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Neutron Diffraction and Mössbauer Studies of Fe-Doped YMN₂O₅

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Abstract

The crystallographic and magnetic properties of multiferroic YMN₂ₓFeₓO₅ (0 ≤ x ≤ 1.0) have been studied by neutron diffraction and Mössbauer technique. The YMN₂ₓFeₓO₅ powders were prepared by sol-gel process. The crystalline structure of the YMN₂O₅ at room temperature was determined to be orthorhombic (Pbam) with lattice constants a₀=7.298 Å, b₀=8.491 Å, and c₀=5.681 Å. The YMN₁₃Fe₇O₃ 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 RMn₂O₅ (R=rare earth materials and Y) was first described by Quezel-Ambrunaz et al ³, who prepared single crystal phase from Bi₂O₃ flux. In general, the structure of RMn₂O₅ at room temperature is known orthorhombic (Pbam). And the Mn⁴⁺ ions are octahedrally coordinated by oxygen, whereas Mn⁵⁺ ions are at the base centre of a square pyramid.

Here we report the neutron and Mössbauer studies for multiferroic Fe-doped YMN₂O₅.

2. Experimental

The polycrystalline YMN₂ₓFeₓO₅ were obtained by the sol-gel process. Yttrium nitrate pentahydrate (Y(NO₃)₂ · 5H₂O), manganese
acetate (Mn(CH₃CO₂)₄ · H₂O), and iron nitrate (Fe(NO₃)₃ · 9H₂O), 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 °C for 12 h. It was dried at 150 °C and finally powdered. The dried mixtures were calcined at 600 °C for 2 h. The final products were crystallized in the temperature range from 700 to 1400 °C for 6 h in air.

The crystal structures of the samples were examined by x-ray diffraction with CuKα radiation and neutron diffraction at the Korea Atomic Energy Research Institute Reactor HANARO. Mössbauer spectra were recorded using a 40 mCi ⁵⁷Co 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 YMn₉₋₆Fe₆O₁₅ 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 YMn₉₋₆Fe₆O₁₅ for all temperature ranges were determined to be orthorhombic of Pbnm. And lattice parameters of the Fe-doped samples were slightly decreased than that of the YMn₉O₁₅.

The Mössbauer spectrum of the YMn₁₅Fe₁₀O₃₅ at room temperature shows a doublet from the electric quadrupole splitting which has a huge value. Above the Néel temperature (Tₙ = 45 K), the quadrupole splitting is given by

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

Here, $\eta$ is the asymmetry parameter of electric field gradient. The value of $\Delta E_Q$ was found to be 1.15± 0.01 mm/s at room temperature for YMn₁₅Fe₁₀O₃₅ that is above $T_n$. It could be interpreted that spontaneous electric polarization for YMn₉₋₆Fe₆O₁₅ 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 YMn₉₋₆Fe₆O₁₅ powders by sol-gel process. Our research presents directly experimental evidence for spin/lattice coupling by neutron and Mössbauer technique.

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References