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Neutron Diffraction and Mössbauer Studies of Fe-Doped YMn_2O_5

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Abstract

The crystallographic and magnetic properties of multiferroic $YMn_{2-x}Fe_xO_5$ ($0 \leq x \leq 1.0$) have been studied by neutron diffraction and Mössbauer technique. The $YMn_{2-x}Fe_xO_5$ powders were prepared by sol-gel process. The crystalline structure of the YMn_2O_5 at room temperature was determined to be orthorhombic (*Pbam*) with lattice constants a_0=7.298 Å, b_0=8.491 Å, and c_0=5.681 Å. The $YMn_{1.8}Fe_{0.2}O_5$ shows a huge electric quadrupole splitting value from the Mössbauer spectrum at room temperature. It can be understood primarily owing to its chemical and crystalline structure.

Keywords: Multiferroic, Neutron diffraction, Mössbauer spectrum,

1. Introduction

Multiferroics possess two or more switchable states such as polarization, magnetization or strain [1]. Despite the possible coexistence of ferroelectricity and magnetism, a pronounced interplay between these properties has rarely been observed [2].

The family of RMn_2O_5 (R=rare earth materials and Y) was first described by Quezel-Ambrunaz *et al* [3], who prepared single crystal phase from Bi_2O_3 flux. In general, the structure of RMn_2O_5 at room temperature is known orthorhombic (*Pbam*). And the Mn^{4+} ions are octahedrally coordinated by oxygen, whereas Mn^{3+} ions are at the base centre of a square pyramid.

Here we report the neutron and Mössbauer studies for multiferroic Fe-doped YMn_2O_5.

2. Experimental

The polycrystalline $YMn_{2-x}Fe_xO_5$ were obtained by the sol-gel process. Yttrium nitrate pentahydrate ($Y(NO_3)_2 \cdot 5H_2O$), manganese

acetate ($Mn(CH_3CO_2)_4 \cdot H_2O$), and iron nitrate ($Fe(NO_3)_3 \cdot 9H_2O$), were used as starting materials. These were dissolved in mixed a solvent system (ethanol : acetic acid : distilled water : diethanolamine = 2 : 1 : 1 : 0.02 mole ratio). The solution was refluxed at 80 ℃ for 12 h. It was dried at 150 ℃ and finally powdered. The dried mixtures were calcined at 600 ℃ for 2 h. The final products were crystallized in the temperature rage from 700 to 1400 ℃ for 6 h in air.

The crystal structures of the samples were examined by x-ray diffraction with Cu$K\alpha$ radiation and neutron diffraction at the Korea Atomic Energy Research Institute Reactor HANARO. Mössbauer spectra were recorded using a 40 mCi ^{57}Co source in a Rh matrix with the spectrometer working at constant acceleration. The magnetic field and temperature dependence of magnetization were measured using a vibrating sample magnetometer under a maximum applied field of 10 kOe in the temperature range from 50 to 400 K.

3. Results and Discussion

We investigated neutron diffraction patterns of polycrystalline $YMn_{2-x}Fe_xO_5$ at various temperatures. The diffraction patterns were refined by Rietveld profile analysis using the FULLPROF program, with the peak shapes approximated by a pseudo-Voigt function. The crystal structures of $YMn_{2-x}Fe_xO_5$ for all temperature ranges were determined to be orthorhombic of *Pbam*. And lattice parameters of the Fe-doped samples were slightly decreased than that of the YMn_2O_5.

The Mössbauer spectrum of the $YMn_{1.8}Fe_{0.2}O_5$ at room temperature shows a doublet from the electric quadrupole splitting which has a huge value. Above the Néel temperature (T_N = 45 K), the quadrupole splitting is given by

$$\Delta E_Q = \frac{1}{2} e^2 q Q \left(1 + \frac{1}{3}\eta^2\right)^{1/2}. \quad (1)$$

Here, η is the asymmetry parameter of electric field gradient. The value of ΔE_Q was found to be 1.15± 0.01 ㎜/s at room temperature for $YMn_{1.8}Fe_{0.2}O_5$ that is above T_N. It could be interpreted that spontaneous electric polarization for $YMn_{2-x}Fe_xO_5$ materials is caused asymmetry distribution between cations and anions. It can be accessed an important point, in that the observation of spin/lattice coupling was directly possible by Mössbauer spectra.

The isomer shift indicates that the valence state of the Fe ions is +3.

4. Conclusion

We have fabricated multiferroic $YMn_{2-x}Fe_xO_5$ powders by sol-gel process. Our research presents directly experimental evidence for spin/lattice coupling by neutron and Mössbauer technique.

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