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Effects of Structural Design, Interface Optimization, and Processing on the Performance of Lithium Battery Anode Silicon Nanomaterials

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Abstract: With an emphasis on the advancements in anode material research, this article offers a comprehensive summary of the major technologies used in lithium-ion batteries, a common type of electrochemical energy storage device. Because silicon has both benefits, such as low cost and high theoretical specific capacity, and significant drawbacks, including electrode pulverization and capacity loss due to volume expansion, it is the main focus of this study. This article goes into great detail on the use of silicon material nanosizing to enhance silicon anode performance, discussing how reducing particle size can mitigate the negative effects of volume changes during cycling. However, the section on compositing and structural design processes lacks sufficient depth, which limits the understanding of how these processes can further improve anode stability and efficiency. Furthermore, the article does not comprehensively cover the diverse methods utilized to enhance silicon anode performance, such as the incorporation of conductive additives or protective coatings. The challenges associated with the practical applications of silicon nanoparticles, such as scalability and cost-effectiveness, are examined in detail; nevertheless, the prospects for further research and technological advancements in these areas are not sufficiently addressed. This paper calls for more in-depth studies and innovations in compositing techniques, structural optimization, and practical solutions to realize the full potential of silicon anodes for advanced energy storage.

Keywords: anode materials for lithium-ion batteries, silicon nanomaterials, structural design, silicon-carbon composite.

1. Introduction

The development of lithium-ion batteries, which have many noteworthy benefits like high energy density and excellent power density, no memory effect, long life, etc., has been prompted by the growing demand for efficient energy storage systems and renewable energy sources worldwide. Since their commercialization in 1991, lithium-ion batteries have become the most popular option for electrochemical energy storage devices. Since their commercialization in 1991, lithium-ion batteries have been widely used in portable electronics and electric vehicles. Large-scale grid storage systems have also been developed using lithium-ion batteries, which are now one of the key technologies advancing the creation of contemporary mobile electronics and electric vehicles [1].

Despite recent advancements in Li-ion battery technology, contemporary innovations face several challenges due to the increasing demand for batteries with enhanced energy densities, greater safety, and increased environmental sustainability. The efficacy of the battery is dictated by the structural and chemical properties of the material constituting the anode component. The development of high-performance anode materials is now the main focus of battery research. This is because it significantly influences the energy output, stability, cost, and safety of batteries.

Silicon is an optimal anode material because to its superior theoretical specific capacity (4200 mAh/g), minimal discharge potential, affordability, and abundance. Silicon has the greatest specific capacity. Although this capacity exceeds the specific capacities of other anticipated nitride and oxide materials, it remains considerably inferior to the capabilities of already used graphite anode materials. The volume of silicon experiences a 400% shift throughout the embedding and delithiation procedures, thus limiting the practical use of silicon anodes. A correlation may be established between this influence and the reduction in capacity, together with the compressive sensitivity of the electrode materials. Considering all these characteristics, it is rather difficult to effectively use silicon anodes.

The use of nanoscale silicon-negative electrode materials is a viable method for addressing this problem. The nanosizing approach increases the specific surface area of the material, hence enhancing its contact area with the electrolyte, which contributes to the battery's high energy storage efficiency. This is achieved by augmenting the material's surface area. This study aims to elucidate how the structural design and compositional attributes of silicon nanoparticles may improve their performance.

2. Influences of silicon nanomaterials on the energy storage performance of lithium battery anode

2.1. Structural design of silicon nanomaterials

Currently, silicon nanowires are often employed because of their volumetric efficiency. Chan [2] synthesized silicon nanowires with an average diameter of 89 nm directly on a stainless steel collector using a gas-liquid-solid technique, thereby alleviating the volume impact of the silicon anode material and significantly enhancing the cycle stability of the silicon anode. The flexibility of the one-dimensional nanowire structure facilitates the timely completion of the silicon anode's embedding/delithiation process. This is due to its release of focused stress, which enhances the structural integrity of the electrode material and mitigates the risk of material rupture and crushing. The one-dimensional nanowire structure allows the deformation of the negative electrode material to be unidirectional, without inducing volumetric changes in other dimensions. This behavior can partially alleviate the volume impact problem. The anode material is significantly diminished as each silicon nanowire may be directly linked to another without requiring additional binders, due to the direct fabrication of silicon nanowires on the collector. Researchers are attempting to transform one-dimensional structures into three-dimensional ones to enhance the surface area of silicon nanoparticles and minimize the transport distance of lithium ions. Mesoporous silicon nanoparticles are extensively utilized because to their substantial specific surface area, exceptionally thin pore walls, and abundant pore volume. These materials can effectively prevent electrode breakage and shorten the transport distance of lithium ions to raise battery power density and prolong battery life[3]. Li[4] prepared mesopore-spongy silicon by using an anodic oxidation method. Using an in-depth transmission electron microscopy study, it was discovered that this material is used as the negative electrode in lithium batteries, can efficiently lessen the significant stress caused by the fluctuation in silicon volume during the charging and discharging process.

2.2. Silicon Nanomaterials Composites

The volume of silicon may expand by up to thirty percent during charging and discharging cycles. Silicon is unsuitable for producing negative electrode materials due to its significant volume change and poor electrical conductivity. To address these challenges, the researchers have explored several approaches of composite technology. One method entails the creation of a "cushioning skeleton" structure that can regulate the material's expansion. Carbon-based anode materials may enhance cycle stability, minimize volume fluctuations while charging and discharging, and provide superior electrical conductivity compared to silicon, making them advantageous for composite materials that include silicon. This is due to the capability of carbon-based anode materials to integrate these attributes. Due of the chemical similarities between silicon and carbon, silicon is frequently used as the foundational element for silicon composites. Silicon-carbon composites may be classified into three categories: porous, yolk-shell, and core-shell[5]. The categories are determined by the morphology of the silicon particles and the configuration of the covering.

In addition to increasing the silicon material's electrical conductivity, the carbon shell serves as a buffer to stop the silicon from displacing or entangling lithium ions, which stops the silicon's volume from increasing. The silicon material's electrical conductivity is enhanced by this carbon shell, which also stops the substance's volume from expanding as the lithium ions are inserted into and extracted from it. Moreover, the carbon shell extends the electrolyte's breakdown and enhances the cycle stability of the electrode material by significantly lowering the direct contact between the silicon and the electrolyte. Using poly(vinyl alcohol) (PVA) as the carbon source material, Hwa [6] performed high-temperature pyrolysis in an inert gas atmosphere to make silicon/carbon composites with carbon shell layer thicknesses ranging from 5 to 10 nm. At 10 nm, silicon and carbon compound. The specific capacity of micron-sized silicon (with a particle size of about 4 μm) and nano silicon without the carbon layer decreased to less than 200 mAh/g after 50 charge/discharge cycles at a current density of 100 mA/g. At 1800 mAh/g, the specific capacity remained still high. Yolk-shell structure is one kind of unique nano multiphase composite material. The spaces left between the silicon core and shell, which are meant to let the silicon core expand and contract, set it apart. Additionally, the purpose of these holes is to provide a stable solid electrolyte (SEI) layer, which improves the material's cycle stability. Zhou[7] created a SiO_2 shell layer on the surface of silicon nanoparticles by using the sol-gel technique. After that, this layer was pyrolyzed using sucrose as a carbon source, which produced an additional layer of carbon capping outside the SiO_2 shell layer. A composite material with the egg yolk-shell structure (Si@void@C) was created by hydrofluoric acid etching, which removed the SiO_2 shell layer. Silicon, the active component, made up 28.54% of the mass of the material. The material maintained a low capacity of 500 mAh/g for 40 cycles after its first discharge, with a specific capacity of 813.90 mAh/g. Si@void@C composites outperformed hollow carbon materials and silicon nanoparticles in terms of cycling performance.

Moreover, stronger structural characteristics are shown by the porous silicon Si@void@C composites during charge/discharge cycles. The porous structure is a wonderful choice for quickly transporting lithium ions and providing a larger specific surface area that permits more active sites for the electrode reaction in order to improve multiplication performance. Yi[8] ground the SiO2 into a powder from micrometers at high temperatures, then used hydrofluoric acid to remove the SiO2 to form a porous silicon structure. This material's 1459 mAh/g specific capacity maintained true after 200 cycles at 1 A/g current density, exceeding that of pure silicon material. This material's 1459 mAh/g specific capacity maintained true after 200 cycles at 1 A/g current density, exceeding that of pure silicon material. Excellent electrical qualities are shown by the specific capacity, which may exceed 700 mAh/g, even with the high current density of 12.80 A/g.

In conclusion, silicon-carbon composites have been built to successfully alleviate the volume expansion issue of silicon during charging and discharging and enhance the electrochemical performance of the electrode materials by adding the core-shell, yolk-shell, and porous designs.

2.3. Other Improvement Methods of Silicon Nanoparticles

The group also looked at silicon nanoparticles and reduced graphene oxide composites as possible materials. Composites made of silicon and reduced graphene oxide do not recycle well. This happens because silicon nanoparticles have a propensity to aggregate at the nanoscale and because graphene's structure does not completely contain silicon nanoparticles. Researchers are trying to find silicon negative electrode materials with better performance by looking at several enhancements for silicon-carbon composites. Li[9] used high-temperature carbonization and ultrasonic dispersion to effectively create a hybrid material comprising NaF, Si, C, and RGO. The main ingredients were graphene oxide solution, phenolic resin, and NaF solution. This material is ideal for use in electrode applications due to its exceptional cycle performance. This might be primarily due to the sodium ions in the NaF solution's capacity to interpenetrate into the graphene oxide interlayer structure. Inhibiting interlayer aggregation substantially improves the uniform dispersion of silicon nanoparticles inside the graphene layer. Furthermore, phenolic resin and reduced graphene oxide were combined to create a composite material with many layers. This structure functions as a helpful buffer against volume variations that occur during charge-discharge cycling and helps to establish a stable solid electrolyte interface (SEI). This configuration somewhat reduces the direct contact between the silicon nanoparticles and the electrolyte. Finally, when the electrolyte degrades, the fluorine ions in the NaF solution may prevent the production of hydrofluoric acid. This prolongs the service life of the electrode structure and prevents hydrofluoric acid from corroding the active components of the electrodes. After 100 cycles, the reversible capacity may reach 1,048 mAh/g if the density is 100 nM/g and the retention rate is above 90% for the next 60 cycles. The performance of metal elements may be improved by both technical developments and the hybridization of silicon nanostructures with metal components. In the end, anode materials—which are conductive mediators and buffer substrates—have a significant effect on the conductivity of metals. In the end, this results in a significant enhancement of the electrode materials' total electrochemical performance. Using elemental copper, which has a high mechanical strength, in combination with the carbon matrix may effectively minimize the volume expansion of silicon particles throughout the charging and discharging process. By combining copper with the carbon matrix, materials with extraordinary electrical conductivity may have an increase in overall electrical conductivity. The material's electrochemical performance will also be enhanced by this. Throughout their investigation, Wang[10] used thermosetting vinyl resin monomer as the reaction medium and carbon source, silicon from silica nanopowder, and copper acetate monohydrate as the first precursor of copper. Using the thermally started polymerization technique, it is possible to produce nanohybrid materials with an average particle size of around 100 nanometers that consist of silicon and carbon as well as silicon, copper, and carbon. These materials consist of silicon, metal, and carbon in equal amounts, with carbon accounting for about half of the total material mass. The ratio of silicon to copper atoms is around 5:1. The trial findings suggest that the cycling performance of the hybrids composed of silicon, carbon, and copper is comparable to that of the hybrids composed of silicon and carbon alone. The total electrical conductivity of Si/C nanohybrids was improved by applying electrochemical impedance spectroscopy on extremely electrically conductive monolithic copper.

3. Summary and Outlook

Silicon materials may encounter substantial problems, including electrode fracture and capacity reduction, due to their volumetric expansion. Silicon materials may encounter substantial problems, including electrode fracture and capacity reduction, due to their volumetric expansion. Enhancing the electrochemical performance of silicon materials may be achieved by structural design and compositing. This may be achieved by mitigating the detrimental effects of volume increase and addressing these particular challenges. Nonetheless, some significant objectives remain to be achieved for silicon-based anode materials. These include enhancing interfacial properties, regulating morphogenesis, and generating environmentally safe materials. Future research should prioritize enhancing the interfacial properties and structural integrity of silicon-based composites. This will facilitate the creation of more efficient, safe, and ecologically sustainable solutions for large-scale energy storage systems and electric vehicles in the future.

Authors Contribution

All the authors contributed equally and their names were listed in alphabetical order.

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