Journal of ELECTRONIC MATERIALS, Vol. 48, No. 3, 2019
https://doi.org/10.1007/s11664-018-6660-4

5TH INTERNATIONAL CONFERENCE OF ASIAN UNION OF MAGNETICS SOCIETIES

Mössbauer Studies of $Li_xFe_{1/3}Mn_{1/3}Ni_{1/3}PO_4$ Cathode Materials

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We report on the crystallographic and magnetic properties of $Li_xFe_{1/3}Mn_{1/3}Ni_{1/3}PO_4$ ($x = 0, 1$) using x-ray diffraction (XRD), a vibrating sample magnetometer (VSM), and Mössbauer spectroscopy. XRD analysis confirmed that the samples have an orthorhombic structure with space group *Pnma*. From the VSM measurements the samples exhibited an antiferromagnetic behavior with a Curie–Weiss temperature $\theta = -162$ K for $x = 1$, and $\theta = -303$ K for $x = 0$. The Néel temperature (T_N) and spin reorientation temperature (T_S) were determined to be 40 K and 10 K for $x = 1$, and 66 K and 25 K for $x = 0$. The hyperfine field (H_{hf}) of $LiFe_{1/3}Mn_{1/3}Ni_{1/3}PO_4$ had smaller values than that of $Fe_{1/3}Mn_{1/3}Ni_{1/3}PO_4$ due to the magnitude of the nearest-neighbor superexchange interaction. Isomer shift (δ) values indicate that the charge states of $LiFe_{1/3}Mn_{1/3}Ni_{1/3}PO_4$ are ferrous (Fe^{2+}), and that of $Fe_{1/3}Mn_{1/3}Ni_{1/3}PO_4$ are ferric (Fe^{3+}). The larger values of the electric quadrupole splitting (ΔE_Q) for the Fe^{2+} phase compared to the Fe^{3+} phased originated from the different lattice and valence electron contributions due to the crystalline field and valence transition. Debye temperatures (θ_D) of 338 ± 5 K ($x = 1$), and 370 ± 5 K ($x = 0$) were obtained for the samples.

Key words: Mössbauer spectroscopy, Curie–Weiss temperature, Debye temperature, crystalline field, spin reorientation