High capacity of Si/SiOx materials as anode and the effects of FEC as an electrolyte additive for lithium ion battery

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The submicro-sized and nanostructured SiOx aggregated powder is prepared by combinational routes of high energy mechanical milling (HEMM) and wet milling. Milled SiOx powder is investigated by particle size analyzer, SEM, TEM, XPS and XRD as well as the control ones. Combining the high energy mechanical milling and CVD temperature treatments not only fracture primary SiOx particles but also form nano-sized Si crystal constructed by amorphous and nanocrystalline phases. We successfully achieved surface modification of SiOx with carbon source as methane and enhanced the electrochemical performance of an SiOx-based anode. A simple planetary ball-milling process followed by heat treatment over a range of temperatures (~500° C) was used to carry out the surface modification. This important investigation confirmed that the heat treatment temperature significantly affected the molecular structure in the modification layer, and its thickness led to a higher discharge capacity. The electrochemical performance using the SiOx as the anode material achieved an excellent capacity of 1587 mAh g-1 after 100 charge/discharge cycles with a 85.8% retention. The capacity regained to ~1500 mAh g-1 with the reversal of the current rate to 0.1C, with very high retention of 80%, indicating significantly enhanced strength of the modified SiOx anode in a lithium ion battery.

The electrolyte additive Fluoroethylene Carbonate (FEC) is well known for the high capacity's reversibility in Si-based anode battery, as it forms the SEI with uniform compositions that can adapt the high volume's change of Silicon. We integrate surface compositions and generated gases to deduce a reasonable FEC reduction path in the battery that consists of LiNixMnyCozO2 (NMC) cathode and Si-based anode. After long cycle, the problem of gas expansion will appear. In this research, we added 10wt% Fluoroethylene Carbonate (FEC) into the electrolyte (EC/DEC/EMC 3 : 2 : 5 w/w with 1M LiPF6). The gas produced by Ethylene Carbonate (EC) and FEC in redox stage was collected and qualified by using FTIR (Gas Analysis). XPS and FTIR (ATR) analysis results indicated that FEC has changed the proportion of interface products such as $(CH_2OCO_2Li)_2$, LiF, $ROCO_2Li$, Li_2CO_3, $Li_xPO_yF_z$, and so on. The electrolyte additive FEC affected the formation mechanism of SEI film in the cycle life of the battery. After the SEI film was formed in the first charge and discharge, the coulombic efficiency of the battery with FEC had been better than that of the battery without FEC, and after long cycles, we found that retention of the battery with FEC was also better.

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