Spin-lattice coupling and frustrated magnetism in Fe-doped hexagonal LuMnO$_3$

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Abstract – Strong spin-lattice coupling and prominent frustration effects observed in the 50% Fe-doped frustrated hexagonal (h)LuMnO$_3$ are reported. A Néel transition at $T_N \approx 112$ K and a possible spin re-orientation transition at $T_{SR} \approx 55$ K are observed in the magnetization data. From neutron powder diffraction data, the nuclear structure at and below 300 K was refined in polar $P\bar{6}_3cm$ space group. While the magnetic structure of LuMnO$_3$ belongs to the $\Gamma_4$ ($P\bar{6}_3cm$) representation, that of LuFe$_{0.5}$Mn$_{0.5}$O$_3$ belongs to $\Gamma_1$ ($P\bar{6}_3cm$) which is supported by the strong intensity for the (100) reflection and also judging by the presence of spin-lattice coupling. The refined atomic positions for Lu and Mn/Fe indicate significant atomic displacements at $T_N$ and $T_{SR}$ which confirms strong spin-lattice coupling. Our results complement the discovery of room temperature multiferroicity in thin films of hLuFeO$_3$ and would give impetus to study LuFe$_{1-x}$Mn$_x$O$_3$ systems as potential multiferroics where electric polarization is linked to giant atomic displacements.

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Hexagonal manganites (h)RMnO$_3$ ($R = $ rare earth) are fascinating systems in the class of multifunctional oxides which present multiferroicity [1–3], dielectric and magnetic anomalies [4], field-induced re-entrant phases [5], metamagnetic steps in magnetization [6] and recently, even found related to cosmology [7]. The primary interest in hexagonal manganites arises from the potential to realize multiferroics since it was found that below the ferroelectric transition temperature, $T_{FE} \approx 1000$ K, they develop electric polarization due to structural distortions and giant atomic displacements [2,3]. hRMnO$_3$ systems often have a low Néel temperature $T_N$ (often $\leq 100$ K) compared to the $T_{FE}$. Strong coupling between lattice, magnetic and electric degrees of freedom is generally observed in hexagonal manganites despite the large separation in temperature between $T_{FE}$ and $T_N$ [8]. The magnetic structure of hRMnO$_3$ presents significant complexity in the form of magnetic frustration where the Mn moments in the ab-plane form 120° triangular lattice [9]. This 2D edge-sharing triangular network is geometrically frustrated with antiferromagnetic nearest-neighbor exchange interaction and gives rise to diffuse magnetic scattering intensity close to $T_N$ [10].
There exist significantly many reports on the magnetic structure of hexagonal manganites in different representations due to the homometric pairs of irreducible representations that yield the same neutron diffraction pattern if the $x$(Mn) is the ideal value of $\frac{1}{2}$. One of the most studied hexagonal manganite, YMnO$_3$ has been reported in several symmetries by different authors —Γ$_3$ [11], Γ$_4$ [12] or Γ$_5$, Γ$_6$ [9]. Earlier investigations suggested Γ$_1$ or Γ$_3$ as the possible magnetic structure for YMnO$_3$ [13].

However, neutron polarimetry studies have confirmed the magnetic structure as Γ$_5$ or Γ$_6$ [9]. On the other hand, hLuMnO$_3$ which shares most of the properties of hYMnO$_3$ has Γ$_4$ ($P6_5cm$) symmetry [10,14]. In both hYMnO$_3$ and hLuMnO$_3$, strong spin-lattice coupling triggered by giant atomic displacements of Mn ion at $T_N$ plays an important role in inducing ferroelectric distortion leading subsequently to multiferroic property.

Compared to hLuMnO$_3$, the ferrite hLuFeO$_3$ is reported to present improved magnetic properties [15]. In a recent study on hLuFeO$_3$, strong exchange coupling leading to high magnetic transition temperatures and spin re-orientation transitions closely connected with structural distortions have been identified [16]. Thin films of hLuFeO$_3$ have shown evidence for a room temperature multiferroic [17] and have been identified as a strong candidate for linear magneto-electric coupling and control of the ferromagnetic moment directly by an electric field [18]. However, bulk LuFeO$_3$ normally crystallizes in orthorhombic $Pbnm$ symmetry thereby precluding the possibility of ferroelectricity. Hence it is desirable to prepare solid solutions of hRMnO$_3$ and hRFeO$_3$ in order to combine the features of giant atomic displacements that lead to ferroelectric polarization and the magnetic transitions at near 300 K. In the present work, the solid solution LuFe$_{0.5}$Mn$_{0.5}$O$_3$ has been synthesized and is studied using magnetization and neutron powder diffraction. The results reveal strong spin-lattice coupling in this material and suggest its potential to be a multiferroic.

The polycrystalline samples used in the present study were prepared by following a solid-state reaction method [4]. High-purity Lu$_2$O$_3$, Fe$_2$O$_3$ and MnO (4N, Sigma Aldrich) were used as the precursors. The synthesized powder sample was first characterized using laboratory x rays. Formation of a single hexagonal phase without impurities was confirmed in this way. Magnetic measurements were performed using a Magnetic Property Measurement System, Quantum Design Inc. Neutron powder diffraction experiments were carried out at the SINQ spallation source of Paul Scherrer Institut (Switzerland) using the high-resolution diffractometer for thermal neutrons HRPT [19] with the wavelength $\lambda = 1.886$ Å in high-intensity mode. About 8 g of powder sample was used to obtain the neutron powder patterns which were recorded at 11 temperature points between 2 K and 300 K. The nuclear and magnetic structure refinements were performed using Rietveld method [20] employing the FULLPROF code [21]. Magnetic structure refinement using representation analysis was performed using the SARA software [22].

Magnetization measurements in zero-field–cooled (zfc) and field-cooled (fc) protocols recorded for LuFe$_{0.5}$Mn$_{0.5}$O$_3$ are presented in fig. 1(a) for 10 kOe. Two magnetic phase transitions are identified at $T_N \approx 112$ K and $T_{SR} \approx 55$ K. At $T_N$, the Néel transition in the 120° triangular lattice takes place. In the case of hLuMnO$_3$ a lower value of $T_N \approx 88$ K was observed. The transition at $T_{SR}$ in LuFe$_{0.5}$Mn$_{0.5}$O$_3$ could be a spin re-orientation transition similar to the one found in hLuFeO$_3$ at 130 K [16]. The $T_{SR}$ in hLuFeO$_3$ is closely related to the interlayer exchange coupling and the atomic displacements due to the $K_1$ phonon mode [16]. The frustration effects in LuFe$_{0.5}$Mn$_{0.5}$O$_3$ are clearly seen in the inverse magnetic susceptibility $1/\chi(T)$ which shows deviation from linear trend even for $T \gg T_N$, as seen from the Curie-Weiss fit in panel (b). From the Curie-Weiss fit, an effective paramagnetic moment value, $\mu_{eff} = 5.41(4)$ $\mu_B$ and Curie-Weiss temperature, $\Theta_{CW} = -946$ K are estimated. The effective paramagnetic moment calculated assuming spin-only contributions is $\mu_{calc} = 5.4$ $\mu_B$. As an estimate of frustration, the ratio $f = |\Theta_{CW}|/T_N \approx 8.5$ is calculated. This value of $f$ signals significant frustration effects and is comparable to the frustration indices of other hexagonal systems collected in table 1. A field scan performed in zero-field–cooled protocol at 5 K is presented in fig. 1(c) where no hysteresis is observed. There is no indication of ferromagnetic contribution to magnetic susceptibility. The maximum magnetic moment obtained at 5 K under 90kOe ($\approx 0.1 \mu_B$/f.u.) is significantly reduced in magnitude compared to the value for the ferromagnetic alignment of Mn$^{3+}$ and Fe$^{3+}$ moments; 5.4 $\mu_B$/f.u. The antiferromagnetic arrangement of moments in the basal plane and of the resulting strong frustration effects leads to this reduction in the observed magnetic moment. In addition to the purely geometrical frustration effects, low dimensionality of the hexagonal plane brought about by the competition between the

![Fig. 1:](image-url)
Table 1: The Curie-Weiss temperature, $\Theta_{\text{CW}}$, the Néel temperature, $T_N$, and the frustration parameter, $f$ of some of the highly frustrated hexagonal manganites. The values for LuFe$_{0.5}$Mn$_{0.5}$O$_3$ are closely compared with those for other related hexagonal systems.

| Compound          | $\Theta_{\text{CW}}$ (K) | $T_N$ (K) | $f$ | Ref. |
|------------------|--------------------------|-----------|-----|------|
| YMnO$_3$         | $-$545                   | 75        | 7.8 | [23] |
| LuMnO$_3$        | $-$740                   | $\approx$ 90 | $\approx$ 8 | [24] |
| (Y, Lu)MnO$_3$   | $-$600 to $-$800         | $\approx$ 70 to 90 | $\approx$ 8 | [24] |
| Lu(Fe, Mn)O$_3$  | $-$946                   | 112       | 8.5 | (This work) |

It is known that the hexagonal manganites undergo a phase transition from centrosymmetric $P6_3/mmc$ to ferroelectric $P6_3cm$ below $T_{FE} \approx 1000$ K [3]. It is found that the nuclear structure of LuFe$_{0.5}$Mn$_{0.5}$O$_3$ remains $P6_3cm$ in the temperature range 300–2 K. The refined lattice parameters and the atomic coordinates for 300 K and 2 K are presented in table 2. The refined Mn position at 10 K is $x = 0.334$. For a perfect 2D triangular network, the ideal value is $x = \frac{1}{3}$ and it is reported to be 0.340 for $h$YMnO$_3$ and 0.331 for hLuMnO$_3$ [24]. The displacements of the Mn atom as suggested by the $x$ position have strong correlation with the magnetic structure. The Mn-Mn interactions between adjacent Mn planes are due to the superexchange mechanism via the apical oxygens of MnO$_5$ bipyramids. When $x = \frac{1}{3}$ all exchange paths are equivalent. However, when $x \neq \frac{1}{3}$, two different paths with two different exchange interactions, $J_{11}$ and $J_{22}$, are formed. Thus $x = \frac{1}{3}$ is a critical threshold value and determines the stability of magnetic structure below $T_N$ [12,15].

Below $T_N \approx 112$ K, a purely magnetic reflection is observed at (101) at $2\theta \approx 23^\circ$ ($d_{hkl} = 4.72$ Å) and enhancement of nuclear intensity at (102) at $2\theta \approx 28^\circ$. 

![Fig. 2: (Colour on-line) The neutron powder diffraction data on LuFe$_{0.5}$Mn$_{0.5}$O$_3$ along with Rietveld refinement for (a) 300 K and (b) 2 K. The magnetic structure is refined in $P6_3cm$ space group. In (b), the magnetic structure is modeled after $\Gamma_1$. The calculated pattern is plotted as a black line and the difference plot as a green line. The Bragg positions are marked as pink vertical bars. In (b), the bottom row of ticks represent magnetic peaks. The inset of (b) magnifies the low-angle reflections (100) and (102). Panel (c) shows the plot comparing the patterns at 75 K and 100 K which highlight an enhancement of intensity for the reflections (100) and (102). Panel (d) shows a comparison of the 2 K data of $h$LuMnO$_3$ and LuFe$_{0.5}$Mn$_{0.5}$O$_3$ to contrast $\Gamma_1$ ($\Gamma_3$) and $T_2$ ($\Gamma_1$).](image)
moments aligned 120° magnetic ordering in the triangular lattice with Mn/Fe moments aligned 120° to each other. The magnetic structure of LuFe₀.₅Mn₀.₅O₃ below Tₘ was solved by assuming k = (0,0,0) propagation vector for the nuclear space group P6₃cm. Representation analysis for magnetic structure then allows six possible solutions: Γ₁ (P6₃mc), Γ₂ (P6₃cm’), Γ₃ (P6₃cm’), Γ₄ (P6₃cm), Γ₅ (P6₃c) and Γ₆ (P6₃) [9,14]. The magnetic structure of hLuMnO₃ belongs to the representation Γ₄ (P6₃cm’) [10,14]. However, non-zero intensity for the (100) reflection which is stronger compared to the (101) one could suggest that the Γ₃ (P6₃cm’) or Γ₁ (P6₃cm) models are the correct one for the Fe-doped compound. The 2K data with the Rietveld refinement fits assuming Γ₁ model is presented in fig. 2(b). The indices of low-angle nuclear and magnetic reflections are marked in the figure. A part of the diffraction data is magnified in the inset of (b) to show the magnetic peaks and the fits. A comparison of the diffraction patterns obtained at 75 K and 100 K which lie between Tₘ and TₙR is presented in panel (c). The reflections at (100) and (102) are seen to undergo an enhancement in intensity with the reduction in temperature. This could be an indication of the progressive change in the magnetic structure below Tₘ. The magnetic refinement above TₙR was performed using the Γ₁ (P6₃cm) and the Γ₃ (P6₃cm’) representations and was found that they both gave equivalent description of the observed data. The analysis was also carried out using the representation Γ₂ (P6₃cm’), however it could not reproduce the experimental magnetic intensities faithfully. Within the present set of measurements, it is not possible to clearly confirm a spin re-orientation at TₙR in this compound. In fig. 2(d) a comparison of the 2K data of hLuMnO₃ and LuFe₀.₅Mn₀.₅O₃ is presented. Note that the (100) peak is absent in the hLuMnO₃ data.

Trimerization instability [2,24], single-ion anisotropy and Dzyaloshinskii-Moriya interactions are anticipated for the P6₃cm structure and could play a role in determining the magnetic ground state. The details of how all these factors lead to a complex magnetic structure is yet to be understood. It was noted in the work by Solovyev et al. [14], using first-principles methods that the different magnetic ground-state models for hYMnO₃ and hLuMnO₂ have close-by energies. In doped compounds of hYMnO₃ and hLuMnO₂, refinement using a combination of different representations have been used to get a better result [24,25].

In fig. 3(a), (b) and (c), the refined atomic positions, x for Mn/Fe and z of Lu1 and Lu2 are plotted as a function of temperature. The atomic displacements are significantly large and comparable to the giant atomic displacements found in hYMnO₃ [2]. Especially, the x position deviates from the ideal value of 1/3 for ideal 2D triangular network. Note that (a) presents an anomaly at TₙR and suggest strong spin-lattice coupling. Huge atomic displacements of all the atoms in the unit cell were found to occur below TₙR in multiferroic h(Y/Lu)MnO₃ leading to strong spin-lattice coupling [2]. The relative shift in Mn x amounts to about 4% which is comparable to the values found for hYMnO₃ [2] or for Ti displacements in a conventional ferroelectric like BaTiO₃ [26]. It is interesting to note that the variations of Mn x in YMnO₃ and LuMnO₂ are in opposite directions, meaning that, in one case, the x value increases from the ideal x value whereas in the other, it decreases. In the case of LuFe₀.₅Mn₀.₅O₃, the Mn x variation resembles closely that of YMnO₃ [2]. In (d), the temperature evolution of magnetic moment is presented and it shows a continuous reduction in magnetic moment and confirms a phase transition at Tₘ, however, at TₙR no anomaly is present. The ordered magnetic moment in LuFe₀.₅Mn₀.₅O₃ at 2K estimated from the neutron diffraction data is 3.3 μB/f.u. which is comparable to the theoretical value of 3 μB for hLuMnO₃ [10].

From the magnetization data on LuFe₀.₅Mn₀.₅O₃, it is clear that two magnetic transitions take place in this hexagonal manganite, at ≈112 K and ≈55 K. The transition at 112 K is confirmed as a paramagnetic-to-antiferromagnetic phase transition. The neutron diffraction data confirms the room temperature nuclear structure as P6₃cm. Further, the 2K data is faithfully analyzed using two magnetic representations—the Γ₁ (P6₃cm) and Γ₃ (P6₃cm’) models. The presence of strong intensity for (100) reflection rules out the Γ₂ (P6₃cm’) and Γ₄ (P6₃cm’ models). Both models Γ₁ and Γ₃ gave reasonable and comparable reliability factors of refinement. However, a reasonable value for the Mn/Fe x position was obtained only with the Γ₁ model. For the other model, the refined x-value was largely off from the ideal value of 1/3. In addition, magneto-electric coupling in hexagonal manganites is only allowed for magnetic structures where the sixfold symmetry axis is not combined with time-reversal symmetry [9]. This excludes Γ₃ (P6₃cm’),
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Fig. 4: (Colour on-line) The refined bond lengths (Mn/Fe)-O(4b) and (Mn/Fe)-O(2a) for LuFe$_{0.5}$Mn$_{0.5}$O$_3$ are presented in (a) and (b), respectively. The anomalies present in fig. 3 are reflected in the bond distances as well, especially close to $T_N$, marked by a vertical dash-dotted line.

The magnetic structure between $\Gamma_1$ and $\Gamma_3$ is inherent. A schematic of the crystal structure of LuFe$_{0.5}$Mn$_{0.5}$O$_3$ must be $\Gamma_1$ below 112 K. In a recent report, Disseler et al. studied the magnetic structure of LuFe$_{0.5}$Mn$_{0.5}$O$_3$ [27]. They observed $T_N \approx 134$ K and the presence of scattering intensity at (100) and (101) reflections above $T_N$ suggesting that correlations related to both $\Gamma_1$ and $\Gamma_2$ were present. First-principles calculations on hexagonal ferrites and manganites [15] do indicate that the amount smaller that the single-ion anisotropy.

Though giant displacements of the atomic positions of Mn and Lu are observed at $T_{SR}$, such an anomaly is not reflected in the temperature variation of magnetic moment. Hence, it is not possible to confirm a possible change of magnetic structure between $\Gamma_1$ and $\Gamma_3$ at or below 55 K. Detailed studies employing single crystals of this composition are required to settle that question. The important result of our work is the observation of giant atomic displacements across the magnetic transition thereby suggesting strong spin-lattice coupling. In order to confirm the effects of atomic displacements that are observed in LuFe$_{0.5}$Mn$_{0.5}$O$_3$ as presented in fig. 3, the bond distances (Mn/Fe)-O were evaluated from Rietveld refinement results. The Mn/Fe-O(4b) and Mn-O(2a) bond distances which are in the basal plane of the hexagonal structure are presented in fig. 4(a) and (b), respectively. It is hence clear that the atomic displacements also reflect in the bond distances and is inherent. A schematic of the crystal structure of LuFe$_{0.5}$Mn$_{0.5}$O$_3$ in $P\bar{6}_3cm$ space group is presented in fig. 5 along with $\Gamma_1$ and $\Gamma_3$ structures.

The magnetic properties of the hexagonal manganite LuFe$_{0.5}$Mn$_{0.5}$O$_3$ are studied in this paper using magnetic measurements and neutron powder diffraction. Frustration effects and, importantly, strong spin-lattice coupling are revealed as a result. It is found that the magnetic structure changes from $\Gamma_4$ for hLuMnO$_3$ to $\Gamma_1$ representation for LuFe$_{0.5}$Mn$_{0.5}$O$_3$ while the nuclear structure remains in $P\bar{6}_3cm$ space group. By perturbing the Mn lattice in the $ab$-plane through substitution of Fe, the temperature of magnetic ordering is enhanced. The atomic positions undergo significant displacements, especially close to $T_N$ and $T_{SR}$ thereby suggesting strong spin-lattice coupling.

Our work attains significance following the recent discovery of room temperature multiferroicity in thin films of hLuFeO$_3$.

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