$Na_2Fe_{0.9}Mn_{0.1}PO_4F$ Composite as Cathode Material: Structural, Magnetic, and Mössbauer Studies

Jae Yeon Seo[1], Hyunkyung Choi[1], Ah-Yeon Lee[2], Seung-young Park[3], and Chul Sung Kim[1]

[1]Department of Physics, Kookmin University, Seoul 02707, South Korea
[2]Center for Research Equipment, Korea Basic Science Institute, Daejeon 34133, South Korea
[3]Center for Scientific Instrumentation, Korea Basic Science Institute, Daejeon 34133, South Korea

Mn-doped sodium iron fluorophosphates $Na_2Fe_{0.9}Mn_{0.1}PO_4F$ were synthesized using ball milling via a solid-state reaction route. The crystal structure and magnetic properties of the as-prepared materials were studied by using X-ray diffraction (XRD), superconducting quantum interference device (SQUID), and Mössbauer spectroscopy. Structural refinement of $Na_2Fe_{0.9}Mn_{0.1}PO_4F$ was analyzed using the Fullprof program. From the XRD patterns, the crystal structure was found to be orthorhombic with the space group *Pbcn*. $Na_2Fe_{0.9}Mn_{0.1}PO_4F$ has a 2-D layered structure composed of a pair of $Fe(Mn)O_4F_2$ octahedrons through fluorine ion sharing, similar to that of Na_2FePO_4F. The temperature dependence of the zero-field-cooled (ZFC) and field-cooled (FC) curves was measured at temperatures ranging from 1.8 to 295 K under an applied field of 100 Oe. We confirmed that the Néel temperature was 2.5 K, which is lower than that of Na_2FePO_4F ($T_N = 3.4$ K). Mössbauer spectroscopy measurements at 4.2–295 K were conducted. At all the temperatures, the spectra were fitted with a double and were determined to be Fe^{2+} ions based on an isomer shift (δ). In addition, the large value of the electric quadrupole splitting (ΔE_Q) is explained by the asymmetric local environment of the Fe ions.

***Index Terms*— Crystal structure, magnetic properties, Mössbauer spectroscopy, sodium–iron–fluorophosphate, superexchange interaction.**