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Crystal structure and magnetic properties of fluorophosphates Na2Fe0.9Mn0.1PO4 F cathode material

Jae Yeon Seo, Mun Hwan Kim, Hyunkyung Choi, Chul Sung Kim

Kookmin university, Korea, Republic of (South Korea); libattery@kookmin.ac.kr

The sodium iron fluorophosphates Na2Fe0.9Mn0.1PO4F was synthesized by solid-reaction state route. A mixture of Na(CH3COO), FeC2O4·2H2O, MnCO3, NH4H2PO4, and NaF was ground. The mixture was first calcined at 350 oC for 3 h under Ar atmosphere and was pressed into a pellet. Theses mixture was sintered at 625 oC for 6 h under Ar atmosphere. The crystal structure and magnetic properties of the as prepared materials were studied by X-ray diffraction (XRD), vibrating sample magnetometer (VSM), and Mössbauer spectroscopy. Structure refinement of Na2Fe1-xMnxPO4F was analyzed using Fullprof program. From the XRD patterns, consistent with Na2FePO4F, the crystal structure of Na2Fe0.9Mn0.1PO4F sample was found to be orthorhombic with space group of Pbcn. Lattice parameters of Na2Fe0.9Mn0.1PO4F are as follows: a0 = 5.2399 Å, b0 = 13.8828 Å, c0 = 11.8028 Å, and V = 858.0840 Å3. Na2FePO4F cathode material has reported two-dimensional (2D) layer structure of PO4 tetrahedra and Fe2O6F3 bioctahedra, which consists of a pair of FeO4F2 octahedra through fluorine ion sharing [1]. The temperature dependence of zero-field-cooled (ZFC) and field-cooled (FC) curves was measured at temperatures from 4.2 to 295 K under applied field of 100 Oe. Mössbauer spectra have been taken at various temperatures ranging from 4.2 to 295 K. We have confirmed that no evidence for long range magnetic ordering by using Mössbauer spectroscopy at 4.2 K.