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Lithium-Iron Phosphates as Cathode Active Materials for Lithium-Ion Batteries

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The transition metal ions connect the diphosphate anions forming a three-dimensional network with channels filled by Li+ cations expected to exhibit high mobility. All compounds order magnetically at low temperatures due the Fe-Fe interactions. Lithium iron phosphate (LiFeP2O7) as cathode active material was synthesized by sol-gel method. Synthesized LiFeP2O7 was characterized by XRD, SEM and EDS.

Key words: EDS, SEM, XRD, Lithium-iron phosphate, Lithium-ion

1. Introduction

The use of layered transition-metal oxides as positive electrode materials for lithium secondary batteries has been studied extensively. Recently, there has been considerable interest in compounds built with phosphate anions such as PO_4^{3-} or $P_2O_7^{4-}$ species because they undergo frameworks where tunnels are accessible for mobile cations such as alkali (Na^+, Li^+) ions. They belong to the wide class of insertion compounds which can be used as positive electrode materials in advanced lithium-ion cells. Also, lithium-ion oxide conductors based on phosphate framework offer some advantages in practical applications due to lower cost, safety, environmental benignity, stability and low toxicity [1-3].

Among them, lithium pyrophosphates $LiMP_2O_7$ (M: transition metal) have been subjected to intense research for the past few years, mainly due to the high mobility of lithium ions which promotes the insertion/extraction reactions. Indeed, there are a large number of crystalline materials containing P_2O_7 groups in the literature with the general formula $LiMP_2O_7$. These phosphates exist in different structures: $LiVP_2O_7$, $LiFeP_2O_7$, $LiCrP_2O_7$ crystallize in the space group P21. In the case of $LiFeP_2O_7$, lithium could be inserted (Fe^{3+} reduction) at 2.95 V against Li/Li^+. Nevertheless, the extraction of lithium from $LiFeP_2O_7$ takes place at high potentials as a result of the high oxidizing power of the Fe^{3+}/Fe^{2+} redox couple [1].

2. Methods and Results

The diphosphate $LiFeP_2O_7$, in which the PO_4 tetrahedra are linked by bridging oxygen to give P_2O_7 groups, crystallizes in the monoclinic system ($P2_1$ space group). The P_2O_7 groups are connected to the FeO_6 octahedron by sharing two oxygen corners, each belonging to a PO_4 unit (Fig. 1).

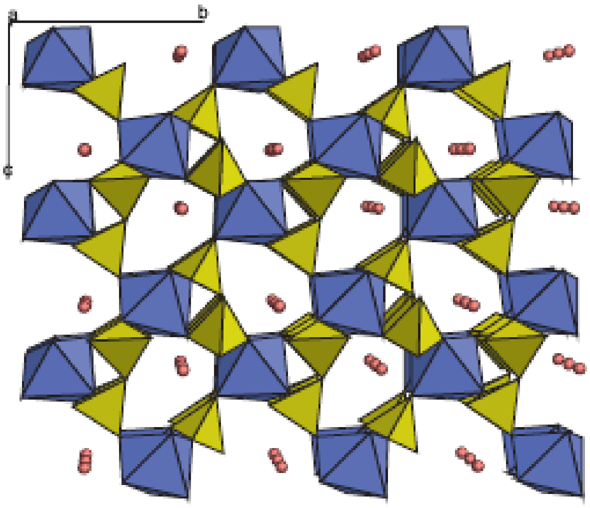

Figure 1. Structure of $LiFeP_2O_7$. Lithium ions are located in tunnels delimited by FeO6 octahedra and PO_4 tetrahedra [1]

This induces a 3D framework in which channels collinear to the [0 0 1] direction are formed and where the lithium ions are located. Moreover, these compounds may present interesting magnetic properties, as iron atoms are connected through super-super exchange paths, involving diphosphate groups (made of two corner-sharing PO_4 tetrahedra). Furthermore, all distances and angles in the studied diphosphates are in good agreement with many other condensed phosphates reported before [1, 3, 4].

The crystallinity of $LiFeP_2O_7$ was assessed from both the SEM and XRD patterns as shown in Figs. 2 and 3, respectively.

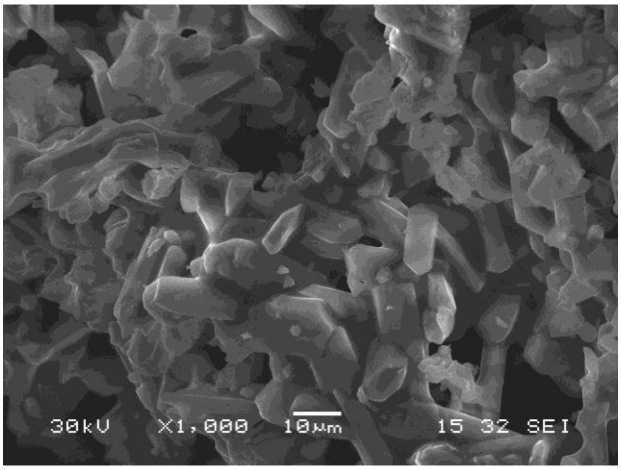

Figure 2: The SEM image of $LiFeP_2O_7$

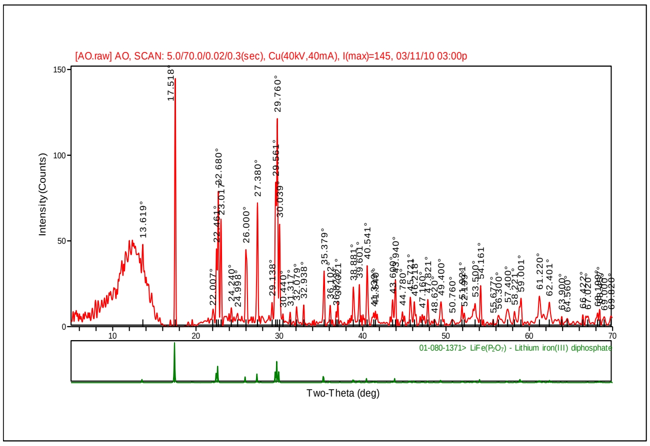

Figure 3: The XRD pattern of $LiFeP_2O_7$

4. Conclusions

The crystallinity of $LiFeP_2O_7$ was assessed from both the SEM and XRD patterns as shown in Figs. 2 and 3, respectively.

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