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Defects and Solutions of Lithium-Ion Battery Cathode Materials

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Abstract. This paper systematically reviews the multi-scale defects and their evolution mechanisms of mainstream cathode materials, including layered oxides, spinel oxides, and phosphates. These materials commonly suffer from bulk lattice distortion, cation mixing, stacking faults, uneven micro-particles, agglomeration, surface microcracks, and lattice reconstruction, which are key factors affecting their performance. Such defects significantly hinder lithium-ion transport, aggravate side reactions with the electrolyte, accelerate transition metal dissolution, and induce oxygen evolution under high voltage, eventually leading to obvious capacity fading, shortened cycle life, and increased safety risks of batteries. To address these defects, coating, elemental doping, particle morphology regulation, and in-situ film formation modification can effectively stabilize interfaces, optimize material structures, improve ion transport efficiency, and suppress side reactions, forming a systematic modification scheme. Future research should focus on multi-scale collaborative modification, clarify atomic-level mechanisms of defects and modifications, develop low-cost and feasible processes, and provide strong support for high-performance energy storage applications.

Keywords: lithium-ion battery, cathode material, defect, modification strategy

1. Introduction

Lithium-ion batteries are key energy storage devices widely used in many fields. Cathode materials determine battery performance but suffer from defects like lattice issues, agglomeration and poor stability, limiting battery performance.

From the perspective of microstructure, lattice structural defects are one of the most common issues, mainly including lattice misalignment, vacancy defects, and grain boundary distortion. Taking layered cathode materials as an example, repeated deintercalation of lithium ions during long-term charge-discharge cycles causes irreversible changes in lattice interlayer spacing, thereby triggering lattice collapse and damaging the integrity of the material's crystal structure [1]. Spinel $LiMn_2O_4$ is prone to lattice distortion due to the Jahn-Teller effect of Mn^{3+}, leading to reduced electrical conductivity of the material [2].

Surface defects also exert a significant impact on battery performance. The surfaces of cathode material particles often contain unsaturated bonds, hydroxyl groups, and microcracks. These defects intensify interfacial side reactions between the material and the electrolyte, forming an unstable

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solid electrolyte interphase film, which not only consumes active lithium ions but may also induce electrolyte decomposition and gas generation, resulting in battery swelling and failure [3].

At the macroscopic morphology level, nano-scale or micro-scale cathode materials tend to agglomerate severely during electrode preparation due to their large specific surface area and high surface energy [4], forming large secondary particles that block internal pore structures, hinder lithium-ion transport channels, and reduce ion diffusion rates. Meanwhile, it causes uneven current distribution inside the electrode, excessively high current density in local areas, and accelerates material aging. In addition, some high-capacity cathode materials also suffer from poor chemical stability. This paper analyzes the mechanisms of doping [5], particle morphology regulation [6], and in-situ film formation modification [7] in improving lithium-ion cathode materials.

These interrelated defects cause capacity fade, short cycle life and safety risks, limiting high-performance battery use. This work analyzes cathode defects and modification methods, supporting material design and safer, higher-performance battery development.

2. Main defects of lithium-ion cathode materials

During the entire life cycle from material synthesis, electrode preparation to electrochemical cycling, cathode materials inevitably generate various defects, mainly including five categories: lattice structural defects, particle inhomogeneity, surface defects, agglomeration, and poor chemical stability. These defects interact and reinforce each other, jointly restricting the energy density, cycle life, and safety performance of batteries.

2.1. Lattice structural defects

Lattice structural defects are the core issues affecting the bulk properties of materials, mainly including cation mixing, lattice vacancies, dislocations, stacking faults, etc. During high-temperature synthesis, site exchange between transition metal ions and lithium ions forms cation mixing, which directly blocks lithium-ion migration channels and leads to initial capacity loss and increased polarization. Excessive lattice vacancies, dislocations, and other defects damage the long-term stability of the crystal structure, induce irreversible phase transitions during cycling, and cause voltage decay and continuous capacity decline.

Research by Professor Mu Shichun's team points out that stacking faults disrupt the interlayer diffusion path of lithium ions, forcing lithium ions to diffuse via a high-energy-barrier mode and significantly reducing the rate performance of lithium-rich layered oxide cathodes. Therefore, precise regulation of crystallographic defects such as stacking faults is crucial for improving the rate performance of lithium-rich materials [8]. Mainstream cathode materials including layered oxides, spinel oxides, and phosphates all exhibit varying degrees of lattice defects, becoming the key bottleneck limiting the intrinsic performance of materials.

2.2. Particle inhomogeneity

Particle inhomogeneity arises from uncontrolled synthesis, showing uneven size, morphology and compactness. It causes inconsistent Li-ion kinetics, local over-deintercalation, particle cracking and side reactions, harming electrode quality.

Aashutosh Mistry's team, through laboratory CT combined with electrochemical diffusion calculations, proved that non-spherical particles destroy the symmetry of lithium-ion intercalation, and the more irregular the particle shape, the more significant the intercalation inhomogeneity,

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directly affecting battery cycle stability [9]. Therefore, achieving uniform regulation of particle size and morphology is an important approach to improving the electrochemical performance of cathode materials.

2.3. Surface defects

Surface defects are the frontier sites for interfacial interactions between cathode materials and electrolytes, directly determining interfacial stability and battery life. They mainly include surface lattice reconstruction, microcracks, step sites, residual impurities, etc. Materials are prone to surface reconstruction during cycling, forming an electrochemically inert rock-salt phase reconstruction layer. Although this layer temporarily suppresses bulk degradation, it significantly increases interfacial impedance. Meanwhile, highly active sites such as surface microcracks and steps catalyze the oxidative decomposition of the electrolyte, forming an unstable and overly thick cathode electrolyte interphase film, which continuously consumes active lithium, increases internal resistance, and induces transition metal ion dissolution.

The dissolved transition metal ions migrate to the anode and damage the anode solid electrolyte interphase film, further exacerbating battery performance degradation. Research on lithium-rich cathode oxides by Wei Jiang et al. reveals that surface defects and bulk defects have different effects on anionic redox kinetics: surface defects can accelerate lithium-ion diffusion and enhance cationic redox activity; bulk defects inhibit lithium-ion migration and reduce cationic redox efficiency; both promote oxygen redox reactions, providing a new perspective for regulating anionic redox in lithium-rich cathodes [10].

2.4. Agglomeration

Agglomeration is the most prominent morphological problem of nano-scale cathode materials. To improve rate performance, cathodes are often designed at the nano-scale, but nano-particles tend to agglomerate severely during electrode preparation processes such as drying, slurry mixing, and coating due to high surface energy. Severe agglomeration not only reduces the tap density of materials and impairs the volumetric energy density of batteries but also causes uneven distribution of active materials inside the electrode, hinders full infiltration of the electrolyte, renders internal particles of agglomerates unable to effectively participate in electrochemical reactions, and drastically reduces active material utilization.

Research on high-nickel cathode slurries by Jeong's team found that under low-speed stirring conditions, conductive nano-particles form spherical agglomerates of tens of microns, leading to drastic changes in slurry rheological properties, affecting electrode coating quality, and ultimately degrading the electrochemical performance of batteries [11]. Therefore, inhibiting particle agglomeration and achieving uniform particle dispersion are key to improving the application effect of nano-cathode materials.

2.5. Poor chemical stability

Poor chemical stability is a comprehensive manifestation of the combined effect of various defects and a core challenge faced by high-voltage and high-capacity cathodes. Many high-capacity cathode materials are prone to lattice structure instability under high-voltage conditions, facing risks such as oxygen evolution and transition metal valence change, triggering capacity fading and safety hazards. Meanwhile, highly active redox couples on the material surface are thermodynamically incompatible

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with the electrolyte, and continuous interfacial side reactions accelerate structural degradation and performance recession.

Research by Errui's team confirms that $LiCoO_2$ cathodes suffer from bulk and surface structural transformation, oxygen release, and intensified interfacial side reactions at 4.6 V high voltage, with rapid decline in chemical stability, severely limiting its high-voltage application [12]. Systems such as high-nickel layered oxides and lithium-rich manganese-based materials also generally suffer from insufficient stability under high voltage, becoming a key bottleneck restricting the development of high-energy-density lithium-ion batteries.

3. Solutions to material defects

To address various defects of cathode materials, four core modification technologies have been formed: coating, elemental doping, particle morphology regulation, and in-situ film formation modification. These technologies systematically solve material defects and improve the comprehensive performance of cathodes through mechanisms such as interfacial stabilization, structural optimization, ion transport improvement, and side reaction suppression.

3.1. Coating

Surface coating technology constructs a functional nano-protective layer on the surface of cathode particles, serving as an effective means to physically isolate the electrolyte, stabilize the crystal structure, and optimize ion or electron transport. It is a mainstream method to solve surface defects, poor chemical stability, transition metal dissolution, and other problems.

Umair's team proposed the coating layer thickness threshold theory, with the optimal thickness usually controlled at 2–10 nm. An overly thin layer fails to provide effective protection, while an overly thick layer hinders lithium-ion diffusion, providing important guidance for coating design [13].

Conductive material coatings (carbon materials, conductive polymers) mainly improve electronic conductivity.To address the insufficient electronic and ionic conductivity of Li-rich $LiFePO_4$ (Li-rich LFP), Shin Park's team compared two carbon coating processes: introducing a carbon precursor before crystal structure formation (C/BLF) and additional calcination coating after structure formation (C/ALF). The study found that the sample prepared by the C/ALF process formed a denser carbon coating layer and constructed a continuous electron transport network. Figure 1(a) shows the charge–discharge curves measured at 0.1 C in the voltage range of 2.5–3.7 V. Figure 1(b) presents the cycle performance at 1 C. After 100 cycles at 1 C, the reversible capacity of the C/BLF electrode is 124.25 $mA \cdot g^{-1}$, while that of the C/ALF electrode reaches a significantly high 134.13 $mA \cdot g^{-1}$, approximately 7% higher than C/BLF [14].

For high-capacity systems such as lithium-rich layered oxides, Yanying Liu's team used $LiCeO_2$ surface functionalization to coat $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$ lithium-rich cathodes.The experimental results shown in Figure 1(c) indicate that the sample with 3% coating amount achieves 86.3% capacity retention after 200 cycles at 5C high rate, with voltage decay only half that of the uncoated sample, revealing the atomic-level pathway of the coating layer inhibiting lattice oxygen migration [15].

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3.2. Doping

Elemental doping introduces heterovalent or isovalent doping ions to regulate the crystal structure, electronic structure, and ion transport properties of materials. It is a core means to fundamentally solve bulk lattice defects such as cation mixing, lattice distortion, oxygen vacancies, and anti-site defects, and can significantly improve the structural stability and intrinsic conductivity of materials.

$LiFePO_4$ (LFP) suffers from low electronic and ionic conductivity and is prone to cation anti-site defects.Xiao Yunhao's team synthesized LFP materials with various aluminum doping concentrations via solid-state reaction. A 1% Al doping content reduced the material defect density from 2.04% to 1.67% and simultaneously increased the lithium-ion diffusion coefficient. The doped sample delivered a discharge capacity of 155.6 $mA \cdot g^{-1}$ at 0.1 C.As shown in Figure 1(d), its specific capacity at a high rate of 5 C was 8 $mA \cdot g^{-1}$ higher than that of the undoped material. This study suggests that reducing anti-site defects through low-level aluminum doping can help improve the electrochemical properties of LFP cathodes, providing a new strategy for enhancing lithium-ion battery performance and managing aluminum impurities during battery recycling [16].

$LiCoO_2$ is prone to irreversible phase transitions, transition metal dissolution, and severe interfacial side reactions under high voltage. Chengjun's team developed highly Al-doped $LiCoO_2$. Pouch cells achieve 95.5% capacity retention after 500 cycles at 4.5 V charging voltage, 79.0% retention after 500 cycles at 4.55 V high voltage, and Figure 1(e) shows that 87.3% retention after 500 cycles at 45 ℃ with optimized electrolyte, supporting the development of high-voltage long-cycle $LiCoO_2$ cathodes [17].

Li_2MnSiO_4 is highly prone to Li-Mn cation anti-site defects with significant anisotropic lithium-ion transport. Kuganathan confirmed via atomic modeling that Al^{3+} doping at Si sites is energetically feasible, increases material lithium content, and improves anisotropic lithium-ion migration, providing an atomic-level scheme for Li_2MnSiO_4 defect regulation [18]. Lee's team proposed a dual doping strategy of aluminum ions and niobium ions—aluminum ions enhance structural stability, and niobium ions optimize primary particle morphology. As shown in Figure 1(f), The prepared high-nickel cathode material achieves 95.6% capacity retention after 500 cycles and 88.3% retention after 1000 cycles, showing excellent long-cycle performance [19].

3.3. Particle morphology regulation

Particle morphology regulation optimizes nucleation, growth, and assembly processes to achieve uniform particle size, regular morphology, and dense structure, solving problems such as particle inhomogeneity, agglomeration, and poor electrolyte infiltration. It is an effective strategy to improve the electrochemical performance of cathode materials.

Hoda Ahmed et al. proposed a synthesis strategy to enhance nucleation and inhibit particle growth and aggregation, applicable to disordered rock-salt oxide systems. Taking $Li_{1.2}Mn_{0.4}Ti_{0.4}O_2$ as an example, this method prepares uniform highly crystalline particles smaller than 200 nm. Figure 2(a) shows the electrode achieves 85% capacity retention after 100 cycles, with an average discharge voltage loss of 4.8 mV per cycle, far superior to samples prepared by traditional crushing processes [20].

Junjie Chen's team compared spray-dried porous $LiMn_{0.6}Fe_{0.4}PO_4$ microspheres with sol-gel samples. The former is assembled from nano-primary particles with better electrolyte permeability and lithium-ion diffusion kinetics.As shown in Figure 2(b) and (c), uniform Mn/Fe distribution suppresses the Jahn-Teller effect and Mn dissolution, achieving 91.9% capacity retention after 400

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cycles at 2C and 90.6% retention after 600 cycles at 5C, significantly superior to control samples [21].

Hai-Yan's team real-time tracked the morphology evolution of high-nickel precursors, revealed the three-stage growth behavior of secondary particles, clarified the regulatory effects of reactant concentration and feeding rate on particle morphology. By controlling reaction conditions in the intermediate stage, particle coarsening is inhibited, preparing uniform secondary particles with ordered internal structure [22]. Lei Yu et al. found that the main failure of single-crystal cobalt-free cathodes stems from anti-site defects and dislocations. Morphology-lattice dual regulation via size homogenization and preferred crystal orientation effectively suppresses structural degradation and voltage decay [23].

Polycrystalline high-nickel layered oxide particles are prone to microcracks during cycling due to numerous grain boundaries, while single-crystal particles have fewer grain boundaries and more stable structures. Xiaozheng et al. converted polycrystalline high-nickel cathodes into sub-micron pseudo-single-crystal particles via ball milling, effectively inhibiting H2-H3 phase transitions and microcrack formation, providing a simple and efficient preparation strategy for long-life cathodes [24].

3.4. In-situ film formation modification

In-situ film formation modification generates a stable and dense protective interfacial film directly on the cathode surface via electrolyte additives or surface in-situ reactions, eliminating the need for additional preparation processes and enabling interfacial modification within the battery system. It is an efficient and convenient method to solve surface defects and interfacial side reactions.

Zhiyuan Lin's team used 2,2,3,4,4,4-hexafluorobutyl methacrylate (HFBM) as an electrolyte additive to construct a polymer coating via in-situ self-polymerization(as shown in Figure 2(d)), effectively suppressing irreversible side reactions. Figure 2(e) shows that Li||$LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ batteries achieve 80% capacity retention after 100 cycles at 1C [25]. Shiping Ma's team in-situ constructed a LiF modified layer on $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ surface via wet chemical method. Figure 2(f) illustrates the preparation process of LNMC811@LiF. The LiF coating protects particle integrity, resists HF corrosion, and promotes lithium-ion diffusion, achieving 90% capacity retention after 100 cycles at 1C and 75% retention after 100 cycles at 2C, much higher than the 52% of the bare sample [26].

Wenzhi Wang et al. successfully modified the surface of single-crystal $LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$ (SC-NCM) via an optimized strategy combining acid treatment and titanium dioxide (TiO_2) coating. This approach can simultaneously remove residual surface contaminants and stabilize the overall structure. Furthermore, even after long-term cycling, the TiO_2 surface coating effectively alleviates internal cracking, phase transitions, and the evolution of the bulk structure. As a cathode material for lithium-ion batteries, as shown in Figure 2(g), the optimized SC-NCM maintains a capacity retention of 87.4% at 1 C over 200 cycles at room temperature, which is higher than that of the pristine SC-NCM (73.5%) [27]. Jiaxiong Wu's team prepared aqueous LFP thin-film cathodes via radio-frequency magnetron sputtering, with in-situ formed interfacial films stabilizing particle structure and alleviating volume effects, significantly improving the cycle stability and capacity retention of LFP in aqueous electrolytes [28].

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Table 1. Summary of cathode material defect modification methods and performance

Method	Material	Rate or Current Density	Cycle Performance	References
Coating	Lithium-rich manganese-based, $LiCeO_2$ coated	5C	200 cycles@84.3%–86.3%	[15]
Doping	Uniform Al-doped $LiCoO_2$	1C	500 cycles@95.5%	[17]
Doping	Al and Nb-doped $Li[Ni_{0.92}Co_{0.04}Mn_{0.04}]O_2$	0.1C	1000 cycles@88.3%	[19]
Particle morphology regulation	Disordered rock-salttype	5C	100 cycles@85%	[20]
Particle morphology regulation	$LiMn_xFe_{1-x}PO_4$	2C	400 cycles@91.9%	[21]
Particle morphology regulation	$LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$	1C	100 cycles@79%	[22]
Particle morphology regulation	$LiNi_xCoyMn_{1-x-}yO_2$	$100mA \cdot g^{-1}$	200 cycles@82.5%	[24]
In-situ film formation modification	$Li\|\|LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$battery	1C	100cycles@80%	[25]
In-situ film formation modification	$LiNi_xCo_yMn_{1-x-y}O_2$	1C	100 cycles@90%	[26]
In-situ film formation modification	$LiNi_{0.6}Co_{0.2}Mn_{0.2}O_2$	1C	200 cycles@87.4%	[27]

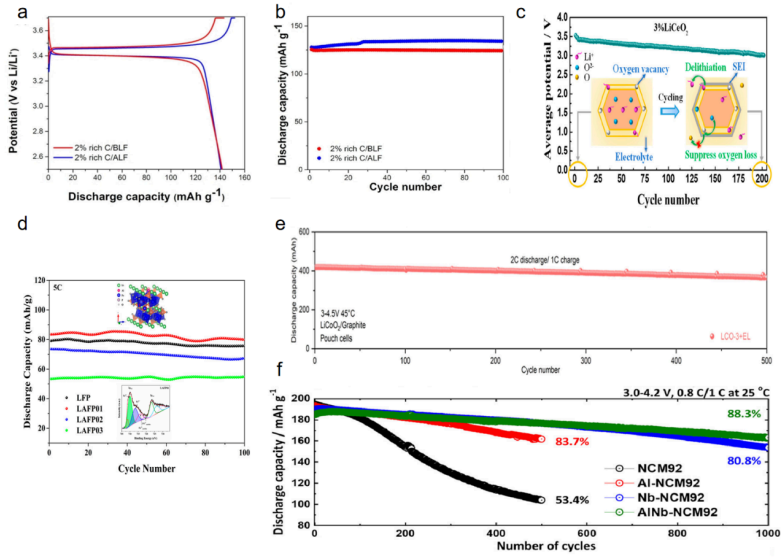

Figure 1. (a) Initial cycle. (b) Cycle performance of C/BLF and C/ALF samples at 1 C. (c) Cycle performance of 3% $LiCeO_2$-coated $Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O_2$. (d) Cycle performance curve. (e) Cycle stability of LCO-3 pouch cell with optimized electrolyte at 45 °C. (f) Long-term cycle performance of pouch full cell with graphite anode, charge at 0.8C, discharge at 1C (25 °C)

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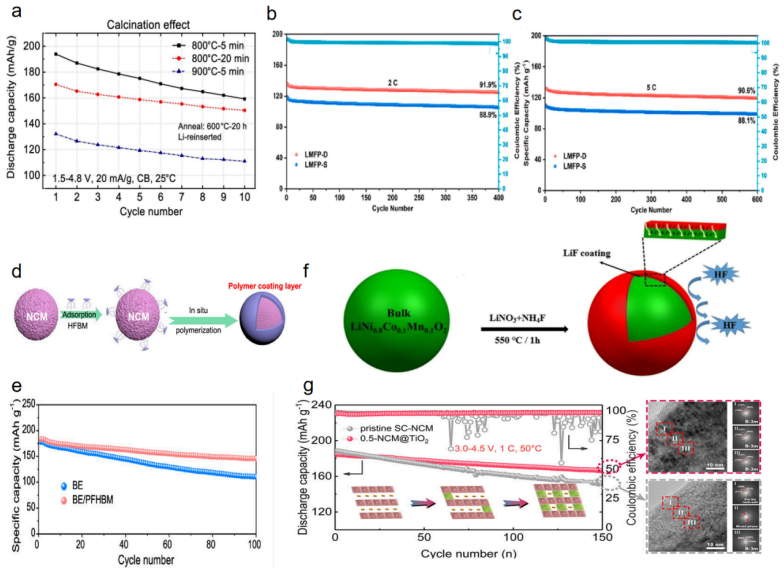

Figure 2. (a) Capacity retention of NM-LMTO at different initial calcination temperatures and times (1.5–4.8 V, 20 mA·g^{-1}). All samples were annealed (600 °C, 20 h) and washed with DIW, followed by a relithiation step. (b) Long-term cycling performance of LMFP-D and LMFP-S at 2C. (c)Long-term cycling performance of LMFP-D and LMFP-S at 5C. (d) Schematic of PCL formed by in-situ self-polymerization on the cathode surface. (e) Comparison of cycle performance with/without HFBM as electrolyte additive. (f) Schematic of modified LNMC811 manufacturing. (g) Cycle performance comparison between optimized SC-NCM and pristine SC-NCM

4. Conclusion

This paper systematically identifies five core defects of lithium-ion battery cathode materials, which synergistically cause capacity fading, short cycle life, and safety hazards, restricting high-energy-density battery development. Four modification strategies including coating, doping, morphology regulation and in-situ film formation can serve as effective optimization solutions. Although lab results are promising, cost, process, and mechanism issues limit large-scale use. Future research should focus on multi-scale modification, atomic-level mechanism analysis, and low-cost scalable processes to upgrade cathode materials and support the new energy industry.

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