ALD Coatings on Cathodes with Increased Performance for Lithium Ion Batteries

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Introduction

LiCoO₂ cathode exhibits a theoretical capacity of 272 mAh g⁻¹. When the battery is charged a cutoff voltage up to 4.2 V, only half lithium can be extracted from LiCoO₂ to Li_{0.5}CoO₂, resulting in the limited capacity (only ~140 mAh g^{-1}) in practical applications. Thus, it is a well accepted strategy to charge LiCoO2 cathode beyond 4.2 V, in order to utilize more lithium ions from the cathode and to increase the specific capacity and the energy density of LiCoO₂. However, the charge cutoff voltage over 4.2 V incurred the dissolution of LiCoO₂ into the electrolyte, thereby causing an increased capacity fade upon cycling. The atomic layer deposition (ALD) technique is a surface-controlled and layer-by-layer process, relying on two sequential self terminating halfreactions.^[1-5] ALD shows significant promise for ultra-thin film coating layers on LIB cathodes. In this study, ALD derived coatings were employed to mitigate the capacity fading of LiCoO₂ in order to satisfy LIB application. In this presentation, we will report the roles of various metal oxides on LiCoO₂ performance.

Experimental

Various metal oxide thin films were directly coated on LiCoO₂ electrode in an ALD reactor. Titanium tetraisopropoxide, tetrakis dimethylamido zirconium and Trimethylaluminum were chosen as Ti, Zr and Al precursors, respectively, while deionized water was commonly used as the oxygen source in the three cases. More details for the ALD deposition can be found in our previous work.^{[1-} ⁵ A typical ALD cycle consisted of a sequential and alternating supply of two precursors as follows: a 0.5-s supply of the metal precursor vapor, a 3-s extended exposure of the precursor to the cathode electrode, a 10-s N_2 purge, a 1-s supply of H₂O vapor, a 3-s extended exposure of H₂O vapor to the cathode electrode, and another 10-s N_2 purge.

Results

ALD derived surface coating layers are effective to increase the cycling performance and the rate capability of the commercial LiCoO₂ cathode in LIBs. Our results demonstrate that various metal oxide coating layers have different influences on battery performance of LiCoO₂ electrode. Different ALD-cycle deposition can result in in some difference enhancing cvcling performance, and the thinnest coatings show the best effect. As shown in Fig. 1, the Al₂O₃ coating shows better cycling performance, and delivers a reversible capacity of 148 mAh g⁻¹ in the 100th cycle. The ZrO₂ coating is better in increasing the rate capability than the TiO₂ and Al₂O₃ ones, and still reaches a reversible capacity of 95 mAh g⁻¹ at a high current density of 700 mA g-1. Several important roles of these layers coating affecting performance improvement will be discussed in detail.

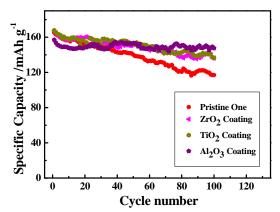


Figure 1 Comparison of various coating layer effect on LiCoO₂ performance

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