# Experimental report

07/04/2017

**Proposal:** **5-31-2528**

**Council:** 10/2016

**Title:** To study the effect of Mn doping on the temperature and field dependent re-orientation of orthoferrite NdFe0.5Mn0.5O3.

**Research area:** Materials

**This proposal is a new proposal**

**Main proposer:** **Ruchika YADAV**

**Experimental team:** Ruchika YADAV

**Local contacts:** Vivian NASSIF

**Samples:** NdFe0.5Mn0.5O3

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D1B | 5 | 1 | 02/03/2017 | 03/03/2017 |

**Abstract:**

The study is based on the Mn substituted orthoferrite NdFe0.5Mn0.5O3. Substition of Mn at the Fe site alters the magnetic properties, though the main characteristic G-type ordering is similar to NdFeO3. Neutron diffraction data (wavelength ~ 1.24Å) reveal that below 250 K, the Fe/Mn spins order in Gamma1(AxGyCz) representation, unlike the usual Gamma4representation observed in NdFeO3 and other orthoferrites. Below 100 K, spins undergo a reorientation and the magnetic structure coexists as Gamma1+ Gamma2, while at 6 K the magnetic structure belongs to only Gamma2(FxCyGz) representation. A second order transition Gamma1 to Gamma2, cannot be explained in terms of Nd-Fe(Mn) isotropic and antisymmetric interactions alone. Also a primary issue here is the simple Gy-type collinear spin arrangement seen below 250 K. without Ax/Cz spin components cannot couple with the Nd spins and cause the spin reorientation transition. It is essential to verify the presence of Cz/Cy-type (010),(100) Bragg peaks, which may be possible with better resolution data. In addition, it would be interesting to study the effect of magnetic field on magnetic structure and reorientation in NdFe0.5Mn0.5O3.

Report for experiment no **5-31-2528** at D1B, ILL

**Topic : Study of spin reorientation in $NdFe_{0.5}Mn_{0.5}O_3$**

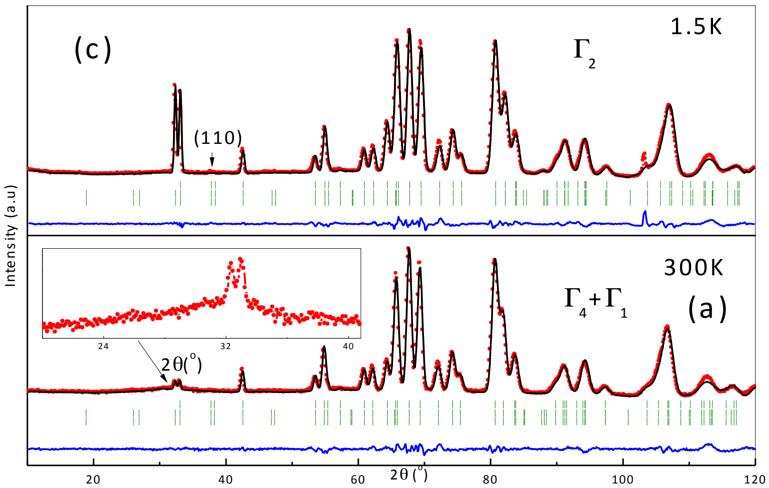
Our material of study is the mixed orthoferrite compound $NdFe_{0.5}Mn_{0.5}O_3$. The crystal structure is orthorhombic(Pbnm) and the lattice parameters is in between that of the two parent compounds $NdFeO_3$ and $NdMnO_3$. The parent orthoferrite $NdFeO_3$ is a well studied compound which is widely known for temperature dependent spin reorientation behavior.It has a very high Neel temperature of 760 K and it orders as a G-type antiferromagnet with ordering vector k=(000) in the representation $\Gamma_4$ ($G_x$, $A_y$, $F_z$). This high temperature magnetic ordering is characteristic of most of orthoferrites and orthochromates. In 200-100 K range a continuous spin reorientation from $\Gamma_4 \rightarrow \Gamma_2$, ($F_x$,$C_y$,$G_z$) occurs in which the easy axis rotates from *x* to *z* direction. At 1.5K, Nd spins order in (Fx,Cy) configuration.

Substitution of Fe by Mn alters the magnetic behavior, even though the ordering vector and G-type nature is same till a very high doping of Mn. For 50% substitution, there occurs a drastic reduction in Neel temperature to 250 K as seen in our ZFC-FC magnetization. In addition, we also see a reorientation like transition causing a split in ZFC-FC at 50 K. To study the magnetic nature we have performed neutron diffraction experiments using D1B instrument at ILL in March 2017. The experiments were performed in the range 1.5 K to 300 K for a duration of 24 hours. At 300 K we observe the emergence of a two low intensity Bragg peak near 32$^o$ which is of magnetic origin. The two peaks correspond to (101) and (011) reflections belonging to G-type magnetic ordering as shown in fig.1a. In addition we also observe a large diffused scattering background, super-posed on the main Bragg peak (inset of fig.1a) which persists even at 100 K. This indicates the coexistence of short range spin-correlations in addition to long range ordering.

At 300 K, the magnetic structure belongs primarily to $\Gamma_4$ ($G_x$, $A_y$, $F_z$) representation wherein moments are along the z-direction. However, we see a small component of $\Gamma_1$ ($A_x$, $G_y$, $C_z$). From 250 K and below, the magnetic structure is refined to $\Gamma_1$ ($A_x$, $G_y$, $C_z$) representation which is exclusively the effect of Mn doping.

This phase persists till 50 K, at which there occurs a development of the $\Gamma_2$($F_x$, $C_y$, $G_z$) phase, thus corresponding to rotation of easy axis from y to z direction. Compared to $NdFeO_3$ our reorientation region is much narrower (50-30 K). Thus between 50 and 20 K the magnetic structure is $\Gamma_1$+$\Gamma_2$. In fig.1b we show the refinement corresponding to 36 K which corresponds to the two representations. Finally at 1.5 K the magnetic structure is entitely $\Gamma_2$ with small ferromagnetic (1-10) peak marked in fig.1c. With decrease in temperature there is a systematic increase in total magnetic moments |M|. At 1.5 K, the total moment is around 2.35 μB for the Fe/Mn site, while it is close to 0.2μB for Nd ion.

The $\Gamma_1 \rightarrow \Gamma_2$ transition is unusual since $\Gamma_1$ is observed in orthoferrites as an outcome of an abrupt spin reorientation transition at low temperatures. Thus Mn substitution results in a three-fold transition viz $\Gamma_4 \rightarrow \Gamma_1 \rightarrow \Gamma_2$, as seen from the intensity ratios of the magnetic peaks (101) and (011), whose systematic variation is shown in fig.2. The predominant $\Gamma_1$ over a wide temperature range can be attributed to a large single ion anisotropy of the $Mn^{3+}$ ion which also shows local Jahn-Teller distortions, which seems to suppress the $\Gamma_4$ phase, characteristic of the $Fe^{3+}$ spins in orthoferrites. Based on our present investigations we propose to analyse the diffused scattering portion of the magnetic peak and subsequently communicate a paper.



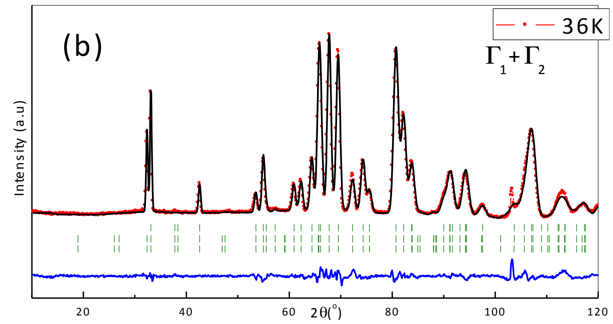




Fig.1 : Refinement of the neutron diffraction data for structural and magnetic part for (a) 300 K, (b) 36 K and (c) 1.5 K. Inset of (a) shows the enlarged portion of the small magnetic Bragg peak.

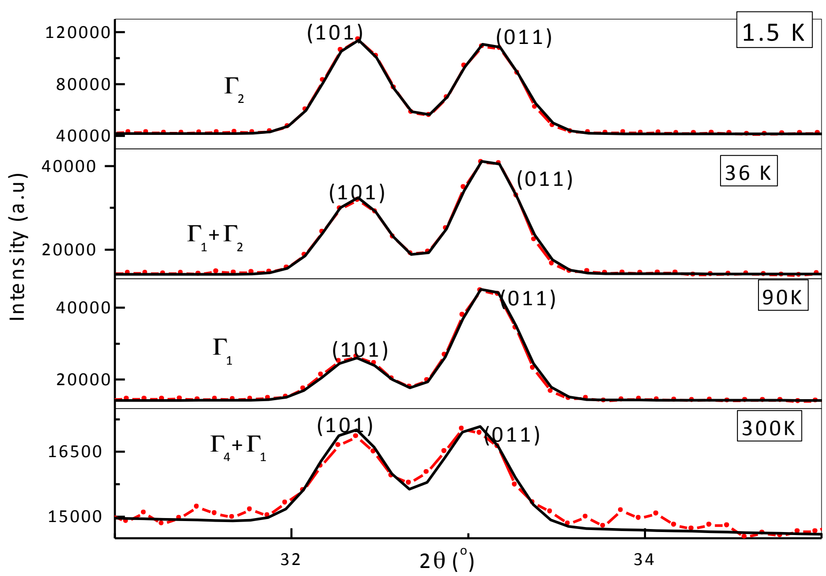



Fig. 2 Variation of the intensity ratio of the G-type magnetic peaks (101) and (011) as a function of temperature.