

Overcoming the Limitations of High Energy Density in Lithium-Ion Batteries: Challenges and Future Directions

Siyi Xia*

International Department, Beijing National Day School, Beijing, 100039, China

*Corresponding author: jaweb@ldy.edu.rs

Abstract. Lithium-ion batteries are crucial to advancing sustainable technologies, particularly in areas like electric vehicles and renewable energy systems. However, the quest for higher energy density remains a persistent challenge due to inherent limitations in their current design. This paper offers a comprehensive review of these challenges, focusing on the key components such as electrodes, electrolytes, and separators. Issues like electrolyte volume, separator thickness, and the properties of electrode materials are discussed in depth, showing how these factors constrain energy density. Moreover, the paper explores innovative solutions, including the use of nanotechnology and the development of anode-free battery designs, which represent promising approaches to overcoming these obstacles. These advancements hold significant potential to greatly improve energy density and overall battery performance. In conclusion, ongoing progress in chemistry, materials science, and nanotechnology will continue to drive the enhancement of lithium-ion batteries, unlocking new possibilities for higher energy densities and more efficient applications across various industries.

Keywords: Lithium-ion battery; nanotechnology; energy density; challenge.

1. Introduction

Batteries are becoming a key enabling technology for the global market for sustainable technologies, such as electric vehicles (EV) and smart grids. The popularity of EVs and the expanding scale of EVs increase the demand for electrical energy, as the energy density, safety and service life of the batteries directly affect the use cost and safety of the whole vehicle [1]. To satisfy the constantly increasing demand, scientists are always trying to develop batteries with the ultimate energy density. From the first rechargeable Li-ion cell almost twenty-five years ago with an energy density of 150 W h kg^{-1} to the Li-ion systems that are used nowadays, which offer volumetric energy densities of 780 W h L^{-1} , we can see an obvious improvement in the data [2]. Although progress has already been made, the request for the battery performance is still not fixed.

With the increasing need, scientists realize that batteries with ultimate energy density are of significance. Thus, many of them have researched to improve the energy density of Li-ion batteries. Ming He et al. wrote *The New-Type Batteries with Ultimate Energy Density* to provide an overview of the development history, underlying theories, present problems, and potential solutions for nuclear, lithium-air, and solid-state batteries [3]. Cao et al. did thermodynamic calculations in their paper on *Batteries with high theoretical energy densities* and found that high-energy-density battery systems could theoretically be made possible by Li, Mg, and Al batteries [4]. Wulandari et al. have done an overview of the Li-ion battery and its development in the early years. The introduction of each component was introduced in previous research [5]. This paper will specifically focus on Li-ion batteries, introduce their basic components, list the challenges faced at the present stage, and produce some possible approaches.

2. Working Mechanism of Lithium-Ion Batteries

Li-ion batteries are devices that convert chemical energy into electrical energy with cathode material made of lithium metal or lithium alloy and use a non-aqueous electrolyte solution. Typically, a Li-ion battery consists of the following four key components: the separator, the electrolyte, the

positive electrode (cathode), and the negative electrode (anode). In a battery cell, the separator functions as an inactive component, while the electrodes and electrolytes are primarily involved in the electrochemical reactions. The components and the basic equations on both sides are shown in Fig. 1 [6]. The specific process is described in the following sentences. The buildup of lithium ions at the cathode, and depletion at the anode is called a concentration gradient. As the battery charges, the lithium ions drift from the cathode side and are finally absorbed by the anode. During discharge, on the anode side, electrons and the outer shell of lithium are released to the electrical pathway, while on the cathode side, the lithium ions return to receive the electrons.

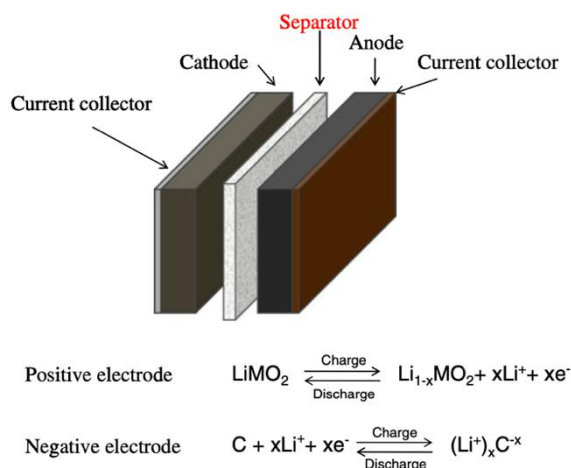


Fig. 1 Schematic of a liquid electrolyte Li-ion cell [6]

3. Limitations on Each Assembly Unit

Several factors affecting energy density have been described in the previous section. In the following part, this paper will discuss the specific challenges faced by each component in improving energy density.

3.1. Challenges Due to Electrode Materials

3.1.1 Anode material

Li-alloy or Li-metal electrodes are used in early lithium-ion batteries. However, the reaction between the liquid organic solvent electrolyte and Li-metal caused many problems, including dendritic growth, capacity loss and some safety issues. To improve energy density and avoid these problems, research has been done on alternative lithium-intercalation compounds to replace the original anode.

Among all compounds, germanium appears to be one of them that performs well increasing in energy density. It has a high lithium capacity of 1623 mA h g^{-1} as well as high electronic conductivity, which is 104 times more than that of silicon. Nevertheless, due to their alloy-based nature, they experience incredibly large volume contractions and expansions ($\sim 300\%$), which lead to a shorter life cycle. High cost and large fading are also factors that need to be improved in the future [5].

3.1.2 Cathode material

Ideally, a cathode in a Li-ion battery should consist of a solid host material with a network structure that facilitates the Li^+ ions to intercalation and de-intercalation. Nevertheless, in terms of discharge capacities, energy densities, and operating voltages, early lithium metal-based batteries did not have great performance.

Lithium manganese-rich (LMR) cathode is one of the materials that attracted attention. Because of its cost-effectiveness, high energy density, good safety profile, and good cycling stability, it has become a promising cathode material [5]. However, continuous energy loss is caused by voltage decay issues and thus hinders the process of commercialization.

3.2. Challenges Due to Electrolytes

There is a distinctive optimal volume of electrolyte in terms of energy density [7]. A low level of electrolyte liquid will result in insufficient wetting of the electrodes, which promotes lithium plating. Thus, during long-term cycling, the continuous electrolyte consumption eventually ends with faster drying, as well as reduced energy density. Meanwhile, excess electrolyte results in increasingly accelerated capacity fading [8] and adds weight, therefore limiting energy density as well as increasing the cost of the battery. According to Thomas et al., in Fig. 2, the electrolyte volume for maximum energy density is shown by the vertical line [7].

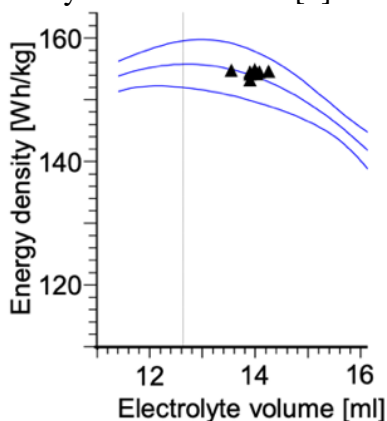


Fig. 2 Electrolyte volume and energy density. The broken line represents the optimal volume in relation to energy density. The lines a and b show the bounds of the confidence interval [7].

3.3. Challenges Due to Separator Thickness

According to Gao-Long Zhu et al., the energy density of batteries can be highly improved by decreasing the thickness of the separator. As shown in Fig. 3, when the separator thickness reduces from 25 μm to 7 μm , the volumetric energy density of the Gr | NCM523 battery will rise by 17.3%. For higher specific energy batteries, for example, Li | S battery, the volumetric energy density increased by 23.4%, which is more significant [9].

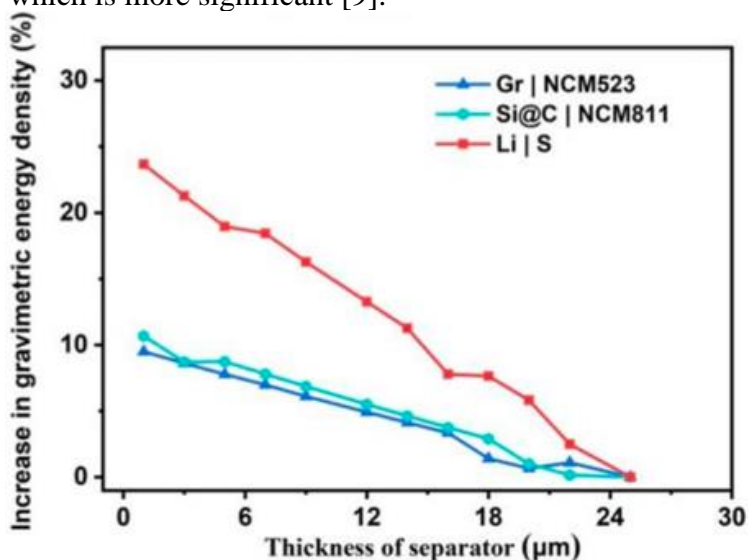


Fig. 3 The increase of volumetric energy density by reducing the thickness of the separator [9]

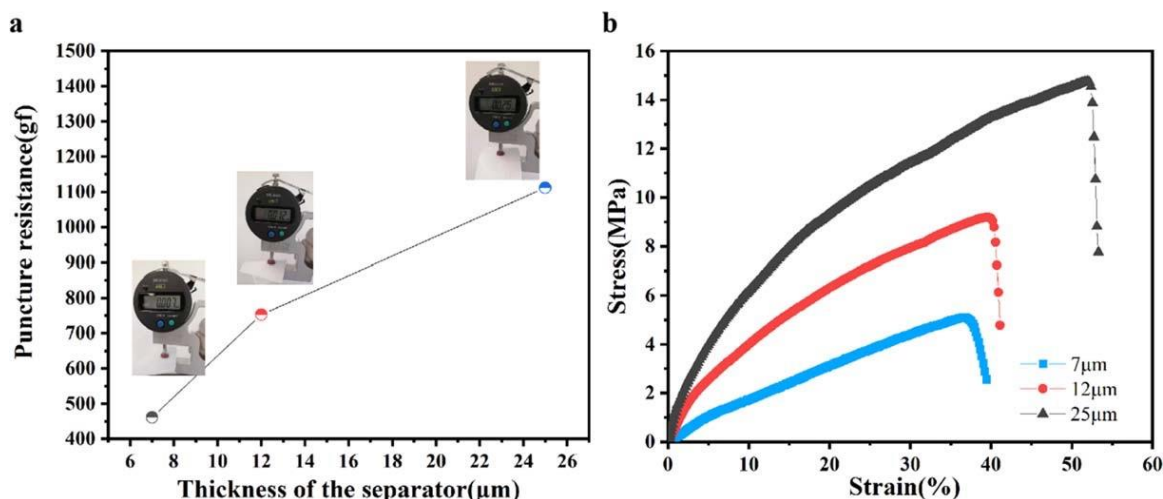


Fig. 4 The performance of the separator with thicknesses of 25 μm, 12 μm, and 7 μm. (a) puncture resistance, (b) tensile strength [7]

However, puncture resistance and tensile strength are both reduced when the separator thickness is thinner. This shows that the mechanical properties of the membrane have clearly weakened (Fig. 4). The mechanical stability will affect electrical performance and the safety performance severely for the traditional separator [9]. An excessively thin membrane may cause width shrinkage [10,11]. Meanwhile, a separator that is too thin can raise the cost and increase the risk of causing an internal short circuit [9].

4. Possible Approaches

In the face of the above challenges, with further research, technology is also constantly improving to solve them. Some of the examples will be listed in the following part.

The use of nanotechnology in batteries has been investigated repeatedly and is considered a very probable solution. It can be easily inferred from Fig. 5 that nano Li-ion has a much better performance in energy density, approximately three times better than Li-ion [12].

Researchers have recently concentrated on modifying the morphology (nanostructured materials) or adding nanomaterials into the structure in order to enhance charging and discharging cycles, raise Li⁺ intercalation and de-intercalation reaction rates, as well as achieve better overall battery performance [5].

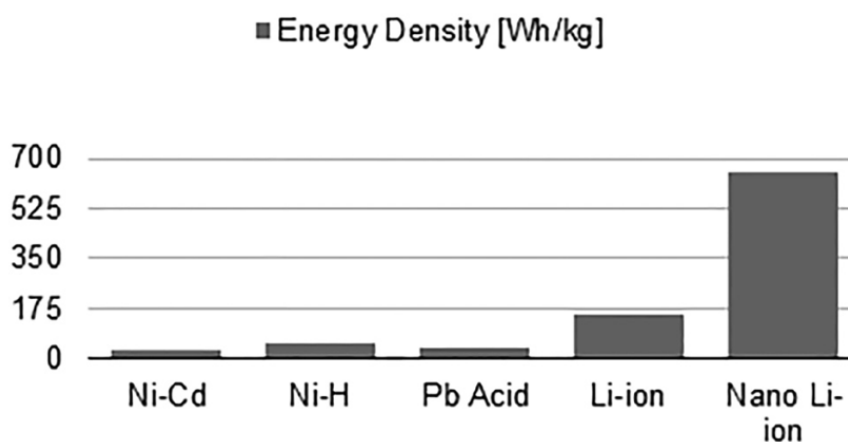


Fig. 5 Visible improvements offered from Li-ion batteries, even before nanotechnology, as compared to older models [12]

Anode-free batteries are a way to raise energy density. Ideally, if the lithium ions extracted from the cathode can be reversibly plated onto the Cu current collector (such as Li metal) and peeled off,

a rechargeable lithium battery with a Cu/separator/cathode/Al configuration can be formed. This battery is called an “anode-free rechargeable lithium metal battery (AFLB)” because it was originally assembled without any active anode material. Notably, the weight and volume needed for the graphite cell are decreased by the lack of a Li host anode material. The energy density of the AFLB will be significantly higher than that of conventional Li-ion batteries because Li has a theoretical capacity of 3820 mAh cm^{-2} , which is more than ten times that of graphite (372 mAh cm^{-2}). This remains the case even after accounting for the increased thickness caused by Li plating during battery charging. This could result in an increase of more than $\approx 50\%$ in the energy density (Wh L^{-1}) of AFLBs relative to conventional Li-ion batteries. The anode-free design works as a Li metal battery after the initial charge process, producing a higher energy density compared to traditional Li-ion batteries and a higher operating voltage of about 0.1 V [13].

5. Conclusion

As was previously mentioned, Li-ion battery energy density presents certain challenges. The electrolyte amount should be carefully controlled in a specific range, and further studies may find a balance between being safe and reducing excessive thickness in the separator. The electrodes need a replacement in materials, as the ones used recently are not perfect at energy density, storage capacity, cycling stability, and safety issues. Therefore, there is still a long way to go to make these batteries commercialized. However, after knowing the challenges, the future of high-energy density batteries is still optimistic. As all property the materials given comes from their structure, especially at the nano scale, nanotechnology is widely used in improving the performance of the materials. Other trials, including the anode-free batteries, are also worth expecting. Hence, it can be hoped that as humans further explore the microcosm and discover the mechanisms as the research goes on, the perfect electrode materials will be found one day. Alternatively, maybe in other ways, new types of lithium-ion batteries could be invented. The study still has some limitations, as factors that may affect the energy density and possible solutions are not fully covered in detail. In the last decades, lots of progress has already been made in the field of lithium-ion batteries, and many researchers have now striven to create better batteries that will improve our life quality. Along with the advancement of chemistry, materials science and technology, there are always some new approaches and techniques. In brief, Li-ion batteries have an unlimited future and are worth the expectation.

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