

The application of nano silicon in the lithium battery

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Abstract. The pollution of environment is becoming increasingly severe, so protecting the environment is urgent and cannot be delayed. The exhaust emissions from automobiles are an important source of environmental pollution. The electric vehicles are a great solution of the exhaust emissions. They only use the electric as energy and hardly emit any harmful gas, such as carbon dioxide, sulfide gas and nitrogen oxide. But the challenges on electric vehicles battery exist. How to effectively solve the different problems existing in current batteries is an urgent issue that needs to be addressed. To find the solution, nano silicon and composite materials based on nano silicon are selected. This research will discuss the application performance of different nano silicon in lithium batteries. Through data analysis, the results show that the nano silicon material is a promising material for lithium battery. In addition, its composite materials are also a good choice for lithium battery.

Keywords: Nano silicon; lithium-ion batteries; electrochemical performance.

1. Introduction

Lithium batteries are the type of battery that uses lithium metal or lithium alloy as the positive/negative electrode materials. Lithium batteries were first proposed in 1912, but due to the reactivity and technical issues of metallic lithium, the technology of lithium batteries did not have market research until the 1970s. Up to now, lithium batteries have become mainstream. Lithium batteries have many advantages, such as high energy density. The energy density of lithium batteries is much higher than that of traditional lead-acid batteries and nickel hydrogen batteries. This also means that in the same situation, lithium batteries can store more energy. Nowadays, electric vehicle technology has been popularized, and lithium batteries have become the first choice for electric vehicle batteries due to their high energy density, which can make electric vehicles lighter in weight and have a longer range of kilometers [1]. Lithium batteries have a longer lifespan than traditional lead-acid batteries and nickel hydrogen batteries, which can reduce the maintenance frequency and cost of lithium batteries. Low self-discharge rate allows lithium batteries to maintain a high level of charge even when not in use for a long time, making them suitable for devices that require long-term storage. Fast charging reduces charging time and improves efficiency due to its high energy density, low internal resistance, and lower memory effect. High voltage endurance, as it can withstand higher voltages, enables it to drive high-power devices. Lithium batteries also have disadvantages, such as being easily affected by the environment. In the case of high temperature overshoot and short circuit, lithium batteries are prone to fire or explosion. At low temperatures, their performance significantly decreases and their discharge capacity decreases. Moreover, lithium metal itself is an active metal, so the production process cost is higher.

Silicon is a promising negative electrode material for the future, and the carbon elements belonging to silicon and graphite belong to the same group of elements. Compared to graphite electrodes, the $\text{Li}_{4.4}\text{Si}$ alloy formed by silicon and lithium can achieve a theoretical lithium storage capacity of 4200 mAh/g, which is 10 times that of graphite electrodes. It can store more lithium ions, making silicon electrodes more commercially valuable and having a higher range as electric vehicle batteries. Silicon materials are environmentally friendly, have abundant reserves, lower costs, and ultimately emit less pollution to the environment. Silicon is difficult to react chemically with electrolytes and does not undergo co embedding with organic solvents, reducing the risk of use. However, silicon electrodes also have their own problems. For example, silicon is prone to shape deformation during charging and discharging, and its maximum self-expansion rate can even reach 300%. This greatly exacerbates

the instability of silicon as an electrode, which also reduces the lifespan of silicon batteries. The emergence of nanotechnology can improve some of the shortcomings of electrode materials themselves. Nanotechnology is a scientific technique for manufacturing materials using individual atoms and molecules, studying the properties and applications of materials with structures and sizes ranging from 1 to 100 nanometers. Nanomaterials have a large surface area ratio due to their small surface area, which increases the contact area between electrode materials and electrolytes, thereby enhancing reaction activity and improving battery capacity and performance. Due to the small size of nanoparticles, this enhances the transport rate of lithium ions in the electrode, which can improve the charging and discharging speed and efficiency of lithium batteries macroscopically. In addition, the nanoscale of silicon particles can effectively alleviate some of the drawbacks of easy expansion of silicon materials themselves and improve the stability of silicon electrode cells. Nanotechnology can also improve the tendency of silicon to expand by controlling the lattice structure and surface properties of materials, enhance the stability and durability of battery materials, reduce material deactivation and corrosion, and ultimately extend the lifespan of batteries. Because the application of nanotechnology can further enhance the battery capacity and energy density of silicon electrode batteries, this enables batteries to maintain high performance while also reducing their volume, making silicon nanobatteries one of the most promising types of batteries in the future. Nano silicon wire (SiNW) is a very good commercially available electrode material, which has been widely used in lithium battery vehicles [2]. This research will discuss the performance of nano silicon in enhancing the electrochemical performance of lithium batteries.

2. Lithium batteries based on nano silicon

2.1. Energy density

Nano silicon materials have significantly improved the energy density of lithium batteries as negative electrodes. Porous carbon nanotube microspheres (CNTs) with lithium metal immersion were prepared by spray drying method, and then molten lithium was melted into the molten metal by melt immersion method to synthesize lithium carbon composite (Li-CNT), which was doped with 10% nano silicon. Li-CNT-Si loaded with nano silicon was formed. Li-CNT and Li-CNT-Si two substances were measured for capacity in the same way. As shown in Fig. 1, Li-CNT-Si containing nano silicon material has a higher battery capacity compared to Li-CNT, up to 2600 mAh/g, which is about 500 higher than 2100 without silicon [3]. It was found that no alloy reaction between silicon and lithium was observed, and no similar crystal formation was observed. Only elemental silicon was present. Nano silicon exists in the negative electrode of lithium batteries, enhancing the wettability of metallic lithium and improving the reaction efficiency between the active material in the electrode and the electrolyte, thereby increasing the battery's capacitance. Nano silicon has some improvement in the physical properties of lithium battery electrodes, enhancing the infiltration rate of lithium ions. Reducing the negative potential of the battery and increasing the positive potential of the electrode are also ways to improve the energy density of the battery. By placing the above materials into the same lithium extraction experiment, the resulting table that the negative electrode with nano silicon added has a lower potential energy, which increases the potential difference between the two poles of the battery and significantly improves the energy density [3]. Compared to micro silicon, nano silicon has a smaller size, improved expansion during charging and discharging, and smaller polarization, which has increased the battery capacity of lithium batteries [4]. From the formula of energy density, there are three ways to improve the energy density of a battery: increasing the specific capacity of the positive or negative electrode of the battery, increasing the positive electrode potential or decrease the negative electrode potential of the battery and increasing the proportion of active components to improve reaction activity. Nano silicon improves the surface physical properties of the negative electrode in lithium batteries, enhances the reaction efficiency between lithium ions in the electrolyte and active materials in the electrode, and may have a catalytic effect on the reaction. In addition, it reduces the potential energy of the negative electrode of the battery and increases the potential

difference of the battery itself. Nano silicon has a stronger storage capacity for lithium ions, which also increases the specific capacity of the negative electrode of lithium batteries. Nano silicon has made significant improvements in each of these three aspects. In terms of battery energy, nano silicon has a great impact on lithium batteries.

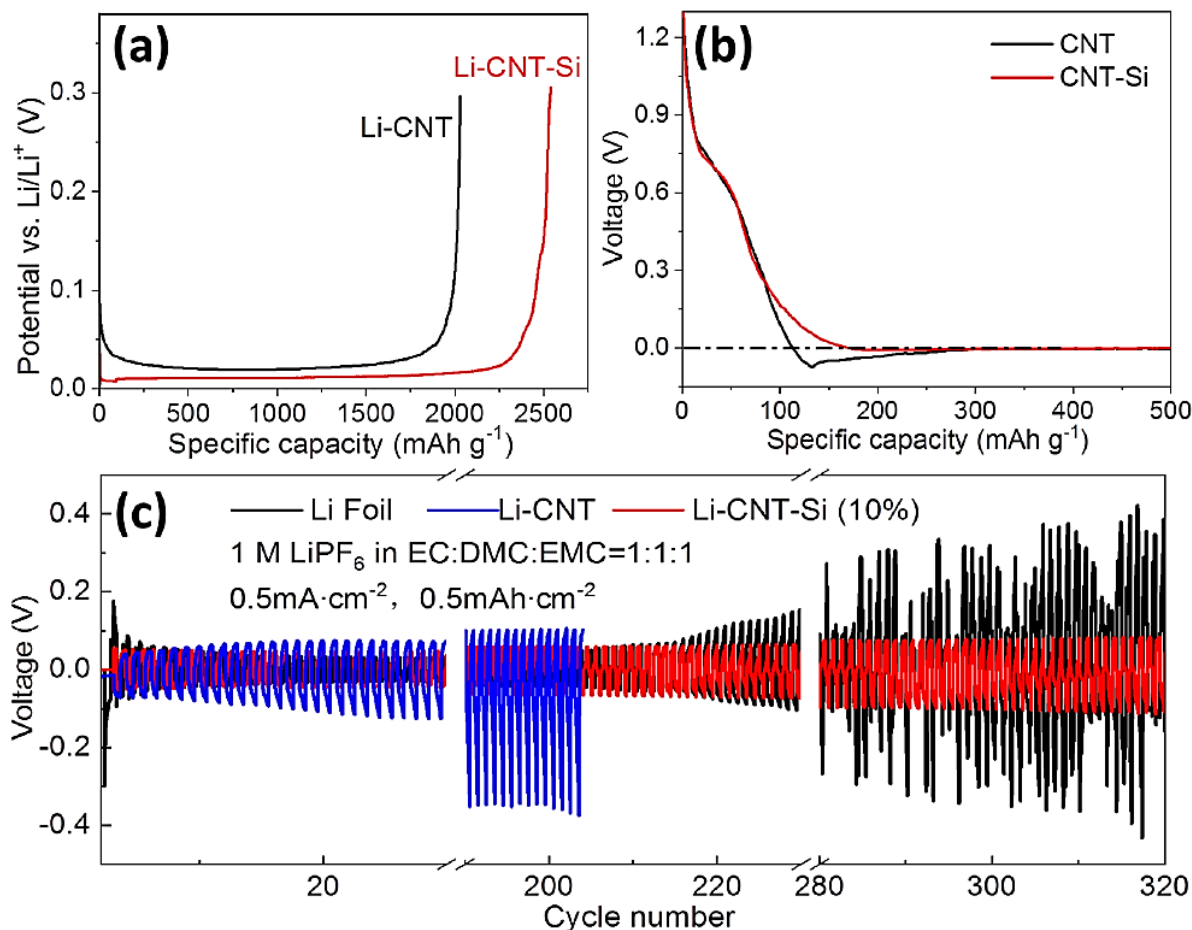


Fig 1. Electrochemical performance of Li-CNT and Li-CNT-Si samples [3]. (a) Constant current discharge curves. (b) Constant current charging curves. (c) Comparison of Overpotential for different samples.

2.2. Lifespan

The lifespan of a battery is also one of the important criteria for measuring its performance. The number of cycles of a battery is one of the important reasons for measuring its lifespan. As the current flows through the charging and discharging process, the electrode material of the battery will also be damaged to a certain extent. Therefore, whether the electrode material of a battery is stable and can accept multiple charging and discharging currents is very important. The coulombic efficiency and the number of cycles of a battery are two important factors for its lifespan. Coulomb efficiency reflects the charge utilization efficiency in batteries and electrochemical reactions, which is influenced by factors such as the surface area, conductivity, and stability of battery electrodes [3]. Silicon itself is a type of material that is easily polarized, and it is prone to expansion during the charging and discharging process of current, and its conductivity is relatively poor. Nanomaterialization reduces the size of silicon materials themselves, which can improve the transmission and scattering mechanisms of positive and negative charges, make the transmission of positive and negative ions freer, increase the concentration of protons, and enhance the conductivity of the electrode itself. Nanomaterials themselves have special electronic structures and electron transport behaviors, which cause slight changes in the properties of the original silicon material and improve the conductivity of the electrode. Nanotechnology reduces the size of silicon particles,

lowers the polarity of silicon itself, alleviates the problem of volume expansion, and improves the stability of the negative electrode in lithium batteries. Nanomaterials themselves have the characteristic of high surface area. The application of nano silicon materials has significantly improved the coulombic efficiency of lithium batteries. Nanotechnology has great stability and improvement ability for silicon materials themselves, but special shaped nano silicon materials can also have unexpectedly good effects. A certain research group has prepared high-performance extremely fine silicon nanowires as negative electrodes, with a first charge capacity of 4200 mAh/g. After 20 cycles at a rate of 0.2 C, the capacity remains at 3500 mAh/g, and at a faster rate of 1 C, the capacity still remains at 2100 mAh/g. The nano silicon material with a silicon hollow spherical shell structure has an empty central part, presenting a hollow spherical shape. The initial capacity is 1420 mAh/g, and after 700 cycles of charging and discharging, there is still 1420 mAh/g. Special structures have unique mechanical properties that mitigate certain points of action that can easily cause nano silicon to expand. The extremely fine nano silicon wires greatly alleviate the internal stress, while the outer layer of the spherical nano silicon material effectively protects the inner layer of silicon [5]. Nano silicon materials as negative electrodes also have significant improvements in the stability of lithium batteries, both in terms of coulombic efficiency and the stability and lifespan of charge discharge cycles. The introduction of special structures also has special physical effects on the nano silicon material itself, improving certain mechanical properties and making it more stable.

2.3. Prevention of the formation of lithium dendrites and SEI

The growth of lithium dendrites is one of the important reasons affecting the safety and stability of lithium batteries. Lithium dendrites are dendritic metallic lithium formed during the reduction of lithium ions. The growth of lithium dendrites can lead to instability at the interface between the electrode and electrolyte during the cycling process of lithium batteries. During the growth of lithium dendrites, the electrolyte is consumed and irreversible precipitates are generated, resulting in a decrease in coulombic efficiency. SEI membrane is a product of the oxidation-reduction reaction of lithium battery electrodes, which plays a protective role between the electrode and the electrolyte. However, the formation of lithium dendrites can also damage the formed SEI film, and the SEI film cannot grow too much, and continuous growth may cause SEI to dissolve in the electrolyte, which in turn leads to an increase in internal resistance and pressure of the battery and in a decrease in battery efficiency. The lithium battery tends to zero at around 37 revolutions per minute, and shows irregular fluctuations at 220 revolutions per minute [3]. This indicates that there is an increase in lithium dendrites, resulting in more dead lithium accumulation at the negative electrode interface, which reduces the conductivity of the lithium battery, increases the interface impedance, and ultimately leads to battery failure. Li-CNT and Li-CNT-Si exhibit relatively stable performance without excessive lithium dendrite formation. This is due to the fact that the particles of nanomaterials are very small, with a pore size of less than 1 nanometer. These tiny particles are difficult to support the generation of dead lithium precipitates, and more often form a smooth thin film on the anode, which better protects the electrode and improves the lifespan of the battery. Compared to Li CNT, Li CNT-Si can store more lithium due to the presence of silicon, reducing the thickness of the SEI film and allowing the battery to operate at a smaller potential. This enables Li-CNT-Si negative electrode lithium batteries to cycle stably for 300 revolutions at lower potentials. Silicon particles have a lower lithium deposition overpotential, which can effectively guide the accurate deposition of lithium ions into the interior of CNT microspheres. Silicon itself is prone to volume expansion during the charging and discharging process, which leads to interface instability and irregular growth of SEI. The SEI film on the silicon surface is uneven and porous, with single-layer, double-layer, and multi-layer film structures, and even a thickness of up to 90 nm. Nanotechnology reduces the particle size of silicon, lowers its volume expansion rate, and enables the protection of SEI films.

2.4. Composite of nano silicon and carbon

Nano silicon materials as negative electrode materials for lithium batteries have made significant improvements, but there are still issues with unstable charging and discharging, as well as easy expansion. Introducing other types of materials and nano silicon will have better performance. Gt SiNW is a newly developed silicon carbon composite material battery composed of nano silicon and graphite [6]. SiNW is evenly distributed around the arranged graphite flakes, effectively protecting the expansion of nano silicon material. It still has 87% of the battery capacity after 250 cycles at a rate of 2 C, and still holds 70% of the battery capacity after 300 cycles. And after 100 cycles, there is only a 20% expansion rate. Through image analysis, 12 nm nano silicon completely covers the graphite sheet, tightly adhering to the surface of graphite. Graphite has better conductivity, which improves the poor conductivity of nano silicon itself. This can also be considered as some synergistic effects between the two materials. During the synthesis process, the organic silane precursor forms a natural organic shell around the nano silicon wire, reducing the contact between the nano silicon and air and minimizing the oxidation of the nano silicon. Due to the uniform distribution of graphite and nano silicon, some nano silicon materials achieve a certain balance when subjected to force, greatly reducing the expansion rate of nano silicon. A carbon coated silicon cone array electrode (SNC-G) was prepared using ion beam etching combined with chemical vapor deposition [4]. The polarity reduction of carbon encapsulation can better leverage the high battery capacity advantage of silicon itself. For the SEI on the electrode surface, irregular SEI appeared on the SNG without carbon encapsulation, and the presence of carbon regularized the nano silicon structure, making the growth of SEI more uniform, protecting the electrode, and extending the battery life.

3. Conclusion

Nano silicon material is a future promising material for the lithium battery anode. The nanosizing silicon could limit the expansion of silicon, so it could longer the life of battery and battery could be more stable. It also protects the sei and prevent the formation of lithium dendrite, and it ensures the high-performance operation of lithium battery. The composition of carbon and nano silicon makes the battery more stable and high efficiency. But due to the nowadays technique limited, the silicon nano material is not better than graphite in the market. In the future, with the technique progress, the silicon expansion could be great limited, and the silicon nano material will be popularized.

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