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Structural and magnetic properties of Mg doped $YbMnO_3$

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ABSTRACT

We have studied the effect of Mg doping on structure and magnetism of multiferroic $YbMnO_3$. Room temperature neutron diffraction studies were carried out on polycrystalline $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) samples to determine phase formation as well as cation distribution and structural properties such as bond length and bond angles. The structural analysis shows that with Mg substitution, there is a marginal change in *a* and *c* parameters of the hexagonal unit cell, *c*/*a* ratio remains constant for $x=0$ and 0.05 samples. Due to changes in bond angle and bond lengths on substituting Mg, there is a slight decrease in the distortion of MnO_5 polyhedra. Magnetic measurements show that the Néel temperature (T_N) increases marginally from 85 K for $x=0.00$ to 89 K for $x=0.05$ sample.

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1. Introduction

Materials in which magnetic ordering can be controlled by electric field and vice-versa are called multiferroic. Such compounds have tremendous potential in practical applications such as spintronics. Rare-earth and yttrium manganites of general formula $RMnO_3$ crystallize in hexagonal structure for R with smaller ionic radius (R=Ho, Er, Tm, Yb, Lu, and Y) [1] or in orthorhombic structure for larger ionic radius (R=La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, and Dy) [2]. Hexagonal $RMnO_3$ compounds are known to show simultaneously ferroelectric as well as magnetic ordering in the ordered phase. The crystal structure of hexagonal manganites consists of MnO_5 polyhedra in which Mn^{3+} ion is surrounded by three oxygen ions in plane and two apical oxygen ions. Mn ions with in Mn–O plane form a triangular lattice and are coupled in terms of spins through the antiferromagnetic (AFM) super exchange interaction. Due to an incomplete AFM coupling between neighboring Mn ions in the triangular lattice, the system forms a geometrically frustrated magnetic state [3–5].

Among rare earth manganites $YbMnO_3$ has been scarcely studied. Magnetization measurements of $YbMnO_3$ showed an AFM transition around 82 K [6]. In the crystallographic structure of $YbMnO_3$, Yb occupies two crystallographic sites (in Wyckoff notations), 2a and 4b of space group $P6_3cm$. There have been many studies on the effect of substitution at Mn site of $YbMnO_3$, whereas we have concentrated on Yb site substitutions. The aim of this study is to understand the effects of partial replacement of Yb^{3+} by Mg^{2+} on the structural and magnetic properties of $YbMnO_3$. We have synthesized Mg-doped $YbMnO_3$ and focused on two compounds $YbMnO_3$ ($x=0.00$) and $Yb_{0.95}Mg_{0.05}MnO_3$ ($x=0.05$) for carrying out the comparative study.

2. Experimental

Polycrystalline samples of $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) were prepared by a standard solid-state reaction method. Stoichiometric amounts of high-purity (purity greater than 99.9%) Yb_2O_3, $MnCO_3$, and MgO powders were thoroughly mixed and subsequently calcined in air at 1200 °C for 24 h, with an intermediate grinding for homogenization. The calcined mixture was cold pressed into pellets, sintered at 1450 °C in air for 24 h. Finally, all the samples were slowly cooled to room temperature for sufficient oxygenation.

The phase purity of samples was checked by powder X-ray diffraction (XRD) on a Brüker D8 Advance X-ray powder diffractometer using Cu Kα radiation. Neutron diffraction experiments were carried out at room temperature at Dhruva, BARC on the UGC-DAE CSR beam line (TT1015) using a neutron beam of wavelength 1.48 Å. All the magnetization measurements were performed on a vibrating sample magnetometer (PPMS-VSM) in

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the temperature range from 2 to 300 K in 100 Oe applied dc magnetic field, in both zero field cooled (ZFC) and field cooled (FC) states of the samples.

3. Results and discussion

In Fig. 1 room temperature XRD patterns of $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) samples are shown. The samples studied here are single phase and the measured patterns can be indexed according to the hexagonal structure with $P6_3cm$ space group (JCPDS No. 38-1246). In Fig. 2 the Rietveld refinement patterns of neutron powder diffraction (NPD) data are shown for both $x=0.00$ and 0.05 samples. The good agreement between observed (black scattered points) and calculated profiles (red continuous line) is indicated by the difference line (blue color). Refined values of lattice parameters and discrepancy factors for $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) are shown in Table 1. The values obtained for $x=0.00$ sample are in good agreement with those reported in the literature [7].

From the values given in Table 1, it is clearly seen that due to Mg substitution, the cell parameter a decreases marginally, while there is a slight increase in c. Overall the cell volume decreases for $x=0.05$ sample when compared to that of $x=0.00$ sample. This decrease in cell volume can be ascribed to ionic size effects, since smaller Mg^{2+} (Shannon ionic radii ~0.890 Å) ion replaces the slightly bigger Yb^{3+} (Shannon ionic radii ~0.925 Å) ion. The observed decrease in cell volume shows that Mg^{2+} does indeed replace Yb^{3+} in the doped $x=0.05$ sample. As the average A-site (i.e. Yb site) radius changes from $x=0.00$ to 0.05, it is expected that the tolerance factor will also change. It is well known for manganites that the average A-site radius plays a crucial role in maintaining the valence state(s) of Mn ions at B-site. Therefore, as the divalent Mg is substituted at Yb^{3+} site, it will not only induce chemical pressure effect but also change the valence of Mn ions from Mn^{3+} towards a mixed-valence state. Presence of Mn^{4+} ion in MnO_5 polyhedra results in Jahn–Teller distortions and this also contributes to variations in lattice parameters; similar explanation was given by Jeuvreya et al. for $YMn_{1-x}Cu_xO_3$ compounds [8].

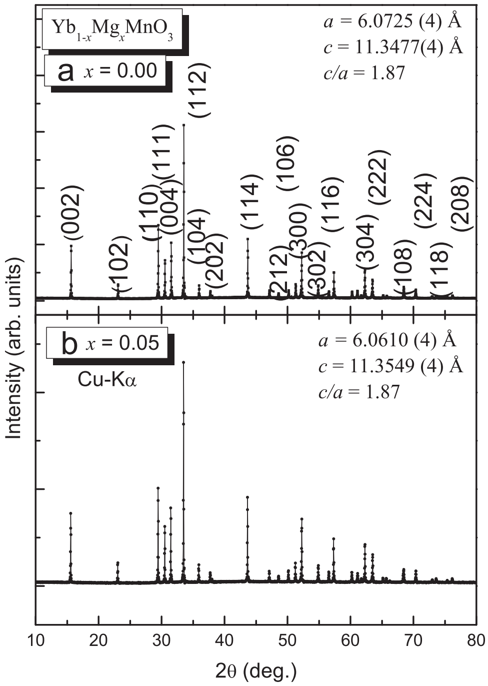

Fig. 1. Room temperature XRD pattern of $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) samples indexed in space group $P6_3cm$.

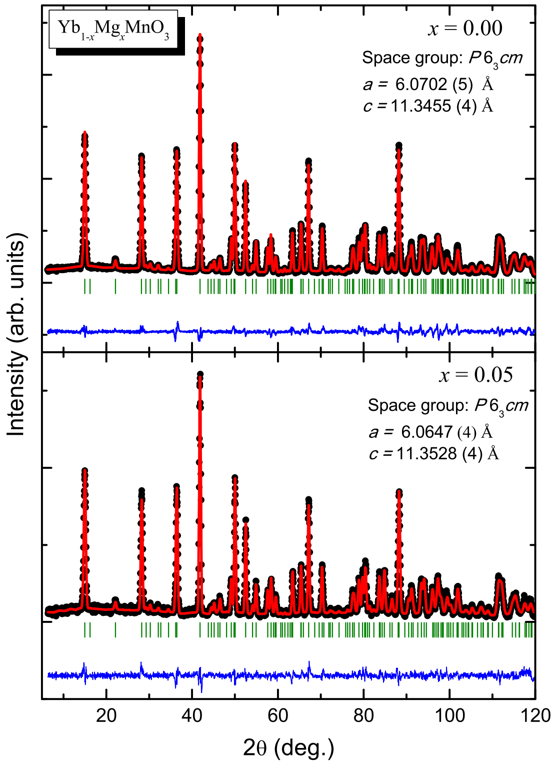

Fig. 2. Rietveld refinement of room temperature neutron diffraction data of $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) samples. The raw data is plotted along with the calculated profile, the difference between observed and calculated data. The vertical tick marks indicate the expected Bragg peak positions. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

Table 1
Structural parameter after the Rietveld refinement of NPD for $Yb_{1-x}Mg_xMnO_3$ ($x=0.00$ and 0.05) samples at room temperature.

$Yb_{1-x}Mg_xMnO_3$	$x=0.00$	$x=0.05$
a (Å)	6.070(5)	6.064(4)
c (Å)	11.345(4)	11.352(4)
V (Å^3)	362.05(2)	361.87(2)
χ^2	3.32	4.03
R_P	5.51	9.21
R_{wp}	7.25	12.6
R_B	4.45	4.73
t (Å)	0.831	0.833

't' is the tolerance factor, given as $t=\left((r_{Yb}+r_o)/\sqrt{2(r_{Mn}+r_o)}\right)$.

Some selected bond distances of Yb–O and Mn–O for $x=0.00$ and 0.05 samples are listed in Table 2. The value of cell parameter a decreases in Mg doped sample when compared to that in pristine sample. This change is ascribed to the decrease in the average ab-plane i.e. Mn–O3 and Mn–O4 bond lengths. Mn–O1 and Mn–O2 bond lengths are along the c axis, and exhibit minor change on doping. The average Mn–O distances in MnO_5 units are significantly shorter in doped sample compared to those of pure $YbMnO_3$.

It is expected that MnO_5 polyhedra will play an important role in the magnetic properties observed in both the samples. Mn–O bond lengths are in agreement with the sum of ionic radii [9]. Moreover, in YbO_7 polyhedron, Yb–O distances are larger in $x=0.00$ sample than those in $x=0.05$ sample, as expected due to

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