Effect of Mg Shallow Doping on Structural and Magnetic Properties of $LiFePO_4$ Triphylite

Hyunkyung Choi, Jae Yeon Seo, and Chul Sung Kim

Department of Physics, Kookmin University, Seoul 02707, South Korea

We examine the structural and magnetic properties of Mg shallow-doped $LiMg_xFe_{1-x}PO_4$ (x = 0.01, 0.05, and 0.1) samples synthesized by the conventional solid-state reaction route. Rietveld refinement of the X-ray diffraction patterns shows the crystal structure and bond lengths of LiO_6 and $Fe(Mg)O_6$. The Néel temperature (T_N), spin reorientation temperature (T_S), Curie–Weiss temperature, and effective moment decreased owing to the decrease in superexchange interactions with increasing Mg^{2+} ions. The Mössbauer spectra of samples below T_N were fitted with asymmetrical eight absorption lines, whereas above T_N were fitted with symmetrical doublet. The change in the value of electric quadrupole splitting and its slop of magnetic susceptibility at T_S suggests that spin reorientation related to the orbital angular moment contributes to the magnetic properties by spin–orbit coupling. The value of isomer shift of samples at all temperatures was Fe^{2+} ion states and it decreased with increasing Mg^{2+} ion owing to decrease in charge density at the Fe nucleus due to the presence of Mg^{2+} ions on the FeO_6 site.

Index Terms— **Antiferromagnetic ordering, cathode, Mössbauer spectroscopy, spin reorientation.**