

Local Atomic Structure of Nanocrystalline K-Li-Mn-O-I Studied with Pair Distribution Function Analysis

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Lithium manganese oxides have recently attracted interest due to their potential application as a cathode material in Li-ion batteries. Recent studies show that nanocrystalline lithium manganese oxides could present significant advantages over their crystalline counterparts. Some of these advantages are structural stability after prolonged cycling, large capacity and smooth discharge curve. We present structural studies of two K-Li-Mn-O-I samples prepared by two different methods, using water or acetone solutions. The nanocrystalline nature of the samples is confirmed by the lack of sharp Bragg peaks in the diffraction pattern. The Pair Distribution Function method is successfully applied to obtain structural information for the two samples from high-energy synchrotron radiation diffraction data. Both materials are layered, but with different distances between the MnO₂ layers. In the case of the water-based material, this distance is considerably larger than for the acetone-based. This result can explain the different electrochemical performance of the two materials.