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Research Progress and Recycling Strategies of Crystalline Electrode Materials for Sustainable Energy Storage

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Abstract. With the massive development of new-energy vehicles and renewable energy, the demand for high-performance, safe, and sustainable energy storage technologies has constantly increased. The increasing demand for electric vehicles and renewable energy systems has accelerated the development of lithium-ion batteries, making them one of the most widely adopted solutions for modern energy storage. However, issues including metal resource consumption, environmental impacts during production, and the recycling of spent batteries have attracted increasing attention. Therefore, exploring electrode materials with high performance, low resource consumption, and excellent recyclability is crucial for future green energy storage technologies. This review focuses on crystalline electrode materials for sustainable lithium-ion batteries and summarizes recent research progress in representative cathode and anode materials. Typical cathode materials, including lithium iron phosphate and lithium manganese oxide, as well as anode materials such as graphite and silicon-based materials, are investigated. Their crystal structures, energy storage mechanisms, and optimization strategies are analyzed. Moreover, recycling and direct regeneration technologies for crystalline electrode materials from spent lithium-ion batteries are reviewed. Life cycle assessment is used as an important tool to evaluate energy consumption and environmental impacts throughout material production and recycling processes. The results demonstrate that optimizing crystal structure design and improving material recyclability can effectively reduce resource consumption and environmental pressure. This review emphasizes the strategies for achieving improved performance, reduced cost, and enhanced sustainability in future energy storage applications.

Keywords: crystal electrode material, sustainable energy storage, structural regulation

1. Introduction

With the rapid development of new energy vehicles, high-performance energy storage technology has become an important foundation for the efficient utilization of recyclable energy. Lithium-ion batteries have been widely used in electronic devices and electric vehicles due to their high energy density, long cycle life, and excellent performance. However, traditional electrode materials still face challenges, including resource dependence, capacity degradation during cycling, and environmental issues associated with spent battery disposal. Therefore, the development of high-performance and sustainable electrode materials has become major research attention.

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Recent studies have shown that crystal structure plays a critical role in determining the ion diffusion, electron transport, and electrochemical performance of electrode materials. The performance of anode materials, such as lithium iron phosphate and lithium manganese oxide, and cathode materials, including graphite and silicon-based materials, has been markedly improved through crystal structure regulation, defect engineering, and composite design. Even so, further development of the relationship between crystal structure and long-term performance, as well as the development of efficient recycling and regeneration strategies, remain essential research challenge.

This review focuses on crystalline electrode materials in sustainable lithium-ion batteries. Through literature analysis and integration, this study investigates the relationship between crystal structures and electrochemical properties, summarizes recent advances in representative cathode and anode materials, and discusses sustainable strategies including material optimization, recycling, regeneration, and life cycle assessment. This study aims to contribute to the future development of high-performance, cost-efficient, and sustainable energy storage materials, while offering potential solutions to current challenges related to resource consumption and environmental impacts.

2. Crystal structures and their influence on electrode performance

The arrangement of atoms within electrode crystals directly determines their electrochemical behavior by affecting the migration, electronic transport, and structural stability. During charge and discharge processes, lithium ions repeatedly migrate between cathode and anode materials through specific diffusion pathways within crystalline frameworks. Therefore, key structural characteristics, including atomic arrangement, lattice parameters, ion diffusion channels, and structural stability, play critical roles in determining lithium-ion transport kinetics, electronic conductivity, reaction mechanisms, and long-term cycling durability [1, 2].

Different crystal structures provide distinct lithium-ion migration environments and consequently exhibit different electrochemical behaviors. Layered structures, commonly found in transition-metal oxide cathodes, provide two-dimensional lithium-ion diffusion pathways that enable efficient ion transport and high theoretical capacities. However, repeated lithium insertion and extraction can induce lattice distortion, phase transitions, and oxygen instability, leading to structural degradation during prolonged cycling. In contrast, spinel structures possess three-dimensional diffusion networks, which facilitate faster lithium-ion migration and improve rate capability. Meanwhile, olivine structures exhibit excellent structural stability due to their strong covalent bonding framework, making them highly resistant to structural collapse during cycling [1, 3, 4]. These differences demonstrate that optimizing electrode materials requires a balance between rapid lithium-ion diffusion and robust structural stability.

Beyond the intrinsic crystal framework, defects and lattice imperfections have increasingly been recognized as important factors influencing electrode performance. Defects such as vacancies, atomic substitutions, and lattice distortions can modify local electronic structures, alter lithium-ion diffusion pathways, and regulate interfacial charge-transfer processes. Appropriate defect engineering can introduce additional active sites, reduce diffusion barriers, and enhance electrochemical reaction kinetics. For example, controlled generation of oxygen vacancies or cation substitutions may improve electronic conductivity and accelerate lithium-ion transport. However, excessive defect concentrations can disrupt lattice integrity, increase structural instability, and promote irreversible side reactions during long-term operation. Therefore, precise regulation of defect type, concentration, and distribution is essential for achieving improved electrochemical performance while maintaining structural durability [5].

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With the development of advanced characterization techniques, crystal-defect engineering has gradually become an essential strategy for regulating the performance of electrode materials at the atomic scale. By purposefully introducing and controlling defects, researchers can modify electronic structures, optimize ion migration pathways, and enhance energy storage properties. Nevertheless, accurately controlling defect formation and understanding their dynamic evolution under practical battery operating conditions remain major challenges. Further research is required to establish the relationship between defect structures and long-term electrochemical degradation mechanisms [5].

In addition to bulk crystal structures, electrode–electrolyte interfaces significantly influence battery stability and lifetime. During repeated cycling, continuous interfacial reactions may result in surface reconstruction, formation of passivation layers, and increased interfacial resistance. A stable interface can effectively suppress electrolyte decomposition, maintain efficient lithium-ion transport, and prevent excessive structural changes. Conversely, unstable interfaces may accelerate capacity fading through electrolyte consumption, transition-metal dissolution, and irreversible crystal reconstruction [2]. Therefore, engineering stable electrode interfaces is as important as optimizing the internal crystal structure.

Moreover, the interaction between crystal structure and mechanical properties plays a crucial role in determining electrode degradation. Lithium-ion insertion and extraction processes are often accompanied by volume variation and internal stress accumulation within electrode particles. Repeated mechanical stress can cause particle cracking, loss of electrical contact, and deterioration of electrode integrity, ultimately reducing cycling performance. Understanding the coupling relationship between chemical reactions, mechanical stress, and crystal evolution provides valuable guidance for designing mechanically stable and durable electrode materials [2].

To enhance both performance and sustainability, various crystal structure regulation strategies have been developed, including elemental doping, surface coating, morphology optimization, and defect engineering. Elemental doping can stabilize crystal lattices and modify electronic structures, while surface coatings can protect active materials from undesirable reactions with electrolytes. Additionally, controlling particle size, crystal orientation, and defect distribution can shorten lithium-ion diffusion distances and reduce structural degradation. These approaches not only improve battery performance but also contribute to longer service life and improved resource efficiency, which are essential for sustainable energy storage technologies [1, 5].

Overall, the relationship between crystal structure and electrochemical behavior provides a fundamental framework for the development of advanced lithium-ion battery electrode materials. By carefully controlling crystal architectures, defect configurations, and interfacial properties, researchers can achieve improved capacity retention, enhanced cycling stability, and more efficient utilization of material resources. Such structural design strategies are expected to play a key role in the development of next-generation sustainable energy storage systems [1, 2, 5].

3. Progress of cathode crystal materials

3.1. Crystal structure and performance of $LiFePO_4$

Among various cathode candidates, $LiFePO_4$ has attracted extensive attention because of its intrinsic safety, economic advantages, and outstanding cycling durability [3].

$LiFePO_4$ exhibits an olivine-type crystal structure composed of FeO_6 octahedra and PO_4 tetrahedra. This stable framework effectively prevents severe structural collapse during cycling. Lithium ions mainly migrate through one-dimensional channels within the crystal structure.

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However, the relatively poor conductivity and limited lithium-ion mobility of this material continue to constrain its application in high-power energy storage systems. To overcome these limitations, researchers have developed strategies including carbon coating, elemental doping, and nanoscale structure design. These approaches improve electron transport and shorten lithium-ion diffusion pathways, resulting in enhanced electrochemical performance [3].

3.2. Crystal structure and performance of $LiMn_2O_4$

$LiMn_2O_4$ is a typical spinel cathode material that has attracted considerable attention due to its low cost, abundant manganese resources, and environmental advantages [4].

The spinel structure provides three-dimensional pathways for lithium-ion migration, allowing $LiMn_2O_4$ to exhibit good rate performance. Compared with layered cathode materials containing nickel and cobalt, $LiMn_2O_4$ provides advantages in terms of cost and resource availability.

However, capacity fading during long-term cycling remains a major challenge. One important reason is manganese dissolution caused by reactions between the electrode and electrolyte. In addition, the Jahn–Teller distortion caused by Mn^{3+} ions can lead to lattice deformation and structural instability, especially at high temperatures or high operating voltages [4, 6].

To enhance cycling stability, researchers have explored methods such as element substitution, surface coating, and particle morphology control. Doping with metal ions can stabilize the crystal lattice, while surface coatings can reduce direct contact between electrode materials and electrolytes. These strategies help suppress structural degradation and improve long-term performance.

3.3. Structural regulation strategies for cathode materials

Structural optimization plays an essential role in improving cathode performance. Element doping can enhance lattice stability, while surface coatings can protect electrode materials from electrolyte corrosion. Furthermore, nanostructured and porous designs can improve lithium-ion diffusion and increase active material utilization [1].

Recent studies have also emphasized the importance of understanding the relationship between crystal structure, mechanical stress, and degradation behavior. Such knowledge provides guidance for designing more durable electrode materials [2].

4. Advances and optimization of anode crystal materials

Graphite is currently the most widely used commercial anode material because of its excellent structural stability, low cost, and suitable electrochemical properties [7].

The graphite crystal consists of stacked graphene layers connected by weak van der Waals forces. During charging, lithium ions are inserted between graphene layers, forming graphite intercalation compounds. The reversible formation of LiC_6 provides stable lithium storage with a theoretical capacity of 372 mAh g^{-1}.

Although graphite has been successfully commercialized, its limited capacity restricts further enhancement of battery energy density toward higher levels. Moreover, under fast-charging conditions, lithium ions may not enter graphite layers efficiently and instead deposit on the surface, causing lithium plating. This phenomenon reduces battery safety and accelerates capacity degradation [7, 8].

Current strategies for improving graphite anodes include surface modification, particle size optimization, and interface stabilization. These approaches aim to enhance lithium-ion diffusion and

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maintain stable electrode structures during repeated cycling.

4.1. Silicon-based anodes: structural evolution and volume expansion

Silicon-based materials are regarded as promising next-generation anode candidates because silicon possesses an extremely high theoretical capacity compared with graphite [9].

During lithium insertion, silicon undergoes an alloying reaction with lithium, resulting in significant volume expansion. The repeated expansion and contraction of silicon particles can cause mechanical fracture, loss of electrical contact, and unstable SEI formation. These problems lead to rapid capacity decay and poor cycling performance.

To address these issues, researchers have developed SiO_2/Si composites, porous silicon structures, and core-shell architectures. These designs provide additional room for volume expansion and improve structural stability. Furthermore, conductive carbon networks are often introduced to enhance electron transport and maintain electrode integrity.

4.2. Optimization strategies for silicon-based materials

Several approaches have been proposed to overcome the limitations of silicon anodes: Designing porous and flexible structures to accommodate volume changes; improving interface stability through surface modification; developing advanced binders to maintain electrode integrity [10].

These strategies provide promising pathways for the practical application of silicon-based anodes.

5. Failure mechanisms and recycling strategies of spent battery materials

5.1. Structural degradation of electrode materials

During long-term cycling, electrode materials experience structural changes, including lattice distortion, particle cracking, active material loss, and increased interface resistance.

These degradation processes reduce lithium-ion transport efficiency and lead to capacity decline. Understanding these failure mechanisms is essential for developing effective regeneration methods [11, 12].

5.2. Direct regeneration technologies

Traditional recycling methods mainly focus on recovering valuable elements through pyrometallurgical and hydrometallurgical processes. However, these approaches often require high energy consumption and may generate environmental impacts [13].

Direct regeneration provides a sustainable recycling pathway by repairing degraded electrode structures and recovering their electrochemical properties [12].

Current regeneration approaches include: lithium compensation; thermal restoration; hydrothermal treatment; electrochemical repair.

These methods can reduce resource consumption and improve the value of recycled materials [11, 12].

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5.3. Future application and sustainability evaluation

Life cycle assessment (LCA) provides an effective method for evaluating environmental impacts throughout battery production, usage, and recycling processes [14].

Future battery development should consider not only electrochemical performance but also cost, resource availability, safety, and environmental sustainability.

6. Conclusion

The increasing demand for electric transportation and renewable energy integration has accelerated the development of lithium-ion batteries as a crucial energy storage technology. However, the increasing demand for batteries has also resulted in challenges such as the consumption of critical resources and the environmental impacts of retired battery disposal. Therefore, developing high-performance, sustainable, and recyclable electrode materials is essential for future energy storage technologies.

This review summarizes recent advances in crystalline electrode materials for sustainable lithium-ion batteries, focusing on both cathode and anode materials. For cathode materials, lithium iron phosphate and lithium manganese oxide are discussed based on their crystal structures, lithium-ion diffusion pathways, and influence on electrochemical performance. Lithium iron phosphate shows excellent cycling stability due to its stable olivine structure, while lithium manganese oxide provides three-dimensional lithium-ion transport channels but suffers from structural degradation during long-term cycling. For anode materials, graphite remains the dominant commercial material because of its stable layered structure, whereas silicon-based materials offer higher capacity but are limited by severe volume expansion and structural instability. Furthermore, this review introduces crystal structure regulation strategies and material modification approaches that can improve capacity, rate performance, and cycling stability. Recycling technologies for spent lithium-ion batteries, including conventional recycling methods and emerging direct regeneration techniques, are also discussed to reduce resource consumption and environmental impacts. In addition, life cycle assessment is applied to evaluate the environmental effects of electrode materials throughout production, operation, and recycling processes.

Although considerable progress has been made, several challenges remain in understanding long-term degradation mechanisms, developing cost-effective recycling methods, and promoting large-scale applications. Future research should target crystal structure optimization, improving material sustainability, and integrating efficient recycling strategies to achieve safer, better-performing, and eco-friendly energy storage systems.

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