

Influence of particle morphology and atomic layer deposition of ZnO on the electrochemical performance of Si/graphite anodes for Li-ion batteries

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Growing global energy demand and transport electrification require more efficient energy storage technologies. Lithium-ion batteries (LIB) are currently the most popular energy storage devices due to their high energy density and flexible design. However, the use of LIBs in next-generation portable electronics and electric vehicles requires improved capacity and power density. Commercial LIB fails to meet these growing demands due to its anode with limited capacity (graphite). Silicon is one of the most promising alternative anode materials because it is the second most-abundant element on earth and has the highest known theoretical charge capacity of $\approx 4200 \text{ mAh g}^{-1}$, which is 10 times higher than existing graphite anodes (capacity $\approx 372 \text{ mAh g}^{-1}$). However, the use of silicon as an anode is challenging due to its high volumetric change (400 %) during lithium insertion and extraction, which leads to particle cracking and pulverization. This eventually leads to fading capacity and limited cycle life. A practical approach to tackle this challenge is to reduce the size of silicon particles, thereby increasing the surface area and number of active sites for lithium-ion flux and reducing internal structural stress during charging and discharging cycles.

This work presents a detailed investigation on the effects of the ball milling on the particle size of silicon, structural and electrochemical behaviour of silicon/graphite composite anodes. Planetary ball milling at lower speed for longer timescale reduced the particle size of as received Si powder from $7 \mu\text{m}$ to $3 \mu\text{m}$, whereas high-energy milling (HEM) of powder at 1000 rpm reduced the particle size to $0.7 \mu\text{m}$ within one hour. The specific surface area increased remarkably from $2 \text{ m}^2 \text{ g}^{-1}$ (as received Si powder) to $30 \text{ m}^2 \text{ g}^{-1}$ for HEM powder. These finer particles provide more active sites for lithium-ion transport, distribute volumetric strain more effectively, thereby minimizing mechanical degradation. As a result, the optimized silicon morphology delivers improved capacity, and long-term cycling stability. This highlights the essential role of particle-size engineering in the development of high-performance silicon/graphite anodes for future battery applications.

Moreover, the electrochemical performance of Si/graphite anode (especially at high charging/discharging rates) was improved by atomic layer deposition of ZnO on the surface of Si particles. The specific discharge capacity increased from 400 mAh g^{-1} to 1000 mAh g^{-1} at 2C rate.