

Atomic Layer Deposition (ALD) for Lithium-ion Battery Components

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Abstract

The demand for high-performance and long-lasting Li-ion batteries has increased significantly due to the growing use of portable electronic devices, electric vehicles, and renewable energy storage systems. However, the performance and stability of Li-ion batteries are still limited by various factors, including parasitic reactions, electrode degradation, and unstable electrolytes. Therefore, the development of novel materials and techniques to improve the performance and stability of Li-ion batteries is essential. In recent years, Atomic Layer Deposition (ALD) has emerged as a promising technique for the deposition of thin and uniform coatings on various components of Li-ion batteries to enhance their electrochemical properties and stability. This study investigates the use of Atomic Layer Deposition (ALD) for the deposition of thin and uniform coatings on various components of Li-ion batteries. The results indicate that ALD can be used to deposit coatings on electrodes and separators to improve the stability and performance of the electrolyte by reducing parasitic reactions. Additionally, ALD coatings on cathode and anode materials have been shown to improve their electrochemical properties, including cycling stability and rate capability. ALD coatings on solid electrolytes also enhance their ionic conductivity and stability. Furthermore, ALD coatings on current collectors improve their stability and reduce their resistance.

Keywords: Atomic Layer Deposition (ALD), Li-ion batteries, Electrolyte coatings, Cathode materials, Anode materials

Introduction

Lithium-ion batteries have gained immense popularity in recent years due to their high energy density, fast charging capabilities, and longer lifespan compared to other rechargeable batteries. The versatility of these batteries has led to their adoption in a wide range of applications, including consumer electronics, electric vehicles, renewable energy storage, medical devices, and aerospace and defense. In consumer electronics, lithium-ion batteries are commonly used to power smartphones, laptops, tablets, and other portable devices due to their small size, lightweight, and ability to deliver high power output. These batteries also provide longer battery life, reducing the need for frequent recharging, which is particularly useful in the fast-paced world of consumer electronics [1].

At their core, Lithium-ion batteries consist of three main components: a positive electrode, a negative electrode, and an electrolyte. The positive electrode, typically made of a lithium-metal oxide compound, and the negative electrode, usually made of graphite, are separated by a thin, porous membrane that allows the flow of lithium ions between them [2], [3]. The electrolyte, a lithium salt dissolved in an organic solvent, acts as a medium for ion transport.

The electrochemical reaction that occurs during charging and discharging involves the movement of lithium ions between the two electrodes. When the battery is charged, lithium ions are extracted from the positive electrode and move through the electrolyte to the negative electrode, where they are stored [4]. This process causes the positive electrode to become positively charged and the negative electrode to become negatively charged [5]. During discharge, the opposite occurs: lithium ions flow from the negative electrode through the electrolyte to the positive electrode, generating an electrical current that powers the device.

There are several different types of Lithium-ion batteries, each with their own unique characteristics and applications. For example, Lithium-ion polymer batteries use a solid polymer electrolyte instead of a liquid electrolyte, which makes them more flexible and lightweight, and therefore well-suited for use in small, portable devices. Lithium iron phosphate (LiFePO_4) batteries have higher thermal stability and longer cycle life than other Lithium-ion batteries, making them a popular choice for use in electric vehicles. Lithium titanate ($\text{Li}_4\text{Ti}_5\text{O}_{12}$) batteries have an even longer cycle life and can charge and discharge at a much faster rate than other Lithium-ion batteries, making them ideal for use in grid-scale energy storage systems [6].

In the realm of electric vehicles, lithium-ion batteries have become the primary source of power, replacing traditional lead-acid batteries due to their high energy density and longer lifespan. The use of these batteries has revolutionized the electric vehicle industry, making it possible for manufacturers to produce cars with a longer range, faster charging times, and better performance [7]–[10]. Furthermore, the use of lithium-ion batteries in electric vehicles has a positive impact on the environment, as it reduces the reliance on fossil fuels and helps to mitigate the effects of climate change [11], [12].

These batteries are used to store excess energy generated by renewable sources, such as solar and wind power, for use when the energy demand is high. This technology helps to address the intermittency issues associated with renewable energy sources, allowing for a more stable and reliable energy supply. Lithium-ion batteries are also being used in grid-level energy storage systems, where they can help to balance the energy supply and demand, reducing the need for expensive and polluting fossil fuel power plants. Lithium-ion batteries are commonly used to power portable medical equipment, such as ventilators, defibrillators, and infusion pumps. These batteries are chosen due to their small size, lightweight, and ability to deliver high power output, which is

essential in emergency situations. The longer lifespan of these batteries also reduces the need for frequent replacements, which can be costly and time-consuming. Lithium-ion batteries are used to power satellites, unmanned aerial vehicles (UAVs), and other high-performance applications. The lightweight and high energy density of these batteries make them ideal for space applications, where weight is a critical factor. Additionally, the ability of lithium-ion batteries to deliver high power output is important in defense applications, where rapid response times are essential [13]. The performance of lithium-ion batteries in EVs is dependent on several factors, including the size of the battery pack, the type and quality of the battery cells used, and the thermal management system used to regulate the temperature of the battery pack [14]–[18]. Battery packs with larger capacities can store more energy and provide greater driving ranges, while high-quality battery cells can offer faster charging times and longer lifespans. The thermal management system is also an important factor in ensuring the performance and longevity of the battery pack. Overheating can cause lithium-ion batteries to degrade and even fail, which can lead to safety concerns [19], [20]. To prevent this, EV manufacturers often incorporate sophisticated thermal management systems that use cooling or heating to maintain the optimal temperature range for the battery pack [21]–[23].

Atomic Layer Deposition (ALD) is a technique used to deposit ultra-thin and conformal layers of materials onto a substrate. The process involves the sequential exposure of the substrate to alternating pulses of gas-phase precursors, which react with the surface to form a monolayer of material, followed by a purge step to remove any unreacted precursors and by-products. The process is then repeated until the desired thickness is achieved. The key feature of ALD is the self-limiting nature of the reaction, which allows for precise control over the thickness and uniformity of the deposited layers at the atomic scale.

ALD is a highly versatile technique that can be used to deposit a wide range of materials, including metals, oxides, nitrides, and sulfides. The process is highly selective and can be used to deposit materials on complex three-dimensional structures, including porous materials and high-aspect-ratio structures. The thickness of the deposited layers can range from a few atomic layers to several hundred nanometers, depending on the deposition conditions. ALD is also compatible with a wide range of substrates, including silicon, glass, metal, and polymers.

Compared to other deposition methods, such as physical vapor deposition (PVD) and chemical vapor deposition (CVD), ALD offers several advantages. PVD and CVD are both relatively simple and cost-effective techniques, but they suffer from poor conformality and thickness control, as well as limited selectivity for certain materials. ALD, on the other hand, offers excellent conformality and thickness control, as well as high selectivity for a wide range of materials. ALD can also be used to deposit materials on a wider range of substrates than PVD or CVD. Additionally, ALD can be used to

deposit materials at lower temperatures, which is important for applications in which the substrate material is sensitive to high temperatures.

Examples of materials that can be deposited using ALD include metal oxides, such as titanium dioxide, aluminum oxide, and zinc oxide, as well as nitrides, such as silicon nitride and aluminum nitride [24]–[26]. These materials are commonly used in a wide range of applications, including semiconductor devices, solar cells, and catalysis. ALD has also been used to deposit metallic materials, such as copper, cobalt, and silver, which are important for applications in interconnects [27]–[38] and plasmonics. ALD can also be used to deposit organic and hybrid materials, such as polymers and metal-organic frameworks (MOFs), which have potential applications in sensors, gas storage, and drug delivery.

Atomic layer deposition (ALD) is a process that involves the deposition of a thin film of material on a substrate by sequentially exposing the surface to alternating precursors. This technique offers exceptional control over film thickness, uniformity, and composition at the atomic scale. One of the most promising applications of ALD is in the field of Li-ion batteries. By using ALD, it is possible to deposit a uniform and conformal coating on various battery components such as electrodes, separators, and electrolytes. This coating can help to prevent unwanted reactions between the electrolyte and the electrodes, which can lead to battery degradation and reduced performance. The use of ALD can also help to improve the stability of the battery, which is important for its long-term performance.

Electrolyte coatings:

In the context of Li-ion batteries, ALD has emerged as a promising method for depositing coatings on the electrodes and separators of these devices. The main advantage of using ALD for battery coatings is the ability to achieve highly uniform and conformal films with sub-nanometer precision. This level of control is particularly important in the case of electrodes, where the coatings must be deposited in a way that does not hinder the diffusion of lithium ions. In addition, ALD can be used to deposit coatings on complex geometries, such as porous electrodes and high-aspect-ratio structures [39]. These properties make ALD a valuable tool for the development of next-generation Li-ion batteries with improved performance and reliability.

One of the key benefits of using ALD for battery coatings is the ability to improve the stability of the electrolyte. The electrolyte is a critical component of a Li-ion battery, as it facilitates the transport of lithium ions between the anode and cathode. However, the electrolyte can also be a source of parasitic reactions that can reduce the capacity and lifetime of the battery. By depositing thin and uniform coatings on the electrode and separator surfaces, ALD can reduce the likelihood of these parasitic reactions occurring. For example, ALD coatings can passivate the surface of the electrode, preventing unwanted reactions with the electrolyte. This can lead to improved stability and a longer

cycle life for the battery. In addition, ALD coatings can help to prevent the formation of solid electrolyte interphase (SEI) layers, which can degrade the performance of the battery over time.

Cathode materials:

In addition to its potential for coating electrodes and separators, ALD can also be used to improve the electrochemical properties of cathode materials in Li-ion batteries. The cathode is the component of the battery that receives electrons from the external circuit during discharge and is responsible for storing lithium ions during charging. The electrochemical performance of the cathode is therefore critical to the overall performance of the battery. By depositing thin and uniform coatings on the surface of the cathode materials, ALD can improve their electrochemical properties and enhance the performance of the battery [40], [41].

One example of the use of ALD for coating cathode materials is the deposition of LiAlO_2 coatings on LiCoO_2 cathodes. LiCoO_2 is a widely used cathode material in Li-ion batteries due to its high energy density, but it suffers from capacity fade and instability at high temperatures. By depositing LiAlO_2 coatings on the surface of LiCoO_2 , researchers have been able to improve the cycling stability and rate capability of the cathodes. The ALD coating is believed to prevent the dissolution of the cathode material and to stabilize the structure of the cathode during cycling. In addition, the ALD coating can prevent unwanted reactions between the cathode material and the electrolyte, further improving the stability and performance of the cathode.

ALD coatings can also be used to modify the surface chemistry of cathode materials. For example, ALD coatings of metal oxides or phosphates can increase the surface area of the cathode material, allowing for more efficient transport of lithium ions. In addition, ALD coatings of metal sulfides or fluorides can increase the capacity and stability of the cathode material. By tuning the composition and thickness of the ALD coatings, researchers can tailor the electrochemical properties of the cathode materials to suit the specific needs of a given application [42], [43].

Anode materials:

ALD has shown great potential in improving the electrochemical properties of anode materials in Li-ion batteries. The anode is responsible for the storage and release of lithium ions during charging and discharging cycles, and its performance is critical to the overall performance of the battery. One way to improve the performance of anode materials is to deposit thin and uniform coatings on their surfaces using ALD. By doing so, the electrochemical properties of the anode can be tuned and enhanced to achieve better performance and stability.

One example of the use of ALD for coating anode materials is the deposition of Al_2O_3 coatings on silicon anodes. Silicon has attracted considerable attention as an anode material due to its high theoretical capacity, but its practical use has been limited by

issues such as large volume changes during cycling and unstable solid electrolyte interphase (SEI) formation. By depositing Al₂O₃ coatings on silicon anodes using ALD, researchers have been able to improve their cycling stability and rate capability. The ALD coating acts as a protective layer that stabilizes the SEI and reduces the negative impact of volume changes on the anode. In addition, the ALD coating can improve the adhesion of the SEI layer to the anode surface, which further enhances the cycling stability of the anode.

ALD coatings can also be used to modify the surface chemistry and morphology of anode materials. For example, ALD coatings of metal oxides or phosphates can improve surface wettability and reduce interfacial resistance, leading to better electron and ion transport. ALD coatings of metal sulfides or nitrides can improve the stability and capacity of the anode material by reducing the formation of SEI layers and the growth of lithium dendrites. By precisely controlling the composition and thickness of the ALD coatings, researchers can tailor the electrochemical properties of the anode materials to achieve optimal performance and stability.

Solid electrolytes:

The use of solid-state electrolytes in Li-ion batteries has been a topic of research due to their potential advantages over liquid electrolytes, such as improved safety, wider operating temperature range, and higher energy density. However, one of the challenges of using solid-state electrolytes is their relatively low ionic conductivity compared to liquid electrolytes. ALD offers a promising approach to address this issue by depositing thin and uniform coatings on the surface of the solid-state electrolytes to improve their ionic conductivity and stability.

One example of the use of ALD for coating solid-state electrolytes is the deposition of LiPON coatings on the surface of the electrolytes. LiPON is a well-known solid-state electrolyte that exhibits high ionic conductivity and stability, making it a promising material for use in Li-ion batteries. By depositing LiPON coatings on the surface of solid-state electrolytes using ALD, researchers have been able to improve their ionic conductivity and stability, leading to better performance and longer cycle life.

ALD coatings can also be used to modify the surface chemistry and morphology of solid-state electrolytes. For example, ALD coatings of metal oxides or phosphates can improve the surface wettability and reduce the interfacial resistance, leading to better ion transport and stability. ALD coatings of metal sulfides or nitrides can improve the stability and conductivity of the solid-state electrolytes by reducing the formation of surface defects and improving the ion hopping between neighboring sites. By precisely controlling the composition and thickness of the ALD coatings, researchers can tailor the electrochemical properties of the solid-state electrolytes to achieve optimal performance and stability.

Current collectors:

In Li-ion batteries, the current collectors play a critical role in the electrochemical reactions and overall performance of the battery. However, the current collectors can also undergo parasitic reactions that can degrade their performance and shorten their cycle life. ALD offers a promising approach to address this issue by depositing thin and uniform coatings on the surface of the current collectors to improve their stability and reduce their resistance.

One example of the use of ALD for coating current collectors is the deposition of TiO₂ coatings on copper current collectors. Copper is a commonly used current collector material in Li-ion batteries due to its low cost and good electrical conductivity. However, copper can also undergo corrosion and oxidation reactions during battery operation, leading to performance degradation and safety issues. By depositing TiO₂ coatings on the surface of the copper current collectors using ALD, researchers have been able to improve their stability and reduce their resistance, leading to better performance and longer cycle life [44], [45].

ALD coatings can also be used to modify the surface chemistry and morphology of the current collectors. For example, ALD coatings of metal oxides or nitrides can improve the adhesion and surface morphology of the current collectors, leading to better contact with the active materials and reduced resistance. ALD coatings of polymers or organic compounds can improve surface wettability and reduce the formation of parasitic reactions at the electrode-electrolyte interface. By precisely controlling the composition and thickness of the ALD coatings, researchers can tailor the electrochemical properties of the current collectors to achieve optimal performance and stability.

Conclusion

ALD has emerged as a powerful tool for depositing thin and uniform coatings on the electrodes and separators of Li-ion batteries. These coatings can improve the stability and performance of the electrolyte by reducing parasitic reactions that can occur at the electrode-electrolyte interface. With its sub-nanometer precision and ability to deposit coatings on complex geometries, ALD is well-suited for the development of next-generation Li-ion batteries with improved performance and reliability. As the demand for high-performance, long-lasting batteries continues to grow, ALD is likely to play an increasingly important role in the battery manufacturing industry. ALD offers a promising approach to improving the electrochemical properties of cathode materials in Li-ion batteries. By depositing thin and uniform coatings on the surface of the cathode, ALD can improve the cycling stability, rate capability, and overall performance of the cathode.

The deposition of thin and uniform coatings on the surface of the anode using ALD can improve the cycling stability, rate capability, and overall performance of the anode. ALD is a promising approach for improving the ionic conductivity and stability of solid-

state electrolytes in Li-ion batteries. The deposition of thin and uniform coatings on the surface of the solid-state electrolytes using ALD can improve their performance, leading to longer cycle life, higher energy density, and improved safety. ALD is a promising approach for improving the stability and reducing the resistance of current collectors in Li-ion batteries. The deposition of thin and uniform coatings on the surface of the current collectors using ALD can improve their performance, leading to longer cycle life, better safety, and higher energy density. With further development and optimization, ALD coatings have the potential to enable the widespread use of high-performance current collectors in Li-ion batteries, contributing to the development of sustainable and efficient energy storage systems.

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