

The Role and Influence of NCM622 Cathode Material in Lithium-Ion Batteries

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Abstract. Under the impetus of global energy transition and the "dual carbon" goals, the demand for lithium-ion batteries has surged. Cathode materials are the core determinant of their performance. Among nickel-cobalt-manganese oxide (NCM) ternary materials, NCM622 (with a Ni: Co: Mn ratio of 6: 2: 2) is widely applied due to its balanced advantages in energy density and safety. However, NCM622 faces challenges such as insufficient high-rate charge-discharge performance, long-term cycle capacity decay, and cost constraints of cobalt resources, which restrict its further application. Additionally, its performance stability under extreme temperature conditions (both high and low temperatures) is unsatisfactory, with capacity fading accelerating sharply in high-temperature environments and ion diffusion kinetics deteriorating noticeably in low-temperature conditions, further impairing its practical application value. This paper focuses on the impact mechanism of NCM622 on the performance of lithium-ion batteries, analyzes the correlation between its crystal structure, chemical composition and the energy density and safety of batteries, explores the ion diffusion kinetics and structural evolution laws, and elaborates on the performance optimization strategies and application prospects.

Keywords: NCM622 cathode material, Lithium-ion batteries, energy density, surface modification

1. Introduction

Driven by the global energy transition and the "dual carbon" goals, lithium-ion batteries have emerged as the core energy carriers for electric vehicles, energy storage systems, and consumer electronics, thanks to their high energy density (NCM622 can reach 191.3 mAh/g), long cycle life (with an 86.5% capacity retention rate after 1000 optimized cycles), and low self-discharge rate. In recent years, the global new energy vehicle market has witnessed explosive growth: in 2023, global electric vehicle sales exceeded 14 million units, and energy storage installed capacity surged by over 60% year-on-year. This rapid expansion has imposed stricter requirements on battery energy density (NCM622 reaches 650-700 Wh/kg) and safety. As a key core component determining the performance of lithium-ion batteries, every technological breakthrough in cathode materials directly influences the development of the entire battery industry [1]. Lithium nickel-cobalt-manganese oxide ($\text{LiNi}_x\text{Co}_y\text{Mn}_{1-x-y}\text{O}_2$, abbreviated as NCM) ternary materials occupy a pivotal position in the lithium-ion battery cathode material market due to their high energy density and excellent

comprehensive performance. Among them, NCM622 (with a Ni: Co: Mn ratio of 6: 2: 2), as a classic formulation in the ternary material system, boasts an outstanding balance between energy density and safety. Compared with low-nickel NCM523, NCM622 significantly enhances the specific capacity and energy density of batteries by increasing the nickel content. In contrast to high-nickel NCM811, its higher cobalt ratio endows the material with better structural stability and thermal safety. It is this superior performance balance that has enabled NCM622 to be widely applied in mid-to-high-end electric vehicles and energy storage systems, becoming a critical material driving the development of the new energy industry [2]. However, current research indicates that NCM622 faces several unresolved issues in practical applications. From existing studies, under high-rate charge-discharge conditions, its insufficient ion diffusion rate leads to degraded rate performance, limiting its use in scenarios requiring high-power output [3]; during long-term cycling, lattice distortion and cation mixing cause capacity fading, affecting the battery's service life [4]; additionally, the scarcity and price volatility of cobalt resources increase material production costs, hindering its industrial promotion [5]. Therefore, this paper focuses on NCM622 cathode materials. It first elaborates on their basic characteristics, such as crystal structure and chemical composition, analyzes their impact on the energy density and safety performance of lithium-ion batteries, then explores the underlying mechanisms affecting performance, including ion diffusion kinetics and structural evolution laws. Finally, combined with its application status and existing challenges, it proposes performance optimization strategies and outlines future development trends, aiming to provide references for further research and application of NCM622.

2. Basic characteristics of NCM622

2.1. Crystal structure characteristics

NCM622 features a typical layered α - NaFeO_2 structure, belonging to the hexagonal crystal system with space group R-3m. Oxygen atoms form a cubic close-packed (ccp) framework, while Li^+ and transition metals (Ni, Co, Mn) occupy octahedral interstitial sites in separate layers. This structure creates 2D lithium-ion diffusion channels between transition metal layers, enabling rapid Li^+ intercalation/deintercalation during charge-discharge—critical for efficient energy storage [6]. However, high-rate cycling or long-term use may cause structural distortion or collapse, blocking diffusion paths and degrading battery performance [7].

2.2. Chemical composition characteristics

NCM622 has a Ni:Co:Mn atomic ratio of 6:2:2, balancing performance comprehensively. Nickel, the core active component, enhances specific capacity via $\text{Ni}^{2+}/\text{Ni}^{3+}/\text{Ni}^{4+}$ redox reactions, though excessive Ni exacerbates cation mixing (Ni^{2+} occupying Li^+ sites), increasing diffusion barriers and reducing stability. Cobalt (Co^{3+}) inhibits $\text{Li}^+-\text{Ni}^{2+}$ disorder, strengthens structural integrity, and supplements capacity via $\text{Co}^{3+}/\text{Co}^{4+}$ redox, but its scarcity raises costs. Manganese (Mn^{4+}) lowers costs (abundant in Earth's crust) and reinforces the layered framework via stable coordination, improving thermal stability, though its low electrochemical activity limits capacity if overused [8].

2.3. Energy density improvement effect

Compared with the low-nickel system NCM523, NCM622 significantly improves the specific capacity of the material by increasing the proportion of nickel. Its theoretical specific capacity can reach 280 mAh/g, and the reversible capacity of actual mass-produced products exceeds 150 mAh/g,

while the actual capacity of NCM523 is usually limited to the range of 130-140 mAh/g. The improvement of specific capacity directly promotes the leap in battery energy density — the energy density of NCM622 batteries can reach 650-700 Wh/kg, which is significantly higher than that of NCM523 batteries (600-650 Wh/kg). Compared with the high-nickel system NCM811, although the latter has more advantages in theoretical specific capacity (270-280 mAh/g) and actual capacity (160-170 mAh/g), and its energy density can exceed 700 Wh/kg, NCM811 has a significant shortcoming in thermal stability [9]. By establishing an optimal balance between energy density and safety performance, NCM622 has been widely used in mid-to-high-end electric vehicles and energy storage systems: in vehicle scenarios, it can extend the driving range to meet users' travel needs; in energy storage scenarios, high energy density helps reduce the volume and floor area of battery packs and improve system integration efficiency [9].

2.4. Safety performance characteristics

Thermal stability is the core evaluation index of NCM622 safety performance. Thermal analysis tests show that the structural stability of NCM622 at high temperatures is better than that of high-nickel NCM811, and its thermal decomposition initiation temperature is higher, which can delay the triggering of thermal runaway chain reactions. For example, NCM622 can still maintain relatively stable thermal decomposition behavior in the charged state of 4.4 V [10]. The critical conditions for thermal runaway depend on the crystal structure integrity, chemical composition uniformity of the material, and the working environment of the battery (such as temperature, charge-discharge rate). Under abnormal working conditions such as high-rate charge-discharge or internal short circuit, the temperature of the battery system rises sharply. When it reaches the critical threshold of thermal runaway, it will trigger a violent exothermic reaction, leading to fire or even explosion. The appropriate amount of cobalt in NCM622 can enhance the rigidity of the layered structure, inhibit structural collapse and oxygen release during cycling, thereby delaying the thermal runaway process and providing a buffer window for safety protection. In practical applications, combined with the real-time monitoring and regulation of parameters such as temperature and voltage by the intelligent battery management system (BMS), the safe working range of NCM622 batteries can be further expanded.

3. Application status, challenges, optimization strategies and development trends

3.1. Research status and challenges

3.1.1. Ion diffusion kinetics

Lithium ions have a specific diffusion path in the layered structure of NCM622. During charge and discharge, lithium ions deintercalate or intercalate from the interlayers of the cathode material. When the battery is charged, lithium ions deintercalate from the lithium layer between the transition metal layers, pass through the electrolyte, cross the separator, and intercalate into the anode material; the opposite happens during discharge. The diffusion of lithium ions in the layered structure mainly occurs along the interlayer channels, and its diffusion rate directly affects the rate performance of the battery. Under high-rate charge-discharge conditions, if the lithium-ion diffusion rate is insufficient, it will lead to intensified battery polarization, a significant drop in battery voltage, and insufficient capacity release, thereby reducing the rate performance. Factors affecting the lithium-ion diffusion rate include the crystal structure integrity of the material, particle size, and the properties

of the electrolyte. NCM622 materials with complete crystal structure and small particle size are conducive to the rapid diffusion of lithium ions. A suitable electrolyte can reduce the resistance of lithium-ion migration, improve ionic conductivity, and thus promote the transport of lithium ions between the positive and negative electrodes.

3.1.2. Structural evolution laws

During cycling, NCM622 will undergo lattice distortion and layered structure degradation. With the increase in the number of charge-discharge cycles, the repeated intercalation and deintercalation of lithium ions will cause changes in the lattice parameters of the material, leading to lattice distortion. When the nickel content is high, the problem of cation mixing intensifies, further damaging the crystal structure of the material. Lattice distortion and cation mixing will block the lithium-ion diffusion channels, making it difficult for lithium ions to intercalate and deintercalate, thus leading to battery capacity decay. This structural evolution phenomenon is more significant in high-temperature environments. High temperature will accelerate the chemical reactions inside the material, worsen the problems of lattice distortion and cation mixing, and seriously affect the cycle life and performance stability of the battery. To inhibit structural evolution, it is necessary to improve the structural stability of the material by optimizing the material preparation process, performing element doping or surface modification, etc. With its excellent comprehensive performance, NCM622 has been applied on a large scale in fields such as mid-to-high-end electric vehicles and energy storage systems. In the field of electric vehicles, mainstream car companies such as Tesla (some models) and BYD (high-end series) use NCM622 batteries as the core power source. Relying on its high energy density, the vehicle's driving range has been significantly increased, effectively solving users' core demands for the practicality of electric vehicle range. In the field of energy storage, NCM622 batteries are widely used in grid-level energy storage and distributed energy storage scenarios: in grid energy storage, they can realize valley electricity storage and peak release, playing a role in smoothing load fluctuations and stabilizing grid voltage; in distributed energy systems, by storing electricity from intermittent renewable energy sources such as solar and wind energy, they significantly improve the new energy absorption rate and energy utilization efficiency.

3.2. Technical bottlenecks and limitations

Although NCM622 has significant advantages, its practical application still faces multiple technical bottlenecks: under high-rate charge-discharge conditions, limited by lithium ion bulk diffusion kinetics and interface transport resistance, the material's rate performance is insufficient, making it difficult to meet the needs of high-power output in electric tools, ultra-fast charging electric vehicles, etc.; during long-term cycles, lattice distortion and cation mixing (Ni^{2+} occupying Li^+ sites) caused by transition metal ion migration continue to intensify, leading to an acceleration in capacity decay rate, a shortening of battery cycle life, and indirectly increasing the full-life cycle cost. In addition, the constraint of cobalt resources constitutes a key limiting factor. As a necessary component of NCM622, cobalt has a highly concentrated global reserve distribution (the Democratic Republic of the Congo accounts for more than 70%), resulting in poor supply chain stability; and the sharp fluctuation of cobalt prices (annual volatility often exceeds 30%) further increases the difficulty of material cost control, weakening the market competitiveness of NCM622.

3.3. Performance optimization schemes (element doping and surface modification technologies)

Surface modification technology, by constructing a uniform and dense protective layer on the surface of NCM622 particles, can not only block the direct contact between the active material and the electrolyte to inhibit side reactions but also maintain efficient lithium-ion transport channels. It is a key means to improve the material's cycle stability, thermal safety, and high-voltage tolerance. At present, a diversified system of surface modification technologies for NCM622 has been formed, among which Al_2O_3 , Li_3PO_4 , ZrO_2 coating, and new composite coating technologies are the most widely used. Their mechanisms and optimization effects are as follows.

3.3.1. Li_3PO_4 coating

The "functional buffer layer" with high ionic conductivity - Li_3PO_4 coating technology is realized through solid-state reaction: NCM622 and lithium phosphate powder are mixed in a mass ratio of 95:5, and calcined at 700-800°C for 4-6 hours under argon protection, so that Li_3PO_4 can uniformly diffuse and deposit on the particle surface, forming a coating layer with a thickness of about 10-15 nm [11]. Compared with Al_2O_3 , the outstanding advantage of Li_3PO_4 is its high lithium-ion conductivity (up to 10^{-6} S/cm at room temperature), which not only does not hinder lithium-ion transport but also promotes interface ion migration. Its mechanism focuses on improving stability in high-voltage and high-temperature scenarios: during charge and discharge at high voltage (such as 4.4 V), NCM622 is prone to structural collapse and release of active oxygen due to excessive delithiation, while the chemical inertness of Li_3PO_4 can effectively capture free oxygen and inhibit the violent reaction between oxygen and electrolyte (the exothermic peak is reduced by 25%); at the same time, the reaction products of Li_3PO_4 and electrolyte can form a stable interface phase, reducing the migration and deposition of transition metal ions. Experimental data show that after 200 cycles at 4.4 V high voltage, the capacity retention rate of NCM622 batteries coated with Li_3PO_4 increases from 75% to 85%, and the initial temperature of thermal runaway increases from 210°C to 240°C, significantly enhancing the safety under high voltage [11]. In addition, in the low-temperature environment of -20°C, its discharge capacity retention rate is 12% higher than that of unmodified materials, showing the optimization effect on wide-temperature performance.

3.3.2. ZrO_2 coating

The "structural stabilizer" under high rate - ZrO_2 coating is prepared by the sol-gel method: zirconium oxychloride is used as the precursor, mixed with citric acid in a ratio of 1:2 to form a sol, NCM622 particles are immersed in the sol, dried, and calcined at 600 °C for 3 hours to form a tetragonal ZrO_2 coating layer with a thickness of 8-12 nm [12]. The high mechanical strength and chemical stability of ZrO_2 make it an ideal protective layer for high-rate scenarios. During high-rate charge-discharge such as 10C, NCM622 particles are prone to large stress due to the rapid intercalation/deintercalation of lithium ions, leading to the transformation of the layered structure to spinel or rock salt phase (i.e., "structural collapse"). The ZrO_2 coating layer can relieve the internal stress of particles through physical constraint, inhibiting structural phase transformation: X-ray diffraction (XRD) analysis shows that after 500 cycles at 10C, the intensity attenuation rate of the layered structure characteristic peak (003) of NCM622 modified with ZrO_2 decreases from 35% to 15%, indicating that the structural integrity is effectively maintained [12]. Performance tests show that its discharge capacity at 10C rate increases from 60% of the theoretical capacity to 75%, and the

rate performance decay rate after 500 cycles decreases by 20%. At the same time, the impedance growth amplitude during high-temperature (60 °C) cycling decreases by 30%, fully demonstrating the synergistic optimization effect of ZrO₂ coating on high-rate and high-temperature stability.

3.3.3. Al₂O₃ coating

The "physical barrier" for inhibiting transition metal dissolution - Al₂O₃, as an oxide with excellent chemical stability and low ion transport resistance, is a classic choice for surface modification of NCM622. Its coating process mainly adopts the liquid-phase deposition method: using aluminum nitrate as the precursor, NCM622 particles are dispersed in a mixed solution of ethanol and deionized water, and the pH value is adjusted to 8-9 to hydrolyze aluminum ions to form aluminum hydroxide colloid, which is uniformly adsorbed on the particle surface, and then calcined at 500-600 °C for 2-3 hours to transform into a γ -Al₂O₃ film with a thickness of 5-10 nm. The choice of this thickness has dual advantages: too thin cannot form a complete protective layer, too thick will significantly increase the lithium-ion diffusion resistance, while the 5-10 nm film can not only completely cover the surface defects of particles but also provide a transport channel for lithium ions through the microporous structure in the film. Its core mechanism is reflected in two aspects: first, the physical barrier effect, the Al₂O₃ film can effectively block the direct reaction between HF (produced by electrolyte decomposition) in the electrolyte and NCM622. Research data show that the dissolution amount of transition metals (Ni, Co, Mn) in unmodified NCM622 during cycling can reach 5-8 ppm, while that after Al₂O₃ coating drops to below 2 ppm, a reduction of more than 60% [13]; second, the improvement of interface stability, the coating layer can induce the formation of a more stable solid electrolyte interface (SEI) film, avoiding the continuous decomposition and consumption of the electrolyte. Actual performance tests show that after 1000 cycles at 25 °C, the capacity retention rate of NCM622 batteries coated with Al₂O₃ increases from 82% to 88%, and after 500 cycles at 45 °C high temperatures, the capacity retention rate increases from 70% to 80%, and the impedance growth rate decreases by 40%, fully verifying its optimization effect on cycle stability [13].

3.3.4. Composite coating

Technology A single coating layer is often difficult to meet multiple performance requirements, so composite coating technology has gradually become a research hotspot. For example, Al₂O₃-Li₃PO₄ composite coating is prepared by a two-step method: first, liquid-phase deposition of Al₂O₃ (inner layer, thickness 3-5 nm), then solid-state coating of Li₃PO₄ (outer layer, thickness 5-8 nm), combining the physical barrier ability of Al₂O₃ and the ion conduction advantage of Li₃PO₄ [14]. Test results show that the capacity retention rate of the NCM622 battery with this composite coating is still 82% after 1500 cycles at 25 °C (only 65% for unmodified materials), the discharge capacity at 5C rate increases by 18%, and the thermal decomposition temperature increases by 25 °C, achieving synchronous improvement in cycle stability, rate performance, and thermal safety. Another type of composite coating is the ZrO₂-LiAlO₂ system, which utilizes the structural stability of ZrO₂ and the high ionic conductivity of LiAlO₂, and can maintain excellent performance in the wide temperature range of -30 °C to 60 °C. Its low-temperature (-30 °C) discharge capacity retention rate is 10% higher than that of single ZrO₂ coating, providing the possibility for application in extreme environments.

4. Conclusions

This paper systematically investigates the impact of NCM622 cathode material on the performance of lithium-ion batteries. The results demonstrate that NCM622, with a nickel-cobalt-manganese ratio of 6:2:2, achieves an excellent balance between energy density (650-700 Wh/kg) and safety. Its layered crystal structure provides efficient channels for lithium-ion diffusion, while the synergistic effect of nickel, cobalt, and manganese ensures the comprehensive performance of the material. However, insufficient ion diffusion kinetics at high rates, structural evolution during long-term cycling (such as lattice distortion and cation mixing), and constraints from cobalt resources remain core bottlenecks restricting its application. To address these issues, technologies such as element doping (e.g., Al^{3+} , Mg^{2+}) and surface modification (e.g., Al_2O_3 , Li_3PO_4 coating) have shown significant optimization effects, which can effectively improve cycle stability and thermal safety. Future research should focus on low-cobalt/cobalt-free modification to reduce costs, develop new electrolytes to enhance ion transport efficiency, and integrate intelligent battery management systems to expand application scenarios. With continuous technological breakthroughs, NCM622 is expected to continue playing a key role in mid-to-high-end electric vehicles, large-scale energy storage, and other fields, providing important support for the sustainable development of the new energy industry.

References

- [1] Wang C G, Liu G L, Jin X R, et al. (2023) Research Progress on Cathode Materials for Lithium-Ion Batteries [J]. Contemporary Chemical Research, 9: 12-14.
- [2] Wang E T, Yang L F. (2022) Preparation and Performance of High Specific Capacity Lithium-Ion Battery Cathode Material $\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$ [J]. Chinese Journal of Applied Chemistry, 39(8): 1209-1215.
- [3] Yang G B. (2024) Grain Boundary Modification and Electrochemical Performance of Ternary Cathode Materials [D]. Harbin Institute of Technology.
- [4] Li C L. (2024) Research on Doping and Surface Modification of Ternary Layered Cathode Material $\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$ [D]. Donghua University.
- [5] Liu J L. (2024) Research on Modification and Mechanism of Lithium-Ion Battery Cathode Materials [D]. Nanjing University of Science and Technology.
- [6] Li H Y. (2023) Research on Kinetics and Coating Modification of High-Nickel Ternary Cathode Material (NCM) [D]. Harbin Institute of Technology.
- [7] Yang P. (2021) Structural Design and Performance Analysis of Lithium Nickel Cobalt Manganese Oxide (NCM622) Cathode Material [D]. Guilin University of Electronic Technology.
- [8] Li K, Huang R, Cong J, et al. (2025) Synchronous Evolution of Structural Morphology and Lithium Storage Characteristics of NCM622 Cathode Material [J]. CIESC Journal, 76(4): 1831-1840.
- [9] Yang M P. (2019) Development and Industrialization of High-Performance Lithium Nickel Cobalt Manganese Oxide (NCM622) Products [R]. Hefei Guoxuan High-Tech Power Energy Co., Ltd.
- [10] Du J Q. (2023) Experimental and Theoretical Research on Thermal Stability of Nickel-Rich Ternary Cathode Thin Films [D]. Xiangtan University.
- [11] Li Y Y. (2023) Research on Modification, Structural Design and Electrochemical Performance of High-Nickel Ternary Cathode Materials [D]. Nanjing University of Science and Technology.
- [12] Wen T, Li X C, Fan J P, et al. (2025) Research Progress on Doping Modification of Ternary Cathode Materials for High-Nickel Lithium-Ion Batteries [J]. Journal of Petrochemical Universities, 38(3): 20-31.
- [13] Cheng Z, Chen S Y, Li X S, et al. (2024) Research on Al_2O_3 Coating Modification of Ternary Cathode Material $\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$ Precursor [J]. Guangzhou Chemical Industry, 52(09): 23-27.
- [14] Pan Y B. (2021) Interface Modification of NCM/CNTs Composite Cathode and Its Application in Lithium Metal Batteries [D]. Huazhong University of Science and Technology.