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ABSTRACTS

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AV-18. Delithiated $Fe_{1-x}Mg_xPO_4$ cathode materials: structural, magnetic, and Mössbauer studies. *H. Choi*[1], J. Kim[1] and C. Kim[1] *1. Department of Physics, Kookmin University, Seoul, The Republic of Korea*

Lithium-ion deficient $Fe_{1-x}Mg_xPO_4$ is a promising cathode material for batteries because of Mg ion is not electrochemically active. $Fe_{1-x}Mg_xPO_4$ (x = 0.01, 0.05, and 0.1) are synthesized by two-step method, which involves combining the solid-state reaction method and the chemical lithium deintercalation method. From the XRD analysis results, the crystal structure of $Fe_{1-x}Mg_xPO_4$ was an orthorhombic structure with *Pnma* space group. The magnetic properties of the sample were determined from vibrating sample magnetometer (VSM) and Mösssbauer spectroscopy, including their magnetic interactions, transition metal oxidation states, and structural ordering. The magnetic susceptibility (χ) of $Fe_{1-x}Mg_xPO_4$ was measured using VSM at temperatures from 4 to 290 K. Typical antiferromagnetic behavior can be found in the below Néel temperature (T_N). The magnetic parameters of $Fe_{1-x}Mg_xPO_4$ calculated from the fitted inverse susceptibility curves χ^{-1}(T). The T_N and curie constant decreases with increasing Mg content, which is consistent with the weakening of the antiferromagnetic exchange and a lower effective total magnetic moment after Mg substitution. Furthermore, for $Fe_{1-x}Mg_xPO_4$, the value of effective moment (μ_{eff}) decreases as expected with increasing Mg content. This can be explained the crystallographically strong deformation of $Fe(Mg)O_6$ octahedra. Mössbauer spectroscopy measurements at various temperatures were performed. The spectra at room temperature was fitted with one doublet, which having the isomer shift (δ) = 0.32–0.43 mm/s (Fe^{3+}). The large electric quadrupole splitting (1.46–1.92 mm/s) value is explained by the asymmetric local environment of the Fe atom. Below the T_N, the spectra of $Fe_{1-x}Mg_xPO_4$ were analyzed the eight resonance absorption lines (including two relatively small intensities). We can be obtained the mechanisms of the processes associated with lithium deintercalation in compounds based on $LiMPO_4/MPO_4$ from Mössbauer spectroscopy data.

[1] S. Yaroslavtsev, S. Novikova and A. Yaroslavtsev, Solid State Ion., Vol. 317, p.149 (2018)

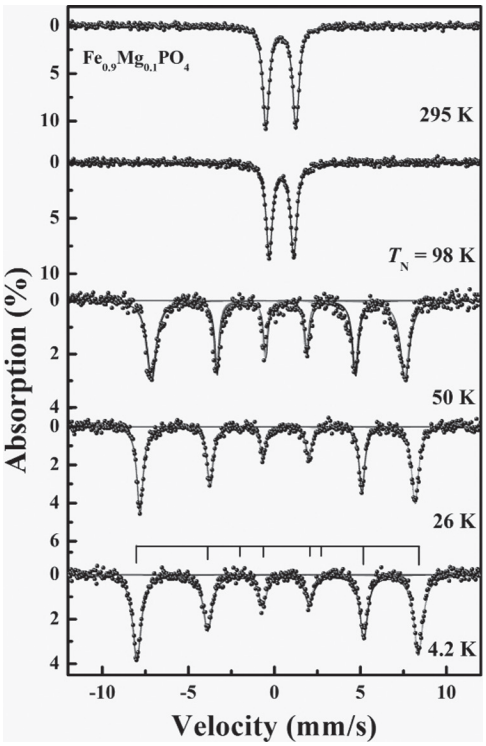

Fig. 1. Mössbauer spectra of $Fe_{0.9}Mg_{0.1}PO_4$ at various temperatures.

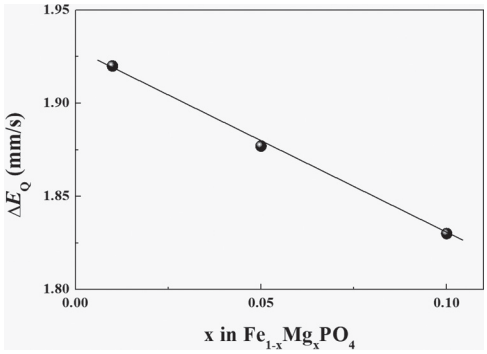

Fig. 2. Mg contents dependence of the electric quadrupole splitting of $Fe_{1-x}Mg_xPO_4$ at 4.2 K.