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Crystallographic and Magnetic Properties of $KFeO_2$.

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Introduction

Recently, the alkali materials[$AFeO_2$: A= Li, Na, K] are increasing scientific interest as promising the low-cost substitutes for cathode materials in rechargeable lithium batteries. Especially, though potassium iron oxide was known as the material with the highest Néel temperatures among iron-oxide compounds[1-2], there have been very few reports on the $KFeO_2$. Since this material is of very unstable nature due to easy oxidation of potassium, it is very difficult to get single phase $KFeO_2$. In this work, we have synthesized successfully single phases of $KFeO_2$, and then studied the magnetic and structure properties.

Experiments and Results

For fabrication of $KFeO_2$ powders, weighted potassium carbonate (K_2CO_3) and iron oxide (Fe_2O_3)[K_2CO_3:Fe_2O_3=1.2:1 at.%] were mixed for 48 h by ball-mill, and then calcined at 1173 K for 10 h. In order to obtain homogeneous material, it was necessary to grind the samples after first firing and press the powder into pellets before heating it for a second time to 1173 K for 20 h. The crystal structure was measured by x-ray diffractometer using Cu-Kα radiation and magnetic properties were measured using a vibrating sample magnetometer (VSM) and Mössbauer spectroscopy with a 40 mCi ^{57}Co source in a Rh matrix. For the analysis of particle morphology, scanning electron microscope (SEM) was used.

The x-ray diffraction patterns for $KFeO_2$ sample showed a single phase, without any segregation of second phase within the instrumental resolution limit. We have presented the observed and calculated peak profile, and Bragg position of a typical x-ray diffraction patterns for $KFeO_2$ In Fig. 1. The crystal structure of the sample is determined to be an orthorhombic structure of Pbca with its lattice constants a_0= 5.557, b_0= 11.227, and c_0= 15.890 Å by Rietveld refinement and then the final Bragg factors R_B was under 5 %.

Fig. 2 shows Mössbauer spectra of $KFeO_2$ powders at below the room temperature. Mössbauer spectra composed of two six-line hyperfine patterns. It is known that in ordered phase the Fe^{3+} ions are two kind of tetrahedral 8c sites (A-site) and 8a site (B-site), for $KFeO_2$. The room temperature spectrum was fitted using the two magnetic components hyperfine fields for A site = 503 kOe, B site = 497 kOe and isomer shift δ = 0.07 and 0.08 mm/s corresponding to Fe^{3+} ions at sites A and Fe^{3+} ions at site B. The hysteresis loops of $KFeO_2$ was measured using VSM under the maxium applied field of 10 KOe at room temperature. It was shown typical antiferromagnetic behaviors, and then *M* at 10 kOe was 0.08 emu/g. Fig. 3 shows the temperature dependence of the saturated magnetization curve under field 10 kOe about the room temperature. An one can see an unusual magnetization be haviors on Fig. 3. It has been shown that $KFeO_2$ was changed an dicastically in to another phases by thermal influence. In order to resolve how the $KFeO_2$ charge into another phase, we have checked Mössbauer spectra after cooled down to room temperature. Fig. 3 shows Mössbauer spectra of a sample that it was after high temperature experiment. We knew very important a result. The magnetization moment, hyperfine field, isomer shift, and quadrupole splitting are 41.8 emu/g, 458 kOe, 0.52 mm/s and 0.008 mm/s, respectively. This result is showing us that the changed phases is Fe_3O_4. Finally, we have concluded that the other phase is Fe_3O_4 from Mössbauer spectra analysis for the powders after high temperature experiment by VSM.

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[2] Z. TMOKOWICZ and A. SZYTULA., J. Chem. Solid. 38, 1112 (1977)

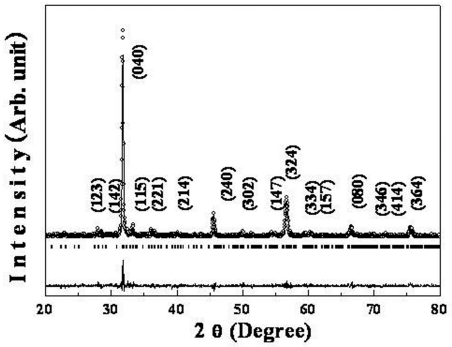

Fig. 1. X-ray diffraction pattern of the $KFeO_2$ powders annealed at 1173 K

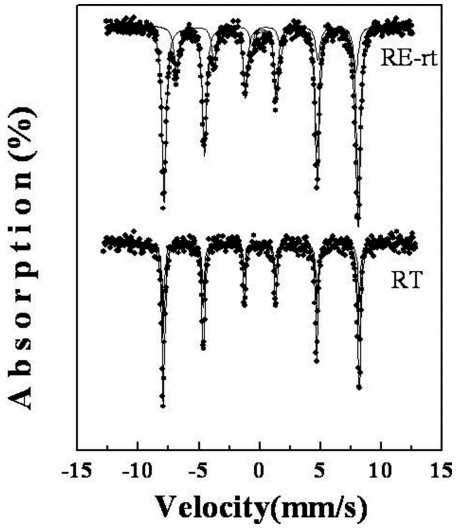

Fig. 2 Mössbauer spectra of $KFeO_2$ measured at RT and at re-RT after high temperature measurement.

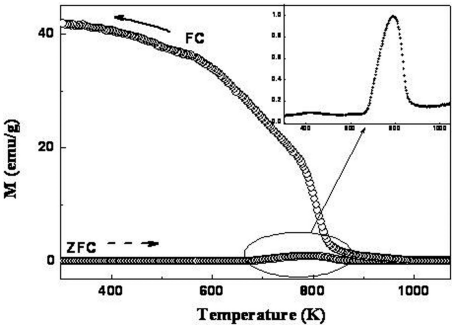

Fig. 3. Temperature vs. magnetization curves of $KFeO_2$ taken under 10 kOe external field