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ABSTRACTS BOOK

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AS-03. Mg shallow doping on structural and magnetic properties of $LiFePO_4$ triphylite.

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INTRODUCTION $LiFePO_4$ triphylite has the disadvantage of low electronic conductivity and slow lithium ion diffusion which lead to poor rate capability. Therefore, various studies to overcome these limitations have been conducted including cation doping and carbon coating [1]. Among various cation, it was reported that Mg doped $LiFePO_4$ showed enhanced rate performance [2]. The aim of this work was to investigate the structural and magnetic properties of Mg shallow doped $LiFePO_4$. We have found that Mg shallow doped in $LiFePO_4$ sufficiently affects the structural and magnetic properties. EXPERIMENT PROCEDURES Mg shallow doped $LiFePO_4$ triphylite precursor was prepared using typical solid-state reaction process. Li_2CO_3, $FeC_2O_42H_2O$, $(NH_4)H_2PO_4$, and $(CH_3COO)_2Mg4H_2O$ in stoichiometric ratios were mixed and the mixture is calcined at 300°C for 4 h in Ar. Then, the powder was pressed into a pellet and annealed at 700°C for 10 h in Ar. X-ray diffraction (XRD) measurements of the samples were performed using Rigaku Ultima IV diffractometer with Cu$K\alpha$ radiation. The XRD patterns were analyzed using FullProf software and Rietveld refinement. The temperature dependence of the dc magnetic susceptibility was measured using a vibrating sample magnetometer (VSM). The magnetization curves were measured in a magnetic field of 100 Oe between 4.2 and 295 K. Mössbauer spectra have been recorded by using a conventional spectrometer of electromechanical-type with the constant acceleration mode. A ^{57}Co (Rh) source has been used and calibration has been done α-Fe foil as a reference sample. The spectra were analyzed within the framework of the Hamilton model. RESULTS AND DISCUSSION Th XRD patterns of Mg shallow doped $LiFePO_4$, $LiFe_{1-x}Mg_xPO_4$ (x = 0.01, 0.05, and 0.1), samples were analyzed by Rietveld refinement and all diffraction peaks are indexed to an orthorhombic crystal structure with the *Pnma* space group. The lattice parameters of $LiFe_{1-x}Mg_xPO_4$ with increasing Mg content showed a slight contraction of the unit cell relative to pure $LiFePO_4$. A slight contraction is due to the difference between the ionic radius of Fe^{2+} and Mg^{2+} in the octahedron. The temperature dependences of the magnetic susceptibility $\chi(T)$ curve under 100 Oe showed a typical antiferromagnetic behavior.(Fig. 1) From these results, it was confirmed that the Néel temperature (T_N) and spin-reorientation temperature (T_S) of $LiFe_{1-x}Mg_xPO_4$ was monotonically decreased from 51 and 22 K for x = 0.01 to 47 and 15 K for x = 0.1. This decrease can be explained due to the weakening of the antiferromagnetic behavior as Mg^{2+} (L = 1, S = 0) ions are substituted for Fe^{2+} (L = 2, S = 2) ions. In order to obtain the experimental effect moment (μ_{eff}) of the samples, the inverse susceptibility was determined by the Curie-Weiss equation from the paramagnetic region. The Mössbauer spectra of the $LiFe_{1-x}Mg_xPO_4$ were obtained at various temperatures ranging from 4.2 to 295 K. The spectrum of the samples at 295 K was analyzed one symmetric doublet with an isomer shift (δ) of 1.10 mm/s and electric quadrupole splitting (ΔE_Q) of 2.95 mm/s, which is typical for octahedral Fe^{2+}. The Mössbauer spectra measured at 4.2 K were confirmed that $LiFe_{1-x}Mg_xPO_4$ had eight asymmetric line indicating that they have both electric quadrupole interaction and magnetic dipole interaction.(Fig. 2) As the temperature decreases, the increased ΔE_Q value was found to decrease below T_S due to spin-orbit coupling. Furthermore, we found that the magnetic hyperfine field value of the samples with temperature showed a large slope value in T_S. These Mössbauer results can be seen to match the T_S values obtained from VSM.

[1] D. Goonetilleke, T. Faulkner, V. K. Peterson, etal., J. Power sources, Vol. 394, p.1-8 (2018). [2] Y. Li, J. Hao, G. Geng, etal., RSC Adv., Vol. 5, p.68681 (2015).

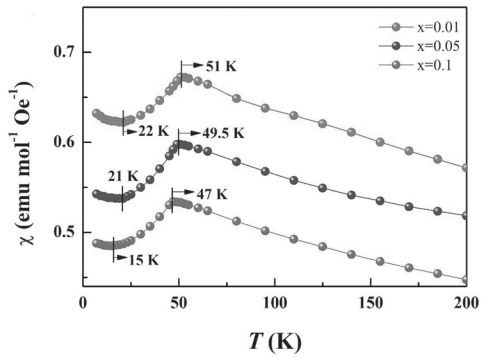

Fig. 1. Temperature dependence of the magnetic susceptibility $\chi(T)$ of $LiFe_{1-x}Mg_xPO_4$ (x = 0.01, 0.05, and 0.1).

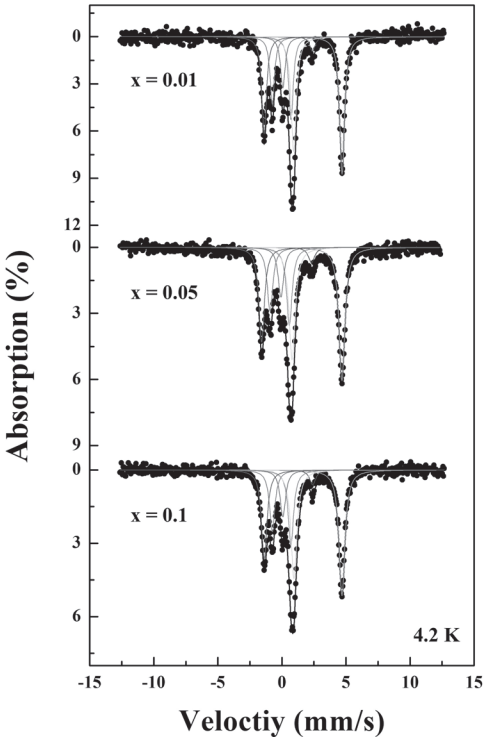

Fig. 2. Mössbauer spectra of $LiFe_{1-x}Mg_xPO_4$ (x = 0.01, 0.05, and 0.1) at 4.2 K.