The Structural Transition and Magnetic Properties of Lithium Deintercalation in $LiFePO_4$

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Lithium deintercalation of $(1-x)$ $LiFePO_4/x$ $FePO_4$ $(0 \leq x \leq 1)$ have been studied with X-ray diffraction (XRD), inductively coupled plasma-atomic emission spectrometer (ICP-AES), and Mössbauer spectroscopy. Lithium deintercalation to obtain $(1-x)$ $LiFePO_4/x$ $FePO_4$ was done by chemical oxidation process using NO_2BF_4. The crystal structure was found to be an orthorhombic with space group *Pnma* for each sample. There exists a mixture of $LiFePO_4$ and $FePO_4$ phase between $x = 0$ and 1. The Mössbauer spectra have been taken at various temperatures ranging from 4.2 K to room temperature. The magnetic Néel temperature (T_N) was determined to be 51 and 114 K for $LiFePO_4$ and $FePO_4$. Also, the iron ions were ferric and ferrous for $LiFePO_4$ and $FePO_4$, both occupying the octahedral sites at various temperatures. We confirmed that the change of Mössbauer spectrum shape as the evidence of two-valence state of iron ions coexists on lithium deintercalation in $LiFePO_4$ from 4.2 K to room temperature.

***Index Terms*—Li-ion battery, Mössbauer spectroscopy, olivine.**