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Voltage-Composition profile and structural analysis of low and high temperature Li_xCoO_2 cathodes

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Abstract – The Li_xCoO_2 is one of the most promising insertion material for cathode electrode. However, the crystalline structure of this material when obtained at low temperature (LT-Li_xCoO_2) is not well determined in the literature. The difficulty in distinguishing the different structures present in LT-Li_xCoO_2 is due to similarities between layered and spinel phases, which generally present highly coincident diffraction pattern. In this work, it was established a correlation between the structure and the electrochemical behavior of this material obtained at low and high temperatures.

The Li_xCoO_2 is one of the most promising insertion material for cathode electrode. This material presents a disordered layered structure (rocksalt) with symmetry R3m when prepared at high temperature (up 700 ºC, i.e. HT-Li_xCoO_2). However, there is no consensus in the literature about the crystal structure of this material obtained at low temperature (LT-Li_xCoO_2). The difficulty in distinguishing the different structures present in LT-Li_xCoO_2 is due to similarities between layered and spinel phases, which generally present highly coincident diffraction patterns. In this work the structures of the Li_xCoO_2 prepared at low and high temperatures were investigated by analysis of synchrotron X-ray powder diffraction (including a quantitative Rietveld refinement) by means of which it was evidenced the presence of two majority phases for Li_xCoO_2 prepared at low temperature, i.e. spinel and layered phase. The intercalation of lithium ions in the Li_xCoO_2 host material was investigated by discharge curves and voltage-composition profile and a correlation was established, for the first time, between this curves and the structure of the Li_xCoO_2 prepared at low and high temperatures. The electrochemical behavior, in agreement with structural results, revealed the existence of two sites of lithium intercalation in both materials and one extra site of lithium intercalation in LT-Li_xCoO_2.

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