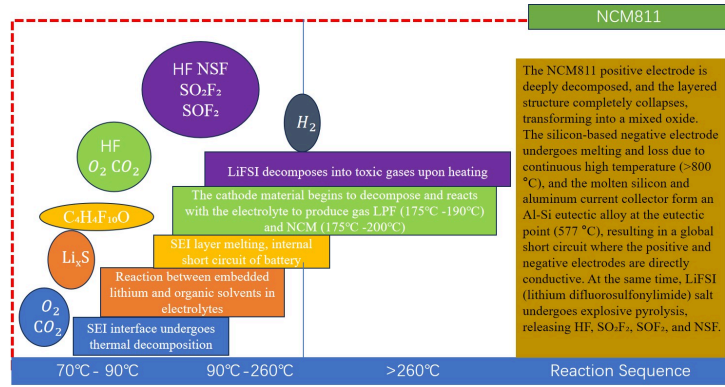


Figure 3. Schematic diagram of gas composition during thermal runaway process [4,11]

The four typical stage characteristics, and its reaction mechanism and thermodynamic behavior undergo significant evolution with increasing temperature. Compared to traditional graphite systems, the thermal runaway of silicon-based high nickel batteries shows three major characteristics: temperature shift, doubled heat release intensity, and increased toxicity risk. This is mainly due to the synergistic effect between the volume effect of the silicon negative electrode and the oxygen release characteristics of the high nickel positive electrode.

3.2. Battery thermal model

3.2.1. Battery heat release process

The heat dissipation process of a battery includes four stages, namely thermal chemical reaction to generate heat, solid-state heat transfer (heat is transferred from the battery core to the outer shell and adjacent batteries), gas jet flow, and environmental heat dissipation. In order to prevent thermal runaway [12], common solutions include positive electrode coating ($\text{Al}_2\text{O}_3/\text{Li}_2\text{ZrO}_3$), which utilizes phase change materials (PCM) to absorb latent heat and suppress initial heat generation; Inserting aerogel felt between electric cores to block solid heat transfer; Design directional pressure relief channels to guide the direction of jet flow, such as the longitudinal pressure relief valve of BYD blade batteries. Or by enhancing environmental heat dissipation, such as the serpentine cooling plate design of Tesla 4680 battery.

3.2.2. Battery heat generation rate

The Bernardi equation is used for the heat dissipation model of NCM811 battery pack [12]:

$$Q = \beta \frac{I_L}{V_B} [(E - U_L) + T \frac{dE}{dT}] \quad (5)$$

To calculate heat generation, where β is the correction coefficient for heat generation rate. Through simulation and experimental comparison, it is found that β is 1.13 during discharge and 0.65 during charging; V_B is the volume of a single battery cell; I_L is the charging and discharging current of the battery; T is temperature; $(E - U_L)$ I_L/V_B is the Joule heating of the battery; $\frac{I_L}{V_B} T \frac{dE}{dT}$ is the electrochemical reaction heat of the battery;

3.2.3. Boundary conditions for battery heat transfer

The boundary condition equation of the battery follows Fourier's law:

$$q_n = -\lambda \frac{\partial T}{\partial n} \quad (6)$$

In the formula, q_n is the heat flux density, W/m^2 ; λ is the thermal conductivity; $\partial T / \partial n$ is the temperature gradient in the normal direction of the isothermal surface of the battery, K/m. Convective heat transfer is directly proportional to temperature difference, expressed by Newton's formula:

$$\phi = hA (T_w - T_f) = hA \Delta T \quad (7)$$

3.2.4. Equation of battery heat dissipation flow field

Due to the Reynolds number of the reaction being greater than 4000, the turbulence model $k - \epsilon$ was used to simulate high-speed airflow injection.

Turbulent viscosity equation :

$$\mu_t = \frac{\rho C_\mu k^2}{\epsilon} \quad (8)$$

3.3. Result

Figure 4 and Table 1 show that thermal propagation triggering times range from 0.33s to 32.62s, while temperature differences vary between 0.22°C and 116.25°C. The simulation results show good consistency with experimental data. The battery reaches its maximum temperature exceeding 1000°C approximately 400s after thermal runaway initiation [12].

Table 1. Maximum temperature, thermal runaway triggering time, and maximum temperature triggering time [12]

No.1	Exp.	Sim.	Gap	No.2	Exp.	Sim.	Gap	No.3	Exp.	Sim.	Gap
T_{1max}	1023.2°C	1040.59°C	17.39	t_{1start}	386.3s	394.9s	8.6	t_{1maxt}	396.91s	369.69s	27.22
T_{2max}	977.3°C	1093.55°C	116.25	t_{2start}	400.62s	368s	32.62	t_{2maxt}	409.28s	389.5s	19.78
T_{3max}	1073.9°C	1011.48°C	37.38	t_{3start}	403.03s	388.87s	14.16	t_{3maxt}	403.77s	394.26s	9.51
T_{4max}	1133.4°C	1033.62°C	0.22	t_{4start}	404.74s	405.07s	0.33	t_{4maxt}	409.67s	405.83s	3.84
26.41 T_{5max}	952.4°C	1083.85°C	131.45	t_{5start}	446.63s	421.23s	25.4	t_{5maxt}	463.81s	437.40s	26.41

The experiment found that the high temperature of the internal modules of the battery and the high-speed jet of the airflow may cause secondary radiation of the flame. It can be attempted to use PCM materials inside the battery module to prevent further expansion of the fire.

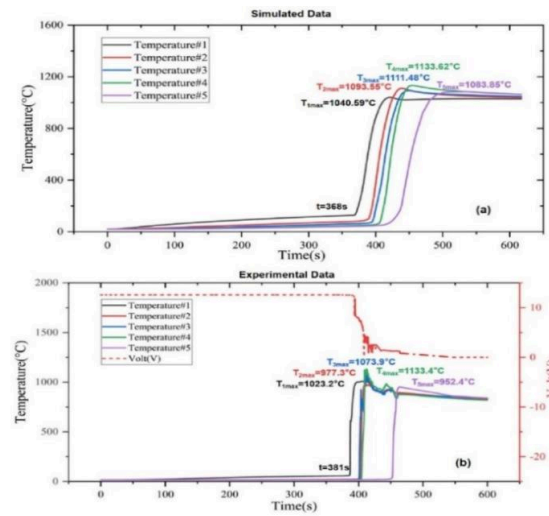


Figure 4. The simulation scheme had a small error compared to the experiment. Li et al. conducted a comparative analysis of thermal profiling data across four designated measurement points in a single-cell NCM811 configuration [12]

4. Collaborative optimization design of energy density and heat dissipation

Lithium-ion batteries present two primary safety concerns. First, thermal runaway may occur under abusive conditions including mechanical penetration, compression, or external heating. Second, heat generation during routine charge-discharge cycles can lead to progressive thermal accumulation. The characterization by electron microscopy confirmed that the intense exothermic reaction is caused by the release of oxygen [10]. The high activity oxygen pulse reacts rapidly with the electrolyte, accompanied by heat release, and the anode and cathode electrodes undergo redox reactions at higher temperatures.

4.1. Overview of battery thermal management systems

BTMS is to ensure optimal operating temperatures and uniform thermal distribution across cells, modules, and packs during high-rate charging/discharging and extreme environmental conditions. BTMS are classified according to cooling medium into three primary types: air-based, liquid-based, and PCM-based cooling systems [13].

The design factors that affect the performance of the cooling system are the geometric shape of the air channel, battery layout, and air flow path. Study demonstrate that conical ducts outperform U-shaped ducts in cooling efficiency, as shown in Figure 5; Fan et al. suggest that reducing the gap spacing between batteries or increasing fan flow can reduce the maximum temperature rise of battery modules, but the gap spacing should be moderate to achieve better temperature uniformity; Enhancing the air-coolant heat transfer area also improves dissipation (Lu et al).

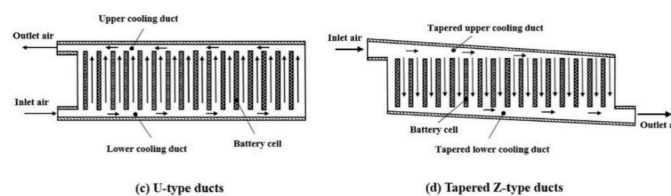


Figure 5. Comparison of U-shaped and conical Z-shaped cooling ducts [13]

Another PCM cooling system requires high latent heat, thermal capacity, conductivity, and proper phase transition temperature [14]. PCM absorbs substantial latent heat through isothermal phase change, supporting thermal stability under high battery loads without excessive temperature rise or gradient. To address PCM's inherently low conductivity, three enhancement methods are typically employed: incorporation of carbon nanomaterials, integration of metal fins, and addition of porous matrices like expanded graphite (EGM).

4.2. Structural modification

At present, chemical modification methods are used to study the thermal runaway risk of NCM811, generally including doping modification, coating modification, and conformity modification [15].

The common doping modification method, Mg^{2+} doping NCM811, can increase the number of cycles. Unlike transition group elements, structural changes are not caused by changes in valence state, thus improving cycling performance. Secondly, after adding Mg^{2+} preserve charge neutrality, partial transition metal cations undergo valence state variations, generating charge carriers that enhance the material's electrical conductivity. Coating modification is the process of covering other material to alter the interfacial contact, thereby increasing the transfer rate of Li^+ and electrons, reducing interfacial resistance, and minimizing the occurrence of side reactions. The MgO coating layer effectively mitigates volume expansion and structural strain during electrochemical cycling. As shown in Figure 6, the coated NCM811 exhibits significantly reduced internal resistance compared to uncoated samples, while simultaneously suppressing SEI film formation and minimizing interfacial side reactions.

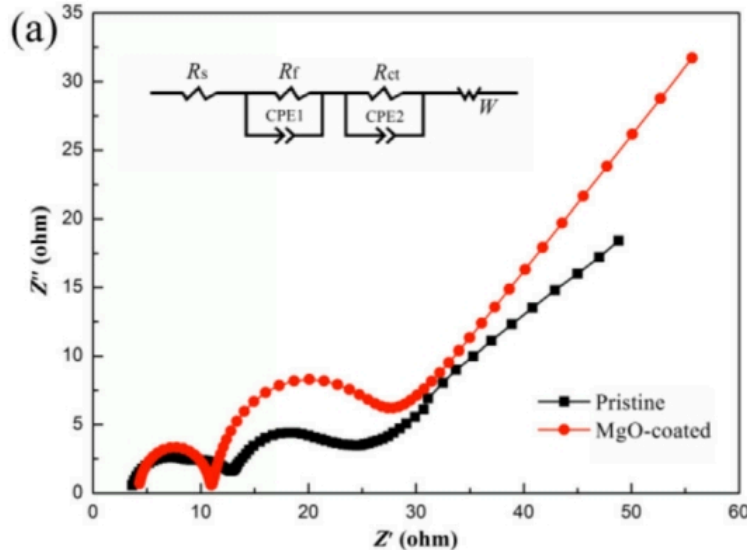


Figure 6. MgO coating reduces the interfacial reaction of NCM811 [15]

Composite modification is a method that combines the above two, such as coating positive electrode materials with graphene. Single layer graphene (thickness 0.335 nm) forms a continuous coating layer, covering the surface microcracks of NCM811 particles and effectively increasing the oxygen diffusion path. Graphene does not undergo oxidative decomposition below 600°C (superior to traditional polymer coating), effectively blocking the escape of high-temperature oxygen. And due to the Young's modulus of graphene being 1 TPa, the coating effectively suppresses the release of fresh oxygen generated by particle breakage during charge discharge cycles on the surface.

5. Conclusion and prospect

Lithium-ion batteries serve as the predominant energy storage technology in electric vehicle propulsion systems. However, battery cost issues and potential thermal runaway problems have constrained the development of the industry. To meet the requirements of increasing the range and lightweight technology of electric vehicles, NCM811 is used as the positive electrode material, with an energy density of up to 300Wh/kg. The silicon-based anode materials offer enhanced energy density, yet their practical application requires mitigation of significant volumetric expansion during electrochemical cycling. The electrolyte system adopts LiFSI to meet the high working voltage requirements of 4.6V or above. It forms a dense CEI/SEI film to suppress side reactions, resulting in a high-capacity retention rate of 85%. In fact, severe thermal runaway exothermic reactions are caused by the release of oxygen, therefore the influence of gas components on thermal runaway cannot be ignored. For example, using structural modification to coat the surface of NCM811 particles with graphene to suppress oxygen generation. In terms of battery cooling management systems, air cooling is a common and main heat dissipation method. Scholars have conducted extensive research on the geometric shape of cooling air channels, battery layout, and air flow paths. At present, the new PCM cooling system has the characteristics of high latent heat and thermal capacity and phase transition temperature within the battery working range and is expected to be further applied in the future.

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