Understanding the effect of Al:ZnO coating on the structural and chemical stabilities of LiNi1/3Mn1/3Co1/3O2 electrode

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LiNi1/3Mn1/3Co1/3O2 (NMC-111) is one of the most promising cathode materials in Li-ion batteries. However, structural and chemical instabilities of the electrode / electrolyte interface at high charge cut-off voltages lead to capacity fading. It is necessary to study the structure and chemistry of electrodes and electrode / electrolyte interfaces in Li-ion batteries since the interfaces determine the local Li-ion transport kinetics and the electrochemical performance. Surface modification using metal oxides is one of the best approaches to suppress capacity fading. In this work, a systematic study on the degradation mechanism of an uncoated NMC-111 powder electrode was presented. Moreover, the effect of an Al-doped ZnO (Al:ZnO) coating layer on the chemical and structural stabilities of NMC-111 electrode cycled at high charge cut-off voltages was analyzed using scanning electron microscopy, analytical transmission electron microscopy, and X-ray photoelectron spectroscopy. The objective of this work is to study the effect of electrode / electrolyte interface on the degradation mechanism and also the effect of coating layer on the stability of electrode / electrolyte interface. The coating layer was applied to commercial NMC-111 powder using a microwave-assisted sol-gel synthesis method. High-resolution TEM imaging, STEM imaging, nano-beam electron diffraction (NBD), electron-energy-loss spectroscopy (EELS), and energy dispersive X-ray spectroscopy (EDX) were carried out using a FEI Titan Themis G3 60-300 TEM. Cross-sectional TEM samples were prepared using a ZEISS cross-beam 340 FIB-SEM. In the case of uncoated NMC-111 electrode, cation mixing, pitting corrosion due to hydrofluoric acid attacking the electrode surface, and an irreversible phase transformation from a trigonal layered to a rock-salt phase occurred, leading to capacity fading. While, in the case of Al:ZnO – coated NMC-111 electrode, cation mixing, pitting corrosion, and the irreversible phase transformation were mitigated. Therefore, the rate capability and capacity retention were improved since the coating layer protected the electrode surface from the direct electrolyte exposure.

Keywords:

EELS, TEM, EDX, NBD, SEM

Reference:

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