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Challenges with the Ultimate Energy Density with Li-ion Batteries

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Abstract. Challenges with the energy density with Li-ion batteries are reviewed. At present, Li-ion batteries are widely used in electronic equipment and electric vehicles, but the energy density is not high. It is important to find out the limitations of the energy density with Li-ion batteries. This essay will start the research with the structure of Li-ion batteries, study the chemistry behind Li-ion batteries and give a summary of the limitations of each battery part which affect energy density. In conclusion, it is the chemistry behind batteries that limits the energy density.

Keywords: Challenges; Li-ion batteries; energy density; chemistry; limitations.

1. Induction

Today, the development of Li-ion batteries is limited by the energy density. Compared with the speed of industrial scale expansion, although the energy density of Li-ion batteries is increasing steadily per year, it is still too slow.

According to the Figure 1, the mass energy density (specific energy) of some substances is as follows: liquid hydrogen: 141.6MJ/kg, gasoline: 46.4MJ/kg, diesel: 44.8MJ/kg, lithium: 43MJ/kg, lithium-ion battery: 0.46-0.72MJ/kg. By comparison, it is evident that there is only a small difference in mass energy density among gasoline, diesel and lithium but a big gap between lithium and lithium-ion batteries. It is very useful and interesting to find out what happened from lithium to lithium-ion batteries and the limitations of the ultimate energy density with Li-ion batteries so that we can solve the problem accordingly.

An overview of the Li-ion battery and its limitations with energy density was given [2,3]. For the electrolyte and separator, it is difficult to get rid of them. The basic reasons will be described in the main body. For electrode materials, some challenges are listed and explained, such as the formation of lithium dendrite and lithium extraction&insertion [4-6]. Electrode materials can not use lithium only or add lithium simply.

On the basis of information above, the challenges with the energy density with Li-ion batteries will be summarized from the working principle, chemical reactions and the inner structure.



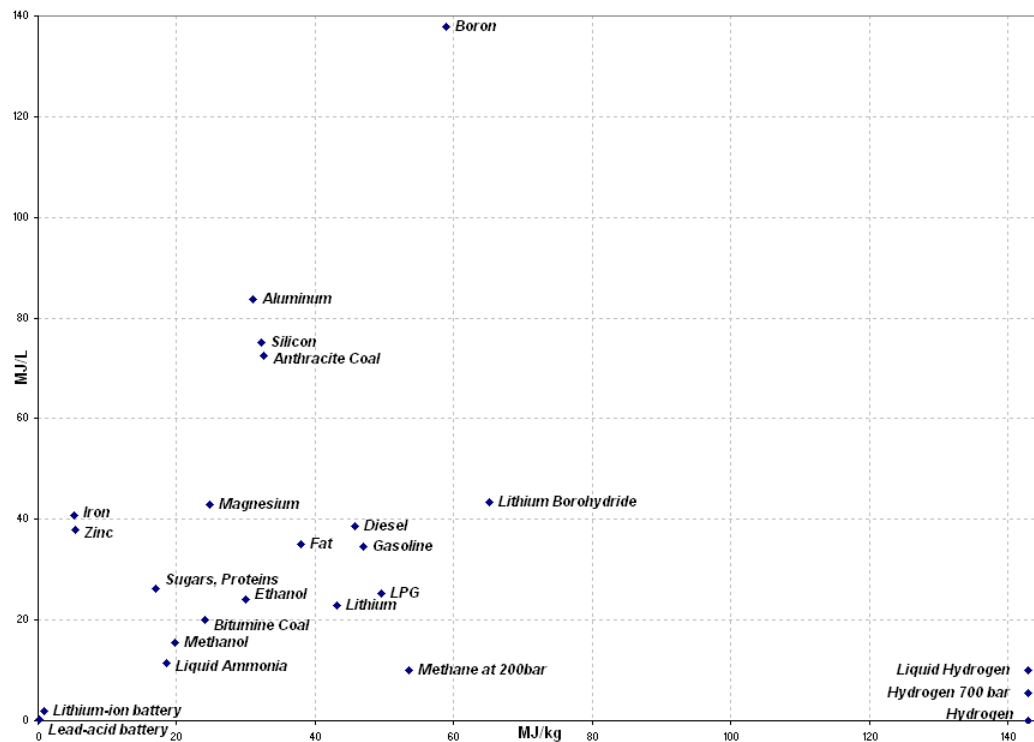


Figure 1. Energy density and specific energy chart of some substances [1]

2. Method

To find out the limitations of the energy density with Li-ion batteries, the research starts with the structure of Li-ion batteries. Then, I study the chemical process and summarize the reasons for energy density with batteries by literature research and qualitative analysis.

3. Results & Discussion

3.1. Basic structure and working principle of Li-ion batteries

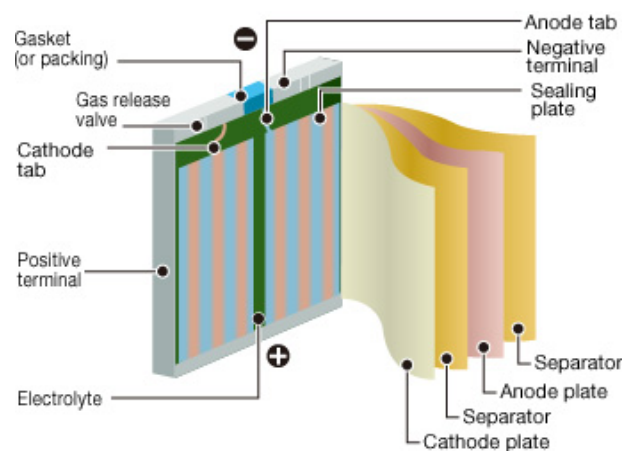


Figure 2. Basic structure of a lithium-ion battery [2]

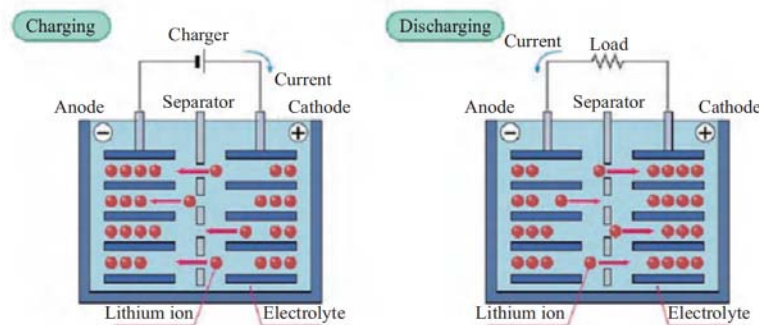


Figure 3. Charging-discharge process of a lithium-ion battery [3]

A Li-ion battery (figure 2) is mainly composed of electrolyte, anode, cathode and separator. Figure 3 shows the charging and discharging progress of a Li-ion battery. During charging, lithium ions are removed from the active material of the positive electrode (cathode), transferred from the electrolyte to the negative electrode (anode) by external voltage, and embedded in the active material of the negative electrode (anode). At the same time, the electrons flow from the positive electrode (cathode) to the negative electrode (anode) through the external circuit. The battery is in the high energy state with the negative electrode (anode) rich in lithium and the positive electrode (cathode) poor in lithium, which realizes the conversion from electric energy to chemical energy. During discharging, the lithium ions are removed from the negative electrode and migrated to the positive electrode and embedded in the lattice. Simultaneously, the electrons flow from the negative electrode to the positive electrode through the external circuit to form the current, which realizes the conversion from chemical energy to electric energy [3].

4. Limitations of each part

In fact, there is not so much lithium in a Li-ion batteries because there are some limitations. And lithium can not be simply added into a Li-ion battery to increase its energy density.

4.1. Electrolyte and separator

Electrolyte, which is generally made of high-purity organic solvent, electrolyte lithium salt and some necessary additives, plays an important role as the carrier of the ion transport in the battery between the two electrodes. However, too much electrolyte is a dead weight, resulting in a lower energy density and unnecessarily increases the costs of the battery [7].

The separator separates the anode from the cathode, which prevents the short circuit caused by the direct contact of electrodes and serves as the medium for the lithium ions in the electrolyte to pass free between electrodes. A good separator is supposed to have: chemical stability (no reaction with electrolyte and electrode materials), wettability (easy to permeate through electrolyte without elongation and contraction), thermal stability (high temperature resistant and isolation performance), mechanical strength (not easily punctured), ionic conductivity (high porosity)[3]. It affects the chemical and safety properties of the battery.

Batteries need the electrolyte and separator to transfer lithium ions in order within the requirements. Therefore, batteries can't get rid of them, although they add extra weight and reduce the energy density. Scientists are searching for the lighter electrolyte and the thinner separator.

4.2. Electrode materials

The problem with Li-ion batteries is that none of the existing electrode materials alone can deliver all the required performance characteristics including high capacity, higher operating voltage, and long cycle life [8].

4.2.1. Anode materials. For higher energy density with batteries, in the case of the same volume, a good material of the anode should be as small and light as possible, and a molecule can release lots of electrons.

As it is mentioned, we hope to transfer lithium ions through the electrolyte and separator in order because it's very important to maintain the stable chemical reaction. But there is no guarantee that lithium ions will be evenly distributed on the anode surface during charging because lithium ions are always disobedient without constraints. The lithium ions that arrive earlier are attached to the anode. Then the subsequent lithium ions are attached to the earlier. Gradually, lithium dendrites are formed.

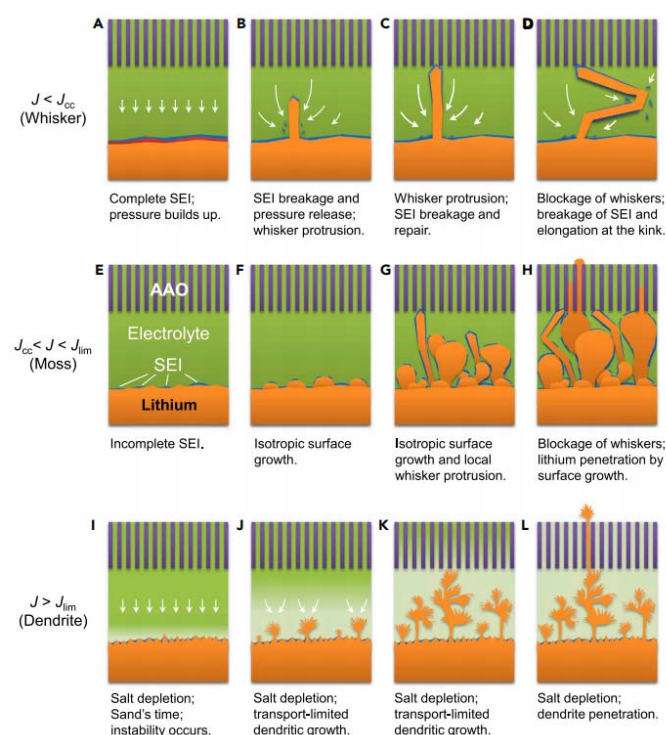


Figure 4. Schematic Summary of the Lithium Growth Mechanisms and Interactions with the Nanoporous Ceramic Separator [6]

From figure 4, the growth of lithium dendrites depends on the applied current density. Under different current densities, lithium grows in different modes and forms different shapes. When the current density is too high, the dendrites will grow wildly [6]. They are thin spikes growing from the anode, which will pierce through the SEI layer and even probably cause a short circuit. So we need to dig some holes for lithium ions to jump in to prevent the phenomenon. Graphite is such a porous material with sheet structure to hold lithium atoms. Therefore, it is widely used as anode materials today. Besides, it is very necessary to reduce the current density and build a high strength protective layer on the anode surface [6]. The problem is solved, but the energy density is diluted. Besides graphite, silicon is also a good material with a much higher capacity than carbon. But it also has a volume effect. Silicon placed in a battery swells as it absorbs positively charged lithium atoms during charging, then shrinks during use as the lithium ion is drawn out of the silicon. This cycle typically causes the silicon to pulverize, degrading the performance of the battery [8].

4.2.2. Cathode materials. At present, cathode materials are mainly LiCoO_2 , LiNiO_2 , LiMnO_2 , LiFePO_4 , $\text{Li}(\text{NiCoMn})\text{O}_2$ [3]. Among them, only about half of lithium ions can be reversible and participate in the extraction and insertion during the charge-discharge process of LiCoO_2 [5].

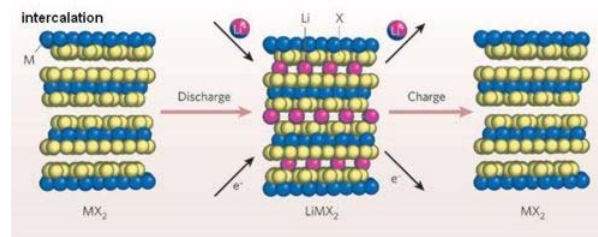


Figure 5. Structural changes of cathode materials during charging and discharging [5]

From figure 5, if lithium ions are excessively extracted from the cathode, the stability and cycle performance of the structure will decrease. Some lithium ions are needed to maintain the structure. Accordingly, the storage capacity of cathode material of lithium-ion batteries is far lower than that of anode material, so the energy density with Li-ion batteries is mainly limited by the cathode material. There are two ways to increase the energy density of cathode materials, one is to increase the specific capacity of cathode materials, the other is to increase the lithium extraction-insertion potential [4].

The extraction or insertion of lithium ion is usually a single electron reaction during charging and discharging. Multi-electron transfer reaction materials are considered to increase the energy density, such as $\text{Li}_3\text{V}_2(\text{PO}_4)_3$, Li_2FeO_4 and $\text{Li}_2\text{FeSiO}_4$ [9-11].

To increase the working potential of materials, among common transition metal, $\text{Ni}^{4+}/\text{Ni}^{3+}$, $\text{Co}^{3+}/\text{Co}^{2+}$ with high redox potential are often considered (Figure 6). A research shows that Ni doping can not only effectively improve the voltage plateau of LiMn_2O_4 material, but also significantly reduce the concentration of Mn^{3+} , slow down the dissolution of Mn, effectively improve the structural stability of the material, so as to improve the cycling performance of the material [12].

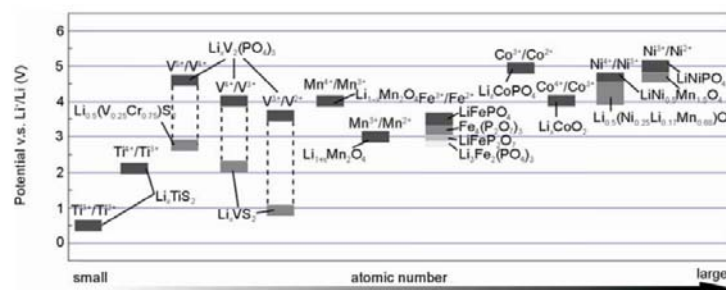


Figure 6. Redox potential of different transition metal [4]

Lithium-rich materials are also a kind of cathode materials with high energy density recently, which have the advantages of high theoretical capacity, high working voltage and low cost. To improve the cycle performance, the most effective structural design method is nano-coating ZrO_2 , TiO_2 , Al_2O_3 . Experiment results show that by coating a suitable inorganic nano-layer on the surface the side reaction between electrode materials and electrolyte can be inhibited and the structural and thermal stability of electrode materials can be improved [13-14].

5. Conclusion

The challenges of energy density with Li-ion batteries have been summed up above. These are always relevant to the chemical process in the batteries. The electrolyte and separator are essential as the passageway of lithium ions. The electrodes need a big storage capacity for charging and discharging repeatedly leading to some extra weight and volume inevitably. For the orderly lithium ions transport, for the orderly distribution of lithium ions and atoms, for the orderly chemical reaction, Li-ion batteries need various accessory materials, which usually are at the cost of energy density though.

Therefore, from lithium to lithium-ion batteries, energy density is sacrificed. However, after knowing the challenges, there is a long way to go. The current situation of energy density with batteries is not optimistic. The perfect electrode materials have not been found yet. New types of lithium-ion batteries still need to be studied further. But there are always some new directions and methods along with the development of chemistry, materials and nanotechnology. The potential of Li-ion batteries is unlimited.

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