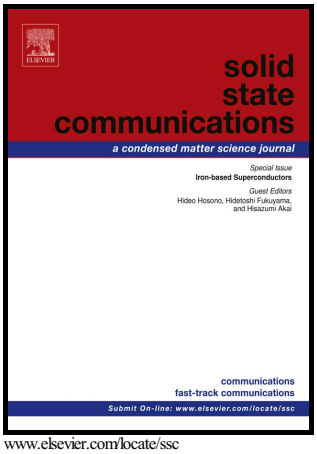

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Investigation of Carbon-Coated Silicon Oxide Phase Changes During Charge/Discharge by Oxygen and Lithium K-Edge X-ray Absorption Fine Structure Spectroscopy

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Abstract

To understand the phase changes associated with the charge/discharge mechanism during cycling, we evaluated the electronic states of oxygen and lithium atoms in the high-capacity anode material SiO-C using O and Li K-edge X-ray absorption fine structure (XAFS) spectroscopy. Multiple peaks observed in the O K-edge spectrum in the 532–548 eV range were likely related to O–Si bonds. During the initial charge, when SiO-C occludes Li, a new peak related to Li–O bonds appeared at 534 eV. During the initial discharge, this peak was maintained at potentials below 0.7 V vs. Li/Li^+, but decreased at higher potentials, suggesting the presence of a phase change point near 0.7 V vs. Li/Li^+. This change was also supported by the Li K-edge spectrum. An examination of the phase change after charge/discharge cycling at negative electrode termination potentials of 0.66 and 1.1 V vs. Li/Li^+ confirmed that the phase structure was stable when cycling at potentials below the phase change point, but unstable at higher potentials. Thus, stable charge/discharge cycling can be achieved by designing batteries with negative electrode termination potentials that are lower than the potential at which the phase change occurs.

Keywords

X-ray absorption fine structure spectroscopy, silicon oxide, anode, charge/discharge

1. Introduction

High-energy Li ion secondary batteries have been developed predominantly for use in miniature mobile devices. Recently, development has progressed in large-scale stationary energy storage for vehicle and stationary applications. In particular, for vehicles, development has achieved battery miniaturization and high-capacity batteries to improve mileage. Development in high-capacity