# Failure Mechanism and Safety Optimization of Lithium-Ion Batteries

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**Abstract.** This work investigates the failure events and safety improvement of lithium-ion batteries as one important clean energy product with clear safety issues. It also sums up the failure ways of the four main parts: cathode structural phase change and low thermal stability, lithium dendrite growth and worsening of lithium anode SEI film, chemical breakdown and hydrolysis of electrolytes, and thermal shrinkage and physical harm of separators. The mix of outside abuse, making flaws, and cycle aging makes battery failure worse and can even cause thermal runaway. For each part, control steps are given, as well as control steps together, such as material and structural improvement, standard use and care, and recycling and reuse. Like the paper does, this one also points out research gaps (e.g., not clearly linked failure ways involving many factors). Future studies should have multi-scale studies and full-life cycle tests, the real-world use of high-performance materials, and the setting up of a full-life cycle safety system, to make sure the safe and steady use of Li-ion batteries.

## 1 Introduction

The clean energy change, pushed by worldwide needs like dealing with climate change and cutting down on use of fossil fuels, puts battery tech, shown by lithium-ion batteries (LIBs), as a key part. LIBs work in electric cars, battery energy storage, power plants, and portable electronic gadgets, making a basic base of the modern green energy setup. But, with the wide use of lithium-ion batteries, their safety problems have become clearer. Events like battery fire accidents in marine transportation have shown the bad results of battery breakdown on people, property, and the environment [1]. To get better specific energy and faster charging speed, finding a middle ground between performance and safety is a hard job. So, knowing the failure way of lithium-ion batteries is key for making sure their trusted and safe use [2]. The study on the failure and safety of lithium-ion batteries is now a hot subject in energy materials. Many experts, both at home and abroad, are doing work on part failure types and changes. They have found the main failure ways of single parts like positive and negative electrodes, electrolytes, and separators, and have made different basic safety protection steps like material change and part improvement [2, 3]. But, more study is still needed on the failure ways under the effect of many factors and on stopping and control methods under extreme working states [4]. But, as the use of lithium-ion batteries in different areas keeps

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growing, the safety problems of lithium-ion batteries have slowly become clear. In 2025, a big accident happened when marine transportation battery caught fire and burned on its own, causing big losses to property and the environment [1]. The industrial field has kept making the electrode and battery structure better to keep making the energy density and fast charging abilities of lithium-ion batteries better, making the conflict between safety and performance more and more clear [3]. So, putting together the failure ways of different battery parts, showing the link between different failure reasons, and giving good ideas for making the safety of lithium-ion batteries better are very important for their dependable and safe use [4]. This paper looks at the battery failure ways, effects, and answers from the view of the main battery parts and puts together some thoughts on making battery safety and lasting power better.

## 2 Basic knowledge of lithium-ion batteries

### 2.1 Basic structure

The main parts of a lithium-ion battery include the positive electrode, negative electrode, electrolyte, separator, and current collector, which work together to store and give out electrical energy [5]. The positive electrode, mostly made of layered oxide materials, is the main thing deciding the battery's working voltage and capacity [2]. The negative electrode, mainly made of graphite materials, shows stability in lithium ion putting in and taking out. The electrolyte, a liquid compound, works as an ion carrier and is usually made of a mix of lithium salts and organic compounds. The separator, put between the positive and negative electrodes, works as a barrier and also as a way for ion movement. The current collector is used to gather and move electrons, making internal flow inside the battery. The need for material traits and the soundness of the other two parts directly change the total performance and safety of the battery.

### 2.2 Working principle

The way lithium-ion batteries work is based on the reversible movement of lithium ions between the positive and negative parts during charging and discharging, following the idea of electric balance. When the battery is charged, lithium ions are taken out from the positive electrode structure, go through the electrolyte and separator, and are put into the negative electrode, with charge moving through the outside circuit. When the battery is used, lithium ions are taken out from the negative electrode, go through the electrolyte, and go back to the positive electrode, with charge moving through the outside circuit to give power to the outside circuit [5]. In the charging and discharging cycles, the movement of lithium ions and the strength of the electrode structure decide the ability to keep the capacity of lithium-ion batteries, while side effects at the surfaces of different battery parts directly change the battery's life and safety.

## 3 Failure mechanisms of key components

The failure of lithium-ion batteries usually starts from the wearing out/failure of one or many parts, often caused by different things. The failures of single parts are connected and build up, finally leading to battery performance drop and safety problems.

### 3.1 Cathode failure mechanism

For layered oxide cathodes, structural and chemical breakdown during long charge-discharge cycles are the main reasons for battery capacity loss and safety drop [2]. After 500 cycles, the permanent loss of active lithium ions in NCM ternary cathodes gets to 15% to 20%, along with the coming out of around 2.3 wt.% of lattice oxygen and the dissolving of transition metal ions ($Ni^{2+}$/$Co^{3+}$/$Mn^{4+}$) at 0.05 to 0.1 mg·$L^{-1}$, directly causing the change of the layered phase of the cathode into spinel or rock salt phase, blocking ion paths, and cutting electronic conductivity by 80% to 90%. Lithium removal makes a volume change of 2.5% to 3.5% in the active particles of the cathode, leading to small cracks, breaking apart, and electrode separation of the active particles. When the number of broken particles goes over 15%, the mechanical structure of the electrode is harmed, making the internal resistance of the battery go up by 40% to 60% [6]. High-nickel cathodes (NCM811/NCM955) show weak stability, with a thermal breakdown start temperature 40~60 ℃ lower than that of NCM523. At a high temperature of 180 ℃ and overcharge at 4.5 V, the oxygen release speed of NCM811/NCM955 is 3~4 times that of NCM523. The heat-making reaction with the electrolyte gives off 800~900 J·$g^{-1}$ of heat, causing an increase in battery thermal runaway by over 50% [4]. The capacity keeping rate of the NCM811 cathode after 800 cycles is under 65%~70%, much lower than the over 85% of the standard NCM622 [6]

### 3.2 Anode failure mechanism

The failure of graphite anodes is mainly caused by lithium dendrite growth and the breakdown of the solid electrolyte interface (SEI) film. During charging, when the local current density on the anode goes over 5 mA·$cm^{-2}$, and the potential is under 0 V (vs. $Li/Li^{+}$), metallic lithium will reduce and form, making needle-like lithium dendrites. The growth speed of these dendrites can get as high as 1~3 μm·$h^{-1}$. When the dendrite size goes past 10 μm, it can get through the commonly used polyolefin separator, causing an internal short circuit between the positive and negative electrodes. During cycling storage, the SEI film goes through repeated growth, breaking, and remaking. Each cycle uses 0.01% to 0.015% of active lithium. After 1000 cycles, the thickness of the SEI film goes up from the first 50~100 nm to 500~800 nm, leading to a 30%~40% drop in battery capacity and a 200%~300% rise in battery internal resistance [7].

During fast charging (10C and above) and working at low temperatures (<0 ℃), the amount of lithium put on the negative electrode goes up by 3 to 5 times, and the speed of side reactions at the interface goes up by 2 to 3 times. During slow charging at -20 ℃, the part of lithium put into the total amount of lithium can go over 25% [8]. When charged at 5C, the cycle life of a graphite negative electrode is 60% to 70% shorter than that of slow charging at 0.5C. Uneven current can cause a rise in the amount of lithium put on by 4 to 6 times in some spots, and the chance of dendrite start goes up by 80%, which speeds up internal short circuits [7].

### 3.3 Electrolyte failure mechanism

The chemical instability of liquid organic electrolytes is a major failure mechanism of batteries [9]. At the interface of cathodes with a high voltage (>4.3 V), the rate constant for the oxidative decomposition reaction of the electrolyte is $1.2\times10^{-4}$ $s^{-1}$. Its inert by-products (such as lithium carbonate and lithium fluoride) precipitate on the electrode, reducing the area of lithium-ion transport voids by 30% to 40% and decreasing ion transport efficiency by 25% to 35%. For anodes, the reductive decomposition of the electrolyte participates in the formation of the solid-electrolyte interphase (SEI) film. If the decomposition is excessive, the electrolyte consumption per single cell can reach up to 5 to 8 μL per cycle, and after 500 cycles, the electrolyte loss can exceed 40% [9].

LiPF6 lithium salt reacts rapidly with moisture in the electrolyte at concentrations >50 ppm, undergoing hydrolysis to produce corrosive substances such as HF and $POF_3$. When the HF content reaches 100 ppm, the corrosion rate of the electrode's active material increases to 10% to 15%, the corrosion and perforation probability of the electrode current collector (copper/aluminium foil) rises by 30%, and the battery's discharge capacity retention decreases by 10% to 15% [9].

The decomposition of the electrolyte generates gases such as $CO_2$, $H_2$, and $CH_4$. When the gas production volume of a single pouch cell exceeds 20 mL, the internal pressure reaches 0.5 to 0.8 MPa, causing the battery to start swelling; when the gas production volume exceeds 50 mL, the battery packaging shell may exhibit gas and liquid leakage [10]. All decomposition reactions reduce the battery's charge-discharge efficiency from a capacity loss of less than 2% to over 99.5% to below 95%. After 800 cycles of charging and discharging, the battery's charge-discharge efficiency stabilizes at around 90% to 92% [9].

### 3.4 Diaphragm failure mechanism

The separator mainly works to keep the positive and negative electrodes apart and let ions go through. The separator failing can directly cause a short circuit inside the battery. Commercial polyolefin-based (PE/PP/PE-PP-PE) separators show poor heat stability. The starting temperature for heat shrinkage of PE separators is 110~120 ℃, with a side heat shrinkage rate getting to 20%~30% at 130 ℃, and full melting and holes at 160 ℃； the starting temperature for heat shrinkage of PP separators is 140~150 ℃, with a side heat shrinkage rate getting to 15%~25% at 170 ℃. The separator can break when hit with mechanical force > 50 N or squeezed stress > 10 MPa； when the length of lithium dendrites goes over 10 μm, they can directly go through commercial separators with a thickness of 12~20 μm [11].

During the making process, the separator may show problems like inclusions, pore size changes more than 2μm, and porosity differences over 5%. These problems are all things that speed up early battery failure. During repeated swelling and shrinking of the battery (with each charge-discharge cycle going from 0.5% to 1%), the harm caused by these problems is 4 to 6 times bigger than before. After 300 cycles, the chance of local short circuits happening in the problem areas goes over 70% [12]. When the separator is broken, the positive and negative electrodes touch locally, which can also make a short-circuit current of 100 to 200 A. The battery temperature can jump to 200 to 300 ℃ within seconds, quickly leading to thermal runaway and the making of toxic gases like CO and $CO_2$ [11]. Also, when the porosity of the separator goes down from 40% to 30%, the lithium-ion conductivity drops by 30% to 40%, further polarizing the battery [11].

## 4 Factors affecting failure and mitigation measures

### 4.1 Key influencing factors

The sources of lithium-ion battery failure include external factors such as use conditions, making flaws, and cycling aging. The aging trend is made worse when these three things interact and make each other stronger. Wrong use of the conditions is the most direct cause. Overcharging can hurt the positive electrode crystallization, let oxygen go off, and cause lithium to build up on the negative electrode. High temperatures (>60 ℃), bad hits, and pressing can quickly break battery parts and cause side reactions [3]. Making flaws are builtin flaws. Problems such as electrode coating mixing, separator dirt, and wrong electrode plate pressure differences can lead to local high currents and uneven stress, causing early flaws [5]. Long-term cycling aging causes permanent damage, such as breaking down of the NCM positive electrode, too much thickness of the negative electrode SEI film, and too much solvent use, leading to a drop in battery capacity, discharge power, and safety performance [2, 13].

## 4.2 Targeted failure suppression strategies for each component

Developing countermeasures based on existing research on the inherent failure mechanisms of lithium-ion batteries in terms of cathode, anode, electrolyte, and separator is a measure to minimize degradation and enhance safety from the root. The strategies are as follows:

### *4.2.1 Positive electrode degradation suppression strategy*

Element doping modification and surface coating modification enhance the structure of the NCM cathode and improve the thermal stability of NCEM. Doping 0.5% to 1% of elements such as Al and Mg in the NCM cathode can reduce lattice oxygen spillover by 50% to 70%, decrease the dissolution amount of transition metal ions to around 0.01 mg $L^{-1}$, and increase the capacity retention rate from 75% to 90% to 92% after 500 cycles [2]. Using a 5 nm to 10 nm thick layer of $LiPO_3$ or $LiAlO_2$ as a surface coating on layered oxide cathode materials blocks direct contact between the cathode and electrolyte, reducing the rate of interfacial side reactions by 50% to 60% and decreasing the growth rate of battery internal resistance by 40% [6].

### *4.2.2 Anode failure suppression strategy*

By adding 1% to 2% of film-forming additives such as fluoroethylene carbonate (FEC) and vinylene carbonate (VC) to the electrolyte, a dense and uniform solid electrolyte interface (SEI) film with a thickness of 100 to 200 nm can be formed on the surface of the graphite anode. This dense film is 10 to 20 times thicker than the original, reducing lithium consumption during cycling to less than 0.002% per cycle, and the degradation after 1000 cycles to 15% to 20% [9]. Tight process control keeps the local current density of the anode during charging to less than 3 mA $cm^{-2}$; stopping the anode potential from going below 0.1 V (vs. $Li/Li^{+}$ ). This can also lower the lithium dendrite growth rate to less than 0.2 μm/h and cut the chance of dendrite nucleation by 80% [7]. Stepwise charging can lower the amount of lithium put down during fast charging (5C) by 70% to 80% [8]

### *4.2.3 Electrolyte degradation suppression strategy*

Using a selected blend of carbonate solvents (ethylene carbonate/dimethyl carbonate/ethyl methyl carbonate) and lithium bis(fluorosulfonyl)imide (LiFSI), a high-voltage stable electrolyte was prepared, which raised the oxidative decomposition potential to 4.8~5.0 V and reduced the decomposition rate constant under high voltage to $5\times10^{-5}$ $s^{-1}$. After cycling at a high voltage of 4.5 V for 500 times, the electrolyte loss could be reduced to less than 20% [9].

### *4.2.4 Diaphragm failure suppression strategy*

Coating a modified polyolefin separator with 3~5 μm thick $Al_2O_3$ and $SiO_2$ ceramic materials can increase the thermal shrinkage temperature of the separator to above 200 ℃, with a transverse thermal shrinkage rate of less than 5% at 180 ℃, and raise the onset temperature of pyrolysis to above 250 ℃. Simultaneously, the puncture force of the separator is increased from 10 $N \cdot mm^{-1}$ to 25~30 $N \cdot mm^{-1}$, and the puncture capability of the separator to lithium dendrites is enhanced by 2~3 times, effectively blocking excessively long lithium dendrites (length > 30 μm). Developing aramid-rich and cellulose-based separators, the thermal stability temperature can reach 250~300 ℃, with no significant shrinkage at high temperatures, a separator puncture force of 40~50 $N \cdot mm^{-1}$, and the mechanical impact resistance of the separator can be improved to over 100 N [11].

## 4.3 Comprehensive mitigation strategies

### *4.3.1 Material and structural optimization strategies*

In terms of materials, the structure and thermal stability of the NCM cathode are enhanced through doping, coating, and structural optimization, inhibiting granulation, transition metal dissolution, and lattice oxygen release [2, 6]; stable electrolytes and film-forming additives are used in the electrolyte to control the uniform and dense formation of the anode SEI film, suppressing the side reactions of redox decomposition of the electrolyte and hydrolysis decomposition of lithium salts, reducing gas production, lithium deposition, and HF decomposition issues [9]; high-temperature resistant, high-mechanical-strength gel-coated ceramic separators or solid electrolytes are developed, and the thermal shrinkage insulation heat resistance and puncture strength of the thickened separator are improved to reduce short circuits and combustion from the source [5, 11].

In terms of structure and manufacturing, improving the electrode coating process and rolling parameters can enhance the uniformity of the coating and mechanical properties, addressing issues such as electrode delamination and pulverization during cycling. By controlling manufacturing conditions and coordination precision, early failures caused by factors such as impurities and misalignment in the separator and electrode sheets can be eliminated [3, 12]. Through multi-component design and interface modification, the interfacial stability at the electrode/electrolyte interface can be significantly improved, extending the service life of the electrode and slowing down the aging phenomenon of internal resistance [2, 6].

### *4.3.2 Implement operation and maintenance, as well as recycling and regeneration strategies*

In the use and operation and maintenance stages, set reasonable charging and discharging windows and temperature ranges, avoiding overcharging, overdischarging, abuse at high temperatures, and high-rate fast charging conditions, to slow down the growth of lithium dendrites and the consumption rate of electrolyte [7, 8]; strengthen transportation fixation and mechanical protection design to prevent impact and compression that may lead to separator fracture and internal short circuit [1]. In the recycling and regeneration stage, combine mechanical, chemical activation, and thermal treatment to achieve lithium replenishment and morphology reconstruction of the spent cathode, enabling "ion transport" and "capacity" regeneration of the discarded layered oxide electrodes [14], reducing resource waste and environmental hazards from recycling discarded power batteries [2, 6]. Establish life-cycle assurance and online monitoring technologies for recycling and reuse, enabling early detection of abnormal changes and timely intervention, further reducing the risk of thermal runaway [2, 4].

## 5 Conclusion

This article comprehensively expounds the failure mechanisms of the four key components of lithium-ion batteries: cathode, anode, electrolyte, and separator, clarifies the coupling effects between external abuse, manufacturing defects, and cycling aging, and reveals the development mechanism of safety accidents from "component failure-performance degradation - ignition". The results of this paper indicate that the main failure modes of the four key components are structural phase transition of the cathode, lithium dendrites in the anode, electrolyte decomposition, and "egg-breaking" of the separator. The coupling between these factors exacerbates the battery failure process. Based on the failure mechanisms, failure prevention strategies such as improving materials and structures, usage and standardization, and waste recycling are effective ways to reduce failure rates, enhance safety, and improve durability.

Current research still has shortcomings: the failure evolution mechanism under multi-factor coupling remains unclear, the accuracy of failure prediction under extreme operating conditions is not high, and the practical application of solid-state electrolytes and high-stability electrode materials has not been achieved. In the future, it is necessary to closely integrate multi-scale characterization, full-life cycle testing, and other methods to further study the battery failure mechanism under complex conditions; further realize the industrialization of solid-state batteries, advanced separators, and high-stability electrolytes; improve the standard system for battery transportation, use, and recycling, establish a battery full-life cycle safety technology system, and facilitate the safe and reliable application of lithium-ion batteries in promoting the transition to clean energy.

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