Improving Distribution of Silicon Nano-particle and Electrochemical Performance of Si/C Composite for LIB Anodes

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Introduction

Silicon is a promising anode material for lithium ion batteries due to its high theoretical capacity (~4200 mAh/g), but its poor performance of cycles prevents its commercialization. It is attributed to the volume expansion during Li-ion insertion/extraction which deteriorates active materials. In addition, it becomes serious when nano-sized silicon particles are used, and its electrochemical properties are determined to the homogeneous distribution of Si nano-particles in a carbon matrix. In this experiment, we prepared silcon nano-particle/graphite (Si/C) composites as an anode material and investigated its physco-chemical and electrochemical properties. Especially, we are trying to distribute silicon nano-particles well on the surface of the carbon. The surface of silicon nano-particle was modified by a reaction with various silane coupling agents (SCA), and this reaction results in the formation of chemical bond between graphite and silicon nanoparticle. The obtained Si/C composite was spheriodized, and the resulting Si/C composites showed better capacity and stable cycleability.

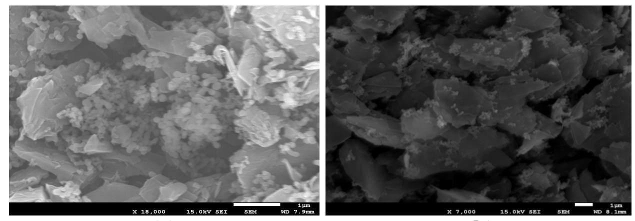
Experimental

Surface modification of30 - 50 nm sized silicon nanoparticle (Nanoamor) with silane coupling agents and graphite matrix (SFG-6 flake type graphite) 30% of H_2O_2 and 6M HNO_3 wers performed. Hydroxyl-terminated silicon nanoparticles were treated with mercapto silane coupling agent (3-mercaptopropyl trimetholxysilane, Shinetsu), and then, the surface-treated silicon nanoparticles mixed with acid treated graphite were refluxed at ~80 ^{o}C overnight. The dispersion of silicon on the obtained active material and the internal resistance were measured by FE-SEM/EDS (FIB-SEM for cross section) and VSP (EC-Lab v-10.23), respectively. For the electrochemical performance measurement, the anode, separator (polypropylene film, Celgard), Li metal as a counter electrode and 1.15M $LiPF_6$ in EC:DEC:FEC (5:70:25) solution (Panax Etec) were used for 2032 type coin-cell assembly, and the cells were tested at 0.2 C (CC-CV mode) in the cut-off range from 0.01 to 1.5 V vs. Li/Li^+ by WBCS3000 cycler (WonAtech, Korea).

Result & Discussion

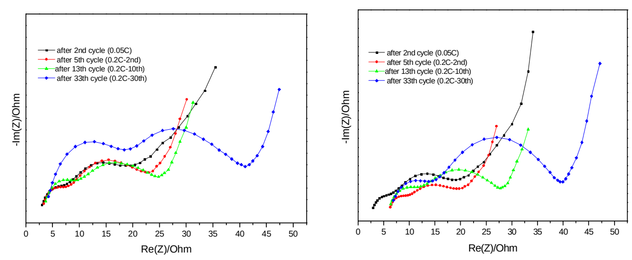
Figure 1 shows the morphology of silicon nanoparticle graphite composites. The aggregation of silicon was suppressed after the treatment of silane coupling agent. It is thought that silane coupling agent which was reacted with hydroxyl functional group of acid-treated silicon nanoparticle reduces effectively its spontaneous aggregation and helps it dispersed on the acid-treated matrix.

Figure 2 shows electrochemical impedance spectra of the reference and surface-modified Si/C composites. Although both cases showed no big differences in SEI resistance, charge-transfer resistance was reduced until ~30 cycles.



(a) (b)

Figure 1. SEM images of the Si/C composite before (a) and after (b) silane coupling agent treatment



(a) (b)

Figure. 2. EIS results of the reference (a) and modified (b) Si/C composites

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References

[1] Hyesun Kim; Jaephil Cho, *Nano letter*, 2008, **8**, No. 11, 3688-3691
[2] Jaephil Cho, *J. Mater. Chem.*, 2010, **20**, 4009-4024