

ANODE MATERIALS FOR LITHIUM ION BATTERIES BY CHEMICAL VAPOR DEPOSITION

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Anode materials such as silicon provide alternatives to carbons used presently as anodes in lithium ion batteries. In theory, delithiation of LiC_6 formed during the charge state should deliver 372 mAh / g. In practice, the discharge capacities of carbon-based anodes are as low as 290 mAh / g. This discrepancy occurs because of the formation of a solid electrolyte interface (SEI) during the first charge state (1) and the slow diffusion of Li^+ between graphite layers.

Lithium ions diffuse faster in $\text{Li}_{4.4}\text{Si}$ alloys that are formed in-situ in Si based anodes. Initial capacities (over 1000 mAh / g) offered by silicon-based anodes decrease during subsequent cycles. Poor reversibility of the alloying reaction at room temperature prevents the successful application of pure silicon powder in lithium ion batteries (2). Several composite materials were prepared (3) in order to prevent the SEI formation in silicon alloy anodes and to increase their performance in batteries. The addition of carbon to silicon powder improves its cycleability (3). Nanodispersed silicon exhibits specific capacities up to 600 mAh / g and good reversibility of the alloying reaction with lithium.

In this study materials containing silicon of sub-micron particle size and silicon-carbon composite materials were prepared. Anode materials containing silicon and carbon-coated silicon were prepared. Chemical vapor deposition (CVD) and metal-organic chemical vapor deposition (MOCVD) methods were used in the syntheses. Toluene was used as a precursor for carbon coatings on silicon powder. The temperature of carbon deposition was 950°C.

In the second part of this study the effects of nitrogen purge and the lack of purging gas on the resulting carbon coating and the carbon-silicon interface were investigated. Silicon wafers (orientation $\langle 111 \rangle$) were the substrates for carbon coating. Toluene was kept as a precursor for carbon coatings on silicon wafers.

HRSEM analysis, EDS analysis, Raman spectroscopy, TEM micrographs, AES/XPS depth profiling and cell cycling experiments were carried out for sample characterization. The cycling properties of pure silicon powder and carbon-coated silicon powder were compared. In the preliminary coin cell test of carbon coated silicon powder (coating temperature $\sim 950^\circ\text{C}$) capacity cutoff was limited to 1000 mAh / g in the voltage range of 0.01 to 1.3 volts. Coulombic efficiency was 92.7 and 98.8 %, respectively, during the initial cycles. Capacity and voltage profiles for this coin cell test are shown in Fig. 1. HRSEM of carbon deposits on silicon powder and silicon wafer are shown in Fig. 2 and 3, respectively.

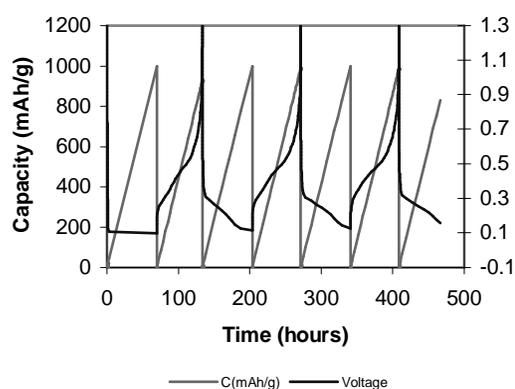


Fig. 1. Capacity and voltage profile for a coin cell containing carbon coated silicon powder.

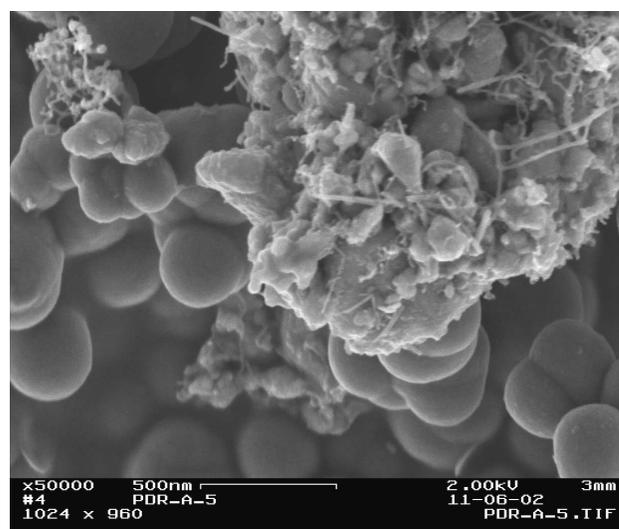


Fig. 2. HRSEM micrograph of carbon deposits on silicon powder.

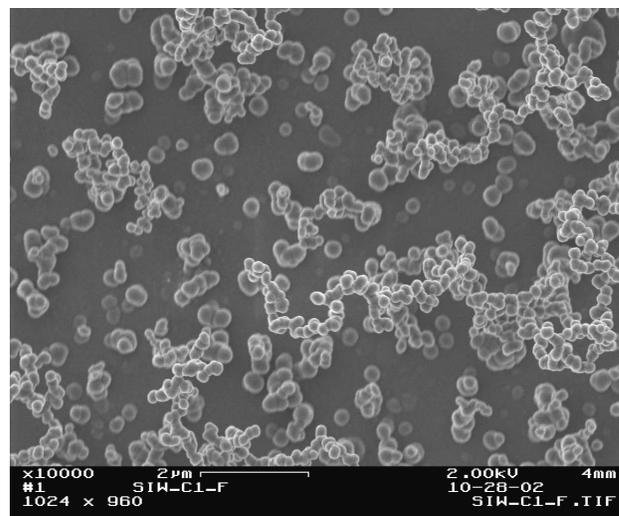


Fig. 3. HRSEM micrograph of carbon deposits on silicon wafer.

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