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Digests of the 2021 KMS Summer Conference The Korean Magnetics Society

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Crystal structure and Mössbauer studies of a-NaFeO₂

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Lithium – ion batteries (LIBs) have excellent electrochemical performance. However, lithium's price is increased due to the low reserves all over the world. As the alternative cathode material of lithium, sodium has attracted attention. It is environmentally friendly, and it is cost-advantage because of the abundance worldwide. Also, the de-intercalation/intercalation properties of sodium-ion batteries (SIBs) are similar to those of LIBs. However, sodium has the disadvantage of being heavy and has a lower energy density than lithium. To solve this problem, sodium layered oxide is recently being studied. NaMO₂ (M = Fe, Co, Ti, Mn, Ni, etc.) has high volume and gravitational density. In this study, the crystal structure, and magnetic properties of NaFeO₂ materials were characterized by X-ray diffraction (XRD), vibrating sample magnetometry (VSM), and Mössbauer spectra measurements.

NaFeO₂ was synthesized using the solid reaction method from Na₂CO₃ (99.5%) and Fe₃O₄ (99%) as starting materials. The mixture mixed at a ratio of 1:1. After grinding the mixture in an agate mortar, there was calcined at 300 °C for 5 h. The calcined mixture was ground again in an agate mortar and compressed using a disk-shaped pellet. The compressed mixture was sintered to 650 °C for 12 h. To confirm the crystal structure of NaFeO₂, it was measured by XRD with Cu-K α radiation ($\lambda = 1.5406$ Å). Mössbauer spectra measured from 4.2 K to 295 K on a Mössbauer spectrometer, and the VSM measured magnetic properties through the zero-field-cooled (ZFC) and field-cooled (FC) measurements from 4.2 K to 295 K with magnetic fields of 0.1 kOe and 1 kOe.

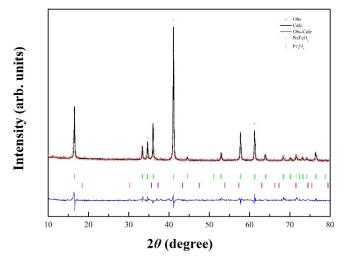


Fig. 1. Refined XRD patterns of NaFeO₂

The crystal structure of NaFeO₂ samples were analyzed using the FULLPROF program after XRD experiment at room temperature. As a result of the analysis, it was found that 5.37% of Fe₃O₄ was present in NaFeO₂ sample. it has a trigonal structure with space group of R-3m. The lattice constants were analyzed as a = b = 3.0251 Å, c = 16.0983 Å. To know the magnetic properties, VSM was experimented from low to room temperature at 0.1

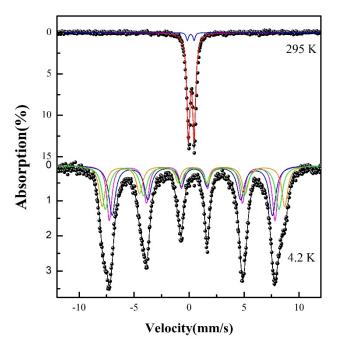


Fig. 2. Mössbauer spectra of NaFeO₂ at 4.2 and 295 K

kOe. it was shown through ZFC-FC data that the Néel temperature (T_N) of NaFeO₂ is 11 K. As a result of Mössbauer spectroscopy analysis from 4.2 K to 295 K, the values of magnetic hyperfine field (H_{hf}) at 4.2 K are H_{hf} (1) = 468.31 kOe, H_{hf} (2) = 453.41 kOe, H_{hf} (3) = 516.00 kOe, H_{hf} (4) = 490.79 kOe, and the electric quadrupole splitting and isomer shift of NaFeO₂ at 11 K are measured to be 0.51 mm/s, and 0.37 mm/s.