JOURNAL OF APPLIED PHYSICS **113**, 17E121 (2013)

Investigation of spin ordering in antiferromagnetic $Fe_{1-x}Mn_xPO_4$ with Mössbauer spectroscopy

Woo Jun Kwon,[1] Bo Wha Lee,[2] and Chul Sung Kim[1,a)]
[1]*Department of Physics, Kookmin University, Seoul 136-702, South Korea*
[2]*Department of Physics, Hankuk University of Foreign studies, Yongin, Kyungki 449-791, South Korea*

(Presented 18 January 2013; received 3 November 2012; accepted 28 November 2012; published online 12 March 2013)

We have investigated the spin ordering in $Fe_{1-x}Mn_xPO_4$, which is a possible cathode material for rechargeable lithium ion battery, with antiferromagnetic structure below Néel temperature (T_N). The prepared $Fe_{1-x}Mn_xPO_4$ ($x=0.0$, 0.1, and 0.3) samples have orthorhombic structures with space group of *Pnma*. These samples show the magnetic phase transition, caused by the strong crystalline field at the MO_6 octahedral sites. According to the temperature dependence of magnetic susceptibility of $Fe_{1-x}Mn_xPO_4$, all samples show antiferromagnetic behaviors. The Néel temperature (T_N) decreases from 114 K at $x=0.0$ to 97 K at $x=0.3$ with Mn concentrations. The magnetization of $Fe_{1-x}Mn_xPO_4$ decreases until the temperature reaches the spin-reorientation (T_S) temperature, and then starts increasing as the temperature increases up to T_N. The T_S of the $Fe_{1-x}Mn_xPO_4$ were found to be 30, 27, and 24 K for $x=0.0$, 0.1, and 0.3. In order to investigate the hyperfine interaction of Fe^{3+} ions in FeO_6 octahedral sites, Mössbauer spectra of $Fe_{1-x}Mn_xPO_4$ have been taken at various temperatures from 4.2 to 295 K. The isomer shift (δ) values of the $Fe_{1-x}Mn_xPO_4$ were between 0.31 and 0.43 mm/s, indicating the high spin state of Fe^{3+} at all temperatures. The magnetic hyperfine field (H_{hf}) and electric quadrupole splitting (ΔE_Q) values of $Fe_{0.9}Mn_{0.1}PO_4$ at 4.2 K were determined to be $H_{hf}=498$ kOe and $\Delta E_Q=2.1$ mm/s. We have also observed the abrupt changes in H_{hf} and ΔE_Q at 27 K for $Fe_{0.9}Mn_{0.1}PO_4$, and decrease the value of T_S of $Fe_{1-x}Mn_xPO_4$ with Mn concentrations. Our study suggests that these changes in $Fe_{1-x}Mn_xPO_4$ are originated from the strong electric crystalline field and spin-orbit coupling of FeO_6 octahedral site. [http://dx.doi.org/10.1063/1.4794374]