Research Progress and Optimization Strategies of Cathodes, Anodes and Electrolytes for Lithium-ion Batteries

Jiaji Li *

China-EU Institute of Engineering and Technology, Shanghai University, Shanghai, 200000, China

* Corresponding author: 81138995@shu.edu.cn

Abstract. The importance of lithium-ion batteries is becoming increasingly clear as the world's need for clean energy grows. However, the challenges of realizing their higher energy density, stability and safety remain to be overcome. This paper discusses the working principle of Li-ion batteries and the importance of their core components, then explores the research significance of cathode, anode materials and electrolytes, respectively, and describes the current mainstream materials and their current challenges and optimization strategies. In terms of positive electrode materials, this paper introduces mainstream materials such as Nickel Manganese Cobalt Oxide (NMC), Nickel Cobalt Aluminum Oxide (NCA), and Lithium Iron Phosphate (LFP), and puts forward strategies to improve energy density and enhance stability; in terms of negative electrode materials, this paper lists core materials such as graphite and silicon, and discusses the issues of volume change and how to improve stability, etc. In the electrolyte section, it not only introduces the mainstream electrolytes such as organic liquid electrolytes and solid electrolytes, but also analyzes and discusses the problems of how to improve their ionic conductivity. By synthesizing these reviews and strategies, this paper aims to promote the progress and development of lithium-ion battery technology and bring new research perspectives and values.

Keywords: Lithium-ion battery, anode material, cathode material, electrolyte.

1. Introduction

Due to the significant impact of global climate change on the earth's ecology, as well as the environmental pollution and economic crisis caused by overdependence on traditional fossil fuels, the search for clean and renewable energy alternatives has become very urgent [1]. In this scenario, lithium-ion batteries have emerged as an important milestone in the technological progress of the 21st century. They play an indispensable role in smartphones and laptops, as well as in electric transportation and extensive grid power reserves. Widespread adoption of this technology has been accompanied by heightened expectations for sustained performance, long-term stability and overall efficiency. However, lithium-ion batteries still face a number of technical and engineering challenges, including short life and high recycling costs. For example, after many charge/discharge cycles, the capacity of the battery degrades, significantly reducing its performance and lifetime, and the potential risks of overheating, short circuiting, and even fire and explosion cannot be ignored. In addition, the high cost of manufacturing and recycling also limits its application and popularization in more fields [2-4].

In order to meet the growing market demand and overcome the technological challenges of lithium-ion batteries, the research field of lithium-ion batteries has made rapid progress in recent years. In the research of positive and negative electrode materials, innovative materials boasting elevated energy storage and high thermal stability continue to be developed, creating opportunities for stable operation of batteries and improving their overall performance. At the same time, scientists are exploring various new ways to improve battery cycling stability and rapid charge/discharge capability. As for electrolytes, the shift from traditional organic liquid electrolytes to solid-state electrolytes not only improves battery safety, but also provides a wider range of operating conditions for batteries. In addition, important breakthroughs have been made in battery interface technology and structural design, providing a solid foundation for improving overall battery performance.

The purpose of this article is to explore in depth the recent advances in Li-ion batteries. Starting from the basic working mechanism of Li-ion batteries, the paper will explain the importance of their

core components, followed by a comprehensive study of these core components, outlining their research significance and listing the main materials. Furthermore, the paper will discuss the major challenges currently faced by cathodes, anodes, and electrolytes and provide optimization strategies. The aim of this paper is to offer researchers and engineers a thorough and in-depth perspective to further advance the development and application of lithium-ion battery technology.

2. Operation and Importance of Lithium-ion Batteries

2.1. Principle of Operation

During charging, the cathode expels lithium ions that traverse the electrolyte and accumulate at the anode. Concurrently, electrons journey from the positive to the negative electrode via an external route. During discharge, the process is reversed. The electrolyte plays a key bridging role in this process, providing a channel to allow lithium ions to traverse, but not allowing the electrons to pass through, ensuring that they can only flow through the external circuit. Taking lithium cobaltate and graphite as an example, the electrochemical reaction equations for the entire cycling process are shown in equations (1)-(3), and the principle is shown in Fig. 1 [5].

Positive reaction:

$$LiCoO_2 \rightleftharpoons Li_{1-x}CoO_2 + xLi^+ + xe^- \tag{1}$$

Negative reaction:

$$6C + xLi^+ + xe^- \rightleftharpoons Li_xC_6 \tag{2}$$

Total response:

$$LiCoO_2 \rightleftharpoons Li_{1-x}CoO_2 + xLi^+ + xe^- \tag{3}$$

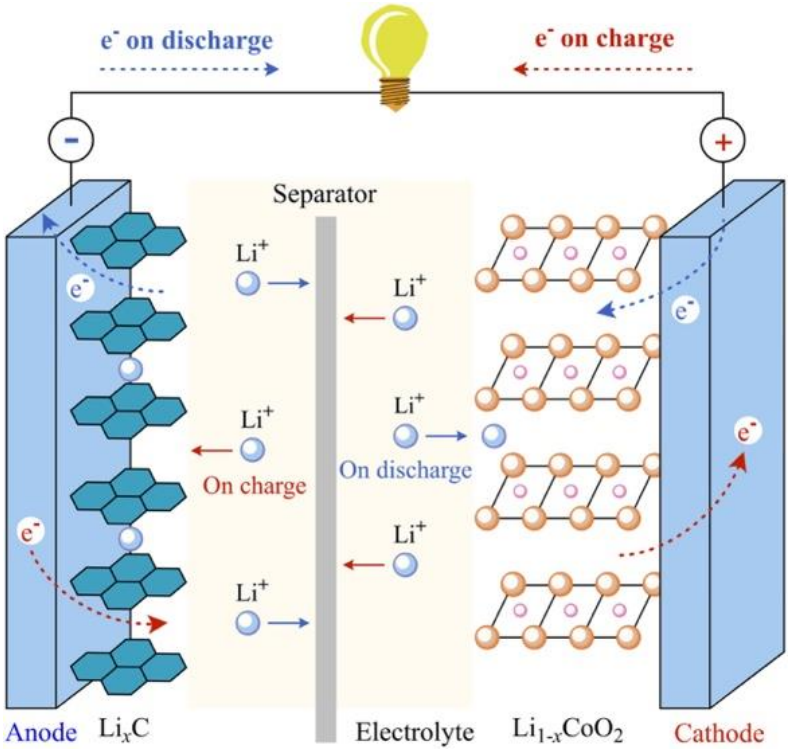


Figure 1. Schematic of an exemplified lithium-ion battery cell.
https://www.nature.com/articles/s41928-018-0048-6

2.2. Importance of Core Components

The selection and design of positive and negative electrode materials and electrolytes are the key factors affecting battery performance. The electrical conductivity, structural stability and interfacial compatibility of these materials with the electrolyte all have a significant impact on the battery's capacity, energy concentration, power output, and longevity. For example, a high-capacity cathode material that reacts violently with the electrolyte can lead to short battery life and safety hazards [6]. Conversely, a good interface can significantly reduce the internal resistance of the battery, thereby increasing its performance and efficiency. In recent years, research on lithium-ion batteries has progressed rapidly, but there are still a number of problems and challenges, and in the following, this paper will focus on the latest advances, challenges, and optimization schemes of these three materials.

3. Cathode

In li-ion batteries, the cathode dictates the overall voltage potential, capacity as well as enduring stability of the battery. As the core of the battery's energy output, its chemical properties, stability and structure play a critical role in the uptake and release of lithium ions. High quality cathode materials should have high voltage, stable chemical properties and good cycling stability.

3.1. Mainstream Cathode Materials

3.1.1. $LiCoO_2$ (LCO)

LCO is the earliest commercially applied cathode material, with a theoretical capacity of 274 $mAhg^{-1}$, an actual capacity of about 185 $mAhg^{-1}$, and an operating voltage of 3-4.45 V. It has the advantages of high voltage, smooth discharge, suitability for high current discharge, high specific energy, and good cycling, and it stands as one of the predominant cathode materials in widespread use. However, due to the relatively high price of cobalt, resource constraints and thermal stability issues, the reliance on cobalt is gradually decreasing, especially in large battery applications such as electric vehicles.

3.1.2. $LiNiO_2$ (LNO)

LNO is the first generation of cathode materials, the theoretical capacity of 274 $mAhg^{-1}$, the actual capacity of up to 200 ~ 220 $mAhg^{-1}$, with high capacity, small loss of capacity over multiple cycles, relatively inexpensive, wide adaptability of raw materials and environmental pollution, etc., but there are difficulties about synthesis, poor stability, and prone to nickel-lithium mixed rows and other shortcomings.

3.1.3. $LiMn_2O_4$ (LMO)

LMO is an early cathode material with a theoretical capacity of 283 $mAhg^{-1}$ and an actual capacity of 160 to 190 $mAhg^{-1}$. With the low toxicity of manganese element and cheap price, the application potential is very high, but there are problems such as the occurrence of deep discharge, loss of electrode composition due to Jahn-Teller distortion, and instability of high-voltage charging electrolyte.

3.1.4. $LiNi_{1-x-y}Co_xMn_yO_2$ (NMC)

NMC is a mixed-metal lithium acid composed of three transition metal elements, Ni, Co and Mn. NMC typically has high energy density and cycling performance. Its performance varies depending on the ratio of Ni, Mn and Co. For example, high Ni versions of NMCs (e.g., $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$) have higher energy density but may be less stable at high temperatures [7]. Due to the relative scarcity and high price of cobalt resources, current research favors the development of high-Ni and low-Co NMC materials.

3.1.5. $LiNi_xCo_yMn_zO_2$ (NCA)

Composed of nickel, cobalt and aluminum, NCAs have a high energy density, making them particularly popular in applications that require high capacity and long range, such as electric vehicles and certain portable electronics. However, they can have thermal stability issues when used for long periods or at high temperatures, and are also more expensive than typical high-nickel materials.

3.1.6. $LiFePO_4$ (LFP)

LFPs are mainly composed of iron and phosphate groups. Compared with NMC and NCA, LFP has a lower energy density, but its excellent thermal and chemical stability makes it attractive for large-scale industrial applications and energy storage, while the long cycle life of LFP batteries and the elimination of the need to use expensive cobalt elements are advantageous from both economic and environmental perspectives. Fig. 2 illustrates a performance comparison among various cathode materials [8].

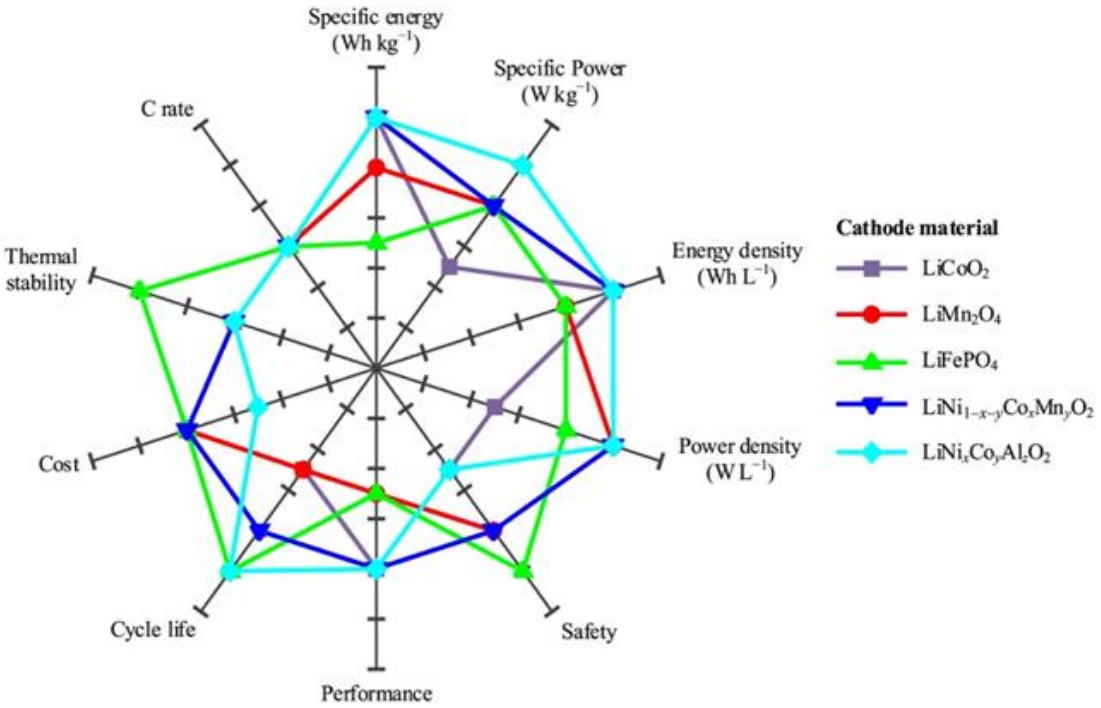


Figure 2. Evaluating cathode substances used in lithium-ion batteries. https://www.sciencedirect.com/science/article/pii/S2352484722005716?via% 3Dihub

3.2. Challenges and Optimization Strategies

3.2.1. Energy density

The energy capacity of li-ion batteries is now a significant constraint hindering the broadening of their use cases. Particularly in applications that require high capacity and long range, such as electric vehicles and avionics, energy density limitations have increased the size and weight of the batteries, limiting the performance and portability of the end products. Currently, the energy density of most cathode materials is limited by their chemical composition and crystal structure, which determine the amount of lithium ions each material can hold per unit volume or weight. To overcome this limitation, scientists have sought to reconfigure the crystal lattice of existing cathode materials, for example by using nanotechnology processing to make the materials nanoscale in size, which can shorten the diffusion path of lithium ions, optimize their reaction kinetics, and thus accelerate the charging and discharging speed of the battery. In addition, the single crystal structure without grain boundaries can resist the formation of microcracks due to volume changes. And the single-crystal material also helps reduce side reactions at the interface, inhibit electrolyte decomposition, and optimize the electrochemical activity of the exposed surface. This not only improves the lithium-ion channels of

the cathode material, but also increases the embedding capacity of lithium ions, further enhancing its energy storage capacity [9]. In addition, it is also very popular to develop and continuously improve cathode materials. For example, nickel-rich and low-cobalt NMCs such as $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ possess greater energy capacity and are more cost-effective than traditional cathode materials such as LCO, and NCAs such as $LiNi_{0.8}Co_{0.15}Mn_{0.05}O_2$ provide higher capacity and voltage platforms, making them more suitable for use in large-scale energy storage devices [10]. In addition, researchers have explored lithium sulfate (Li_2SO_4) as a cathode, which has a theoretical capacity many times greater than existing materials. Yet, the advancement of novel materials often presents new challenges, such as cost and thermal stability issues, that require further research and optimization.

3.2.2. Stability

The stability of cathode materials is a key issue in lithium-ion battery research. When batteries are used at high voltages, high temperatures and under long-term cycling conditions, chemical and structural instability of cathode materials can occur, leading to capacity loss and rapid degradation of battery performance. In addition, reactions with the electrolyte can cause irreversible structural changes that affect the cycling stability of the cathode material. These problems not only limit battery life, but can also create safety hazards.

Coating technology, as the first line of defense to protect the cathode material, is commonly employed to enhance the surface of cathode materials for augmented stability. By applying a slender safeguarding coating, such as zirconia and alumina, on the exterior of the cathode substance, it efficiently prevents direct interaction between the cathode substance and the electrolyte, reduce the side reaction, improve its thermal stability, and protect the internal material structure. In this way, the battery's lifespan through cycles is significantly improved and the rate of capacity degradation is dramatically reduced [11].

In addition, doping is another effective way to improve stability. By doping other elements such as calcium, magnesium, and aluminum into the crystal structure, the electronic structure of the material can be optimized, its electrical conductivity can be improved, and its crystal lattice can be stabilized [12]. This minimizes the material's volumetric fluctuations during charge and discharge cycles, thus inhibiting the formation of cracks, but also improves its resistance to oxidation and corrosion. Thus, the high-voltage endurance of the cathode material is ensured, and long-cycle conditions is significantly improved.

4. Anode

Anode materials play a critical role in lithium-ion batteries, determining their energy density, lifetime, safety, and charge-discharge efficiency. Since energy storage and transfer occurs primarily between the electrodes, the selection and refinement of anode materials are critical. A superior anode material ensures that the battery has high energy density, long life and safety.

4.1. Mainstream Anode Materials

4.1.1. Graphite

Graphite is one of the most commonly used anode materials, consisting mainly of multiple layers of carbon atoms, which has stable cycling performance and good electrical conductivity, but has its natural limitations in terms of electrical capacity (about 372 $mAhg^{-1}$). It is widely used for batteries in mobile phones, laptops and other portable electronic devices.

4.1.2. Silicon

The potential electrical capacity of silicon as an anode material is much higher than that of graphite, reaching about 4200 $mAhg^{-1}$, but despite its high electrical capacity, silicon undergoes a lot of volumetric expansion and contraction during lithium-ion embedding and de-embedding, leading to structural rupture and thus reducing cycling stability, and to address this issue, researchers are exploring silicon nanoparticles, silicon-based composites, and the combination of silicon and graphite.

4.1.3. Lithium Titanate (LTO)

LTO is another anode material, usually in the form of $Li_4Ti_5O_{12}$, which has a higher operating voltage, better safety, and does not undergo significant volume changes during charging and discharging like other anode materials such as silicon. Because of its excellent performance, LTO is often used in applications that require frequent charging and discharging, such as certain types of power tools and fast-charging systems. However, LTO has a lower energy density and higher manufacturing cost than traditional anode materials such as graphite.

4.1.4. Li-metal

Li-metal is favored as an anode choice owing to its exceptionally high theoretical capacity potential. (about 3860 $mAhg^{-1}$) and very low potential [13]. Li-metal batteries possess the potential to attain superior energy densities theoretically. However, they are susceptible to the growth of dendrites. Specifically, during charge and discharge cycles, the deposition and removal of lithium ions on the lithium-metal surface can lead to the formation of irregular lithium "dendrites". These protruding formations have the potential to puncture the battery separator, leading to internal short-circuits and posing significant safety risks. The performance distinctions among various anode materials are illustrated in Fig. 3 [8].

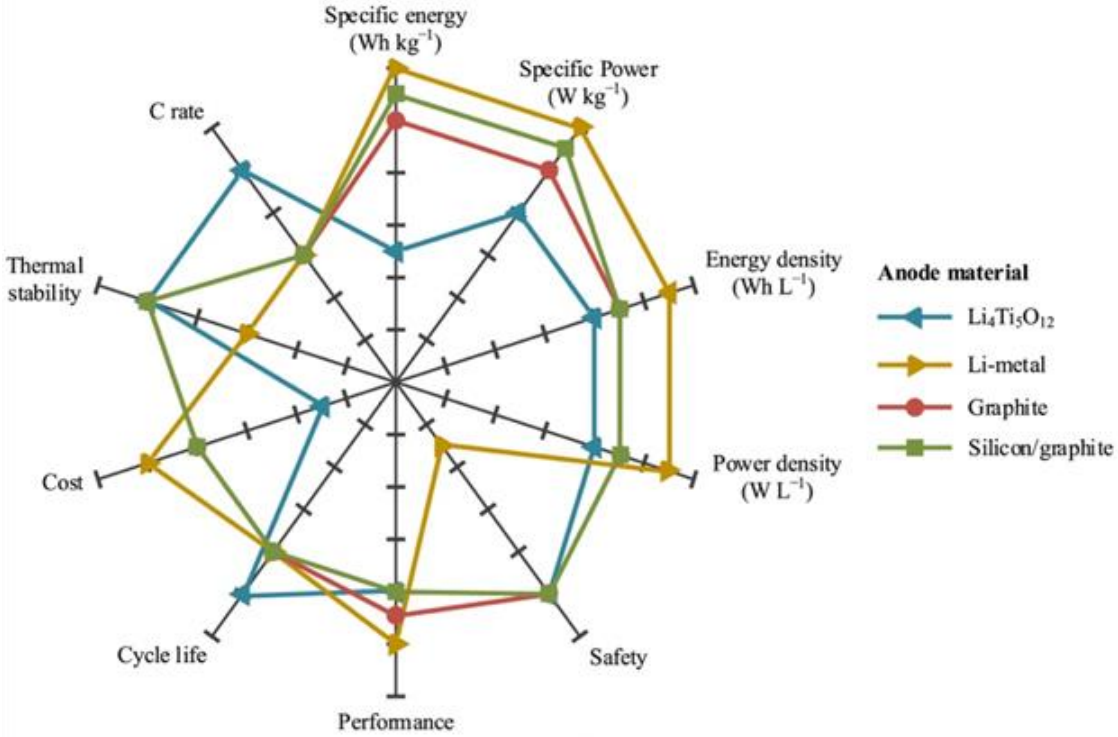


Figure 3. Evaluating anode substances used in lithium-ion batteries. https://www.sciencedirect.com/science/article/pii/S2352484722005716?via% 3Dihub

4.2. Challenges and Optimization Strategies

4.2.1. Volume expansion and contraction

Throughout the charge and discharge cycles of a lithium-ion battery, the anode material absorbs and releases lithium ions, resulting in significant volume expansion and contraction. Particularly with high-capacity anode substances like silicon, the volume fluctuation can multiply several times. This repeated volume change can not only cause the anode material to fracture, which reduces the repetitive charge-discharge efficiency of the battery, but can also cause an intracellular electrical failure, increasing the safety risk.

To combat the volume expansion problem, composite design has become the key to the solution. By combining anode materials with high capacity but drastic volume changes with other materials

with better volume stability, such as silicon and carbon composites, we can to some extent balance the properties between these materials. For example, carbon can provide a stable skeleton for silicon, allowing enough space for the silicon to expand, thus reducing the risk of fracture [14]. In addition, carbon plays the role of increasing the electrical conductivity in the composite, which ensures good battery performance during charging and discharging.

Nanosizing is also one of the strategies to address the volume variation of anode materials. Designing the anode material to nanometer size helps to provide a shorter and more efficient diffusion path for lithium ions. This means that as lithium ions rapidly enter and exit the anode material, the small particle size contributes to an even distribution of volumetric stresses, thereby reducing internal stresses in the material. At the same time, the expansive surface area of the nanoparticles guarantees comprehensive interaction with the electrolyte, further improving the battery's charge and discharge rates. It should be noted, however, that the nano-sized design must take into account the overgrowth of the SEI layer that may result from the reaction with the electrolyte, which is a key point for the next optimization step.

4.2.2. Stability

The stability of anode materials is a key factor in the cycling performance and lifetime of li-ion batteries. During charging and discharging, the reaction of the anode surface with the electrolyte results during the creation of a volatile solid electrolyte interface (SEI). As the number of charge/discharge cycles increases, the SEI layer can continue to grow, fracture or peel off, resulting in effective lithium-ion loss and increased internal resistance. More seriously, the inhomogeneous SEI layer can lead to localized overheating, increasing the safety risk of the battery.

The stabilization and homogeneity of the SEI layer is critical to the long life and stability of the battery. And synthetic SEI technology, i.e., controlling the formation of a stabilized SEI layer by pretreatment or addition of specific chemicals, has been widely studied. By choosing the right chemical composition and formation conditions, a more uniform and compact SEI layer can be obtained. An ideal synthetic SEI can form a smoother conductive ion path, which promotes the rapid transfer of Li+ and ensures that the battery continues to operate stably. Has excellent electrochemical stability and resilience to better cope with the volume expansion of lithium metal. The formation of lithium dendrites can be stopped by strong mechanical properties or high modulus of elasticity. In addition, it also has excellent barrier function and electronic insulation properties to avoid the adverse reaction between lithium metal and electrolyte [15].

Coating technology is primarily employed to create a slender protective coating on the surface of the negative electrode material to prevent undesirable reactions with the electrolyte. For example, by uniformly applying an oxide, carbon or other material as a coating to the negative electrode particles, the area in direct contact with the electrolyte can be significantly reduced, thereby extending the life of the battery. Such coatings not only prevent the overgrowth of unstable SEI layers, but also enhance the electron transport and structural integrity of the anode material, further enhancing the performance and stability of the battery [16].

5. Electrolytes

Electrolytes play a critical role in lithium-ion batteries by connecting the positive and negative electrodes of the battery and providing a transport path for lithium ions from one pole to the other. The electrolyte not only affects the conductivity and internal resistance of the battery, but its interaction with the electrode materials also affects the safety and the battery's cycle endurance. An effective electrolyte should have high ionic conductivity, chemical and enhanced heat resistance, along with superior synergy with the electrode constituents. Selecting and optimizing the right electrolyte is key to ensuring that lithium-ion batteries can operate safely and reliably in a wide range of applications.

5.1. Mainstream Electrolytes

5.1.1. Organic liquid electrolytes

This was the first electrolyte used and is still the dominant electrolyte today, usually consisting of lithium salts and organic solvents. Lithium salts such as $LiPF_6$, $LiBF_4$, $LiClO_4$ are the main source of ions in the electrolyte, and these lithium salts can be dissolved in organic solvents and release lithium ions that can be transferred during charging and discharging. In particular, $LiPF_6$ is the most commonly used lithium salt in commercial lithium-ion batteries due to its excellent electrochemical stability and ionic conductivity. Organic solvents, commonly ethyl carbonate (EC), dimethyl carbonate (DMC), and diethyl carbonate (DEC), are often used in a solvent mixture to achieve better electrolyte performance. In addition to dissolving lithium salts, these solvents provide suitable mobile channels for lithium ions to migrate quickly and efficiently in the battery.

Although organic liquid electrolytes play a critical role in batteries, they have inherent drawbacks such as flammability, volatility, and in some cases chemical instability, which limit some applications of lithium-ion batteries, especially in high-temperature or high-pressure environments. To address these issues, researchers are still actively searching for alternative or optimized electrolyte systems.

5.1.2. Solid electrolytes

Solid electrolytes offer a higher level of safety than organic liquid electrolytes because they are generally nonflammable. They also offer a wider electrochemical window, which opens the possibility of developing high-voltage battery materials. However, solid electrolytes have poor ionic conductivity, which can limit the discharge rate of the battery, although potential interface challenges between the solid electrolyte and the electrode substance might arise, which can lead to increased resistance or unstable chemistry, in addition to solid electrolytes having processing difficulties and mechanical brittleness that need to be improved [17]. Common solid electrolytes include polymer electrolytes, ceramic electrolytes, etc.

Polymer electrolytes are made from polymer materials such as polyethylene oxide (PEO) and lithium salts. These electrolytes have excellent flexibility and processability, making them easier to integrate with electrode materials. However, the ionic conductivity of such materials is relatively low, especially at room temperature. This can limit the charging and discharging rate of the battery and affect its overall performance. In addition, as the temperature increases, the polymer can become destabilized, leading to structural damage and degradation of electrical properties.

Ceramic electrolytes, represented by $Li_7La_3Zr_2O_{12}$ (LLZO) and $Li_{10}GeP_2S_{12}$ (LGPS), are also currently receiving a great deal of attention in the battery field, mainly because of their outstanding high ionic conductivity, a property that allows them to provide comparable performance to liquid electrolytes over a wide temperature range. In addition, they provide chemical stability to electrodes and excellent barrier properties, especially in preventing lithium dendrite ingress. This physical barrier greatly enhances battery safety and eliminates the risk of solvent leakage from liquid electrolytes. However, due to its natural brittleness, this can lead to micro-cracks or fractures during battery assembly and use, while these voids can reduce the actual contact area with the electrodes, which in turn increases the interfacial resistance, hindering ion transport.

5.2. Challenges and Optimization Strategies

Electrolytes are used as ion transport media in lithium-ion batteries, and their ionic conductivity directly affects the performance and efficiency of the battery. Lower ionic conductivity means that lithium ions are transported less efficiently during battery charging and discharging, resulting in a decrease in the energy output and input efficiency of the battery. In addition, low conductivity can lead to an accumulation of lithium ions in the battery, which increases the risk of short circuits and thermal runaway. Therefore, optimizing the electrolyte's ion transfer rate is critical to improving the overall efficiency of the cell.

The ion transport properties of the electrolyte can be significantly improved by introducing specific additives such as lithium hexafluorophosphate ($LiPF_6$) and lithium hexafluoroborate ($LiBF_4$)

into the electrolyte. For example, certain organic solvents or lithium salts can be used as additives to improve the migration rate of lithium ions in the electrolyte by adjusting the microstructure of the electrolyte. In addition, the additives can also help to form an SEI, which further promotes efficient ion transport while improving the stability of the battery [18].

At the same time, research and development of a wide range of new materials with high ionic conductivity should be continuously focused. For example, highly ion-conductive polymers such as polyethylene oxide (PEO)-based materials or ceramic materials such as LLZO ($Li_7La_3Zr_2O_{12}$) and LATP ($Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$), which have ionic conductivity close to or exceeding that of liquid electrolytes with excellent stability, have shown excellent electrochemical performance at the laboratory level [19, 20]. These materials have unique structural properties that allow them to have higher ionic conductivity. In the future, these new materials are expected to replace or combine with conventional liquid electrolytes to provide higher performance and longer battery life.

6. Conclusion

Lithium-ion batteries, as a storage solution for renewable energy sources, are becoming more and more important today as environmental issues and global energy crisis problems increase. In this study, we delve into the operational principles of lithium-ion batteries and highlight the significance of their core components in detail. In the investigation of cathode materials, this study not only focuses on the leading materials such as NMC, NCA and LFP, but also discusses the strategies to improve energy density and stability, etc. For anode materials, this study analyzes the challenges of volume change and stability improvement along with key materials such as graphite and silicon, and provides targeted solution strategies. In the field of electrolytes, this paper not only introduces electrolytes such as organic liquids and solids, but also focuses on their problems and optimization methods in terms of safety and ionic conductivity. In the future, researchers should continue to focus on the development of new materials, technology updates, and further solutions to existing challenges to ensure the safe and efficient use of lithium-ion batteries. This paper provides ideas for understanding and improving lithium-ion batteries, with the goal of accelerating technological innovation in this field and providing valuable references for research in related fields.

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