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XANES and EXAFS analysis of LixMn2O4 as thin-film cathode material for lithium-ion batteries

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Owing to their light weight and high energy density, lithium-ion batteries (LIBs) are currently the method of choice for energy storage for numerous applications and are dominating the rechargeable batteries market. However, it is well accepted that the interfaces of the LIBs electrode materials are the source of problems in terms of capacity fading and safety. Atomic layer deposition (ALD) is considered as great technique to address these shortcomings, allowing the production of highly uniform and conformal films with an accurate thickness and growth control at the sub-Å level, making it an enabling technology for 3D all-solid state thin-film LIBs. Among the available cathode materials for these batteries, lithium manganate spinel is a promising candidate due to its low cost, low toxicity, high voltage, high specific capacity for storage of electrochemical energy, and minimal structural changes during charge/discharge cycling. In the present study, thin films of LiXMn2O4 spinel with different level of lithiation were produced by means of ALD. The synthesis process consisted of the deposition of a 100-nm MnO2 parent oxide film on a Si wafer that was subsequently lithiated using a precursor of lithium tert-butoxide and water (LiOt Bu +H2O). To gain fundamental understanding of this lithiation process, the atomic structure of this material was investigated by means of XAS at the CLÆSS beamline from the ALBA synchrotron radiation facility. Signals were collected at the Mn-K edge (6.5 keV) simultaneously in TFY (total fluorescence yield) and TEY (total electron yield) modes. From the XANES region, it was demonstrated that the Mn oxidation state decreases as a function of lithitation cycles, while from the EXAFS analysis, it was shown that there are not corner-sharing octahedral in the spinel cathode material in comparison to the parent oxide MnO2 with rutile structure. Further analysis and interpretation are under way, specially focused on polarization and strain studies (in-plane and out-plane-bond distances and strains).

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