

Analysis of SiO Anode for Lithium-ion Battery

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Recently, SiO has attracted attention as a promising negative-electrode material due to its relatively high lithium content, which provides greater energy density than lithium-intercalated carbons. It has also been cited for its long cycle life (Fig. 1)¹⁾. Conversely, it has been reported that lithium alloys, such as Si, show very large change in volume during charge and discharge, leading to stresses that cause the alloy to disintegrate and the anode to lose capacity upon cycling. This difference in cycle performance is believed to arise from the difference of chemical structure of Si and SiO, however it has not been studied intensively. Thus, we have analyzed the chemical structure of the anode using X-ray photoelectron spectroscopy (XPS).

We deposited SiO films on Cu foil by vapor deposition. Charge and discharge cycle tests were done using half cells, and after the cycle we brought out the anode. We evaluated three states of SiO chemical structure with XPS. The states we evaluated are the as deposition state, the initial charge state, and the initial discharge state. In order to avoid contact with oxygen, sample handling was carried out under inert gas during disassemble the battery to XPS measurement. The thickness of the 500 nm of the layer was removed using Ar sputtering to reduce the risk of surface contamination.

The spectra are fitted into five peaks corresponding to five different Si oxidation states on the basis of the binding energy previously reported^{2,3)}. As can be seen in Fig. 2, the Si oxidation states are mainly attributed to Si³⁺ and Si⁰. We have confirmed that silicon oxide still remains after the initial charge.

Table 1 shows the abundance ratio of Si oxidation states of Si 2p spectra. Si²⁺ abundance ratio decreased during initial charge, and increased during initial discharge. In contrast, Si⁰ abundance ratio increased during initial charge, and decreased during initial discharge.

These results indicate that the Si oxidation states of SiO can be reversibly changed from Si²⁺ to Si⁰, which is apparently a key factor of the long SiO cycle life.

Acknowledgment

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References

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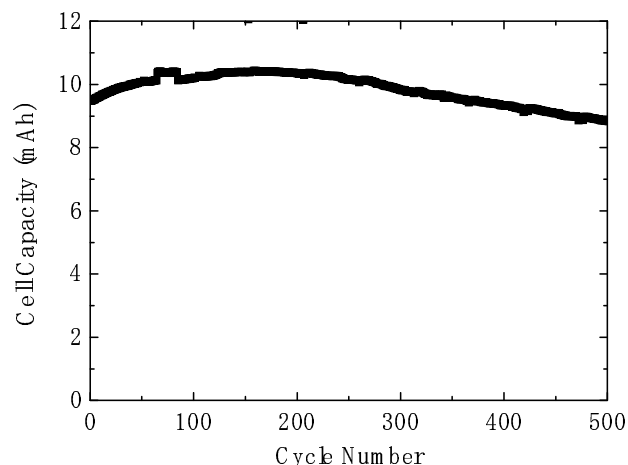


Fig. 1 Cell cycle life using SiO anode

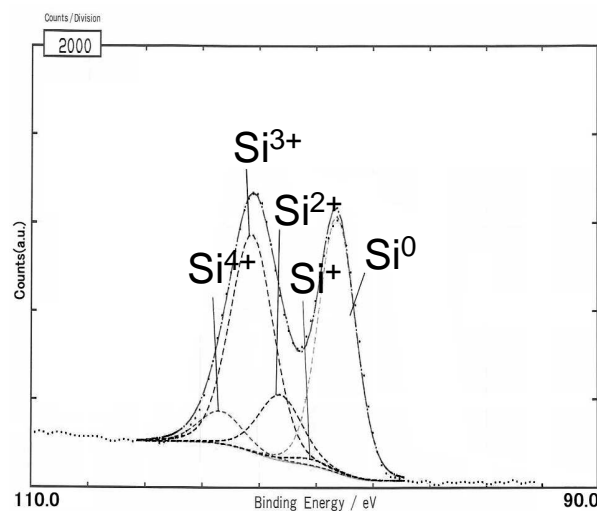


Fig. 2 Si2p core level spectra of SiO after initial charge

Table 1 Abundance ratio of Si oxidation states of Si 2p spectra (a) as deposition, (b) after initial charge and (c) after initial discharge

	Si ⁰	Si ⁺	Si ²⁺	Si ³⁺	Si ⁴⁺
(a)	23.6%	0.9%	34.2%	39.7%	1.5%
(b)	40.3%	1.2%	12.1%	40.4%	6.0%
(c)	21.5%	-	27.9%	42.1%	8.5%