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Structural, Magnetization and Spin Wave Analysis in Layered 5d Iridate Sr2IrO4

Imtiaz Noor Bhatti[1] and A. K. Pramanik
School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India

E-mail: inbhatti07@gmail.com

Abstract. Magnetic behavior has been studied in 5*d* layered compound Sr_2IrO_4. The material shows reasonable spin-orbit coupling effect. A canted type antiferromagnetic spin ordering induced by Dzyaloshinskii-Moriya antisymmetric interaction arising from IrO_6 octahedral distortion is observed. Our structural analysis shows a rotation of IrO_6 octahedra by ~11.3^o around *c* axis which works as precursor for (canted) weak ferromagnetic phase. Temperature dependant magnetization shows transition temperature ~225 K and field dependent magnetization shows low moment 0.055 μ_B/f.u. Our spin-wave analysis of low temperature magnetization data shows very high stiffness constant ~3365 meVÅ^2, which is interesting for this low moment spin canting system.

1. Introduction

Recently 5d transition metal oxides (TMOs) specially iridates and osmates have received extensive attention of researchers due to potential for exotic physics driven by competing interactions viz. crystal field effect (CFE), spin-orbital interaction (SOI) and onsite Coulomb interaction (U). Moreover, crystallographic structure of material also plays vital role. Over the past several years the most comprehensively studied iridate is Sr2IrO4; being iso-structure and iso-electronic to high TC cupric superconductor La_2CuO_4. The Sr_2IrO_4 draw interest as it has been theoretically predicted to be superconductor electrons/hole doping. The layered perovskite Sr_2IrO_4 believed to stabilize in J_{eff} = ½ ground state and it is a magnetic insulator. In 5*d* iridates active interactions such as: crystal field effect (CEF), on site coulomb interaction (U) and spin orbit coupling (SOC), compete among each other setting new balance which promote novel electronic and magnetic phases in these materials. It is recently found that the electronic ground state is influenced by strong SOC of Ir ion in an octahedral environment which splits the t_{2g} band into lower J_{eff} *=3/2* quartet and upper J_{eff} *=1/2* doublet. The J_{eff} *=1/2* band is so narrow that modest U opens a Mott gap by splitting it into upper and lower Hubbard bands, thus driving it to unconventional Mott insulator.[1] The Sr_2IrO_4 belongs to K_2NiF_4 family of compound and crystallize in reduced tetragonal structure with space group I41/acd. The reduced symmetry is due to rotation of IrO_6 octahedral around c-axis and play key role in physical properties of Sr_2IrO_4. [1-7]

The magnetic ground state in Sr_2IrO_4 is believed to be canted type antiferromagnetic (AFM) which gives ferromagnetic component with magnetic ordering around 225 K to this material. The spin canting is rendered by Dzyaloshinskii-Moriyam anti-symmetric interaction driven by SOI and rotated IrO6 octahedra. Further, the establishment of novel J_{eff} *=1/2* ground state has induced exotic properties in iridates [3-8].

In this report we focus on magnetism of Sr_2IrO_4. Our experimental data reveals a transition to weak FM state ~225 K. In low temperature regime the magnetic behavior is understood through spin wave analysis.

[1] Inbhatti07@gmail.com

2. Experimental Detail

The polycrystalline sample of Sr_2IrO_4 is prepared using standard solid state method using ingredients $SrCO_3$ and IrO_2. The high purity ingredients were thoroughly mixed and grinded for five hours. The well ground powder then calcinated at 900 ^{0}C for 24 hour with heating and cooling rate of 3 ^{0}C. The calcinated powder is further grounded for half an hour and pressed into pallet and sintered at 1000 ^{0}C and 1100 ^{0}C for 24 hours each with intermediate grindings to achieve sample homogeneity. We have followed the same sample preparation procedure reported elsewhere.[9,10,11] The phase purity of the sample has been checked using powder x-ray diffraction (XRD) with a Rigaku MiniFlex diffractomer with CuKα radiation. The structural analysis is done on XRD data using FullProof software. DC magnetization (M) data have been collected using a vibrating sample magnetometer (PPMS, Quantum Design).

3. Result and Discussions

3.1. Structural study

XRD pattern of Sr2IrO4 is shown in Fig. 1 along with Rietveld analysis. The analysis shows the sample is in single phase without any chemical impurity, and crystallizes in tetragonal phase with I41/acd symmetry. The refined lattice parameters are a = b = 5.4980(2) Å and c = 25.779(1) Å. We also find a rotation of IrO_6 octahedra by ~ 11.3° around c axis.

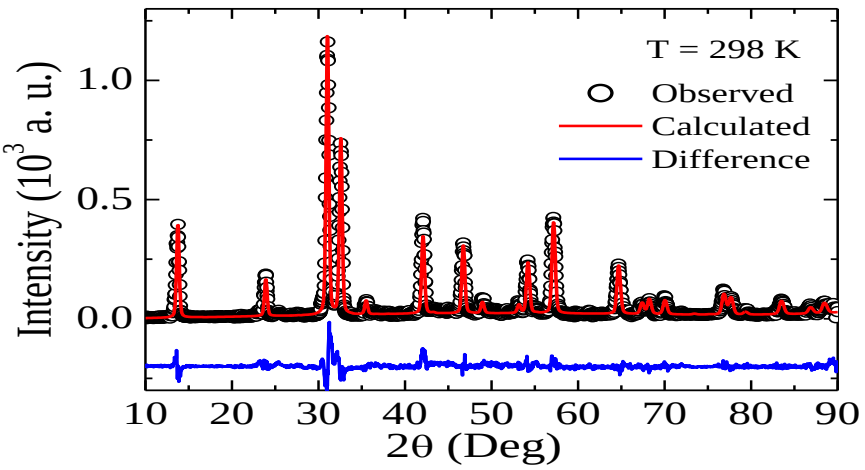

Figure 1. XRD pattern collected for Sr_2IrO_4 has been shown along with the Reitveld refinement..

3.2. Magnetization and spin wave analysis

Fig2(a) shows the temperature dependant magnetization M(T) data collected in ZFC and FC protocol in the temperature range of 5 K – 320 K in an applied field of 10 kOe. The M(T) data show a transition to weak FM state with T_c ~ 225 K. Moreover, Curie-Weiss law [$\chi = M/H = C/(T-\theta_p)$] is found to follow above T_c with θ_p = 233 K which is in favor of FM ordering (Fig 2b). We estimate an effective paramagnetic moment μ_{eff} = 0.56 μ_B/f.u.

The hysteresis in isothermal magnetization M(H) at T = 5 K shown in Fig. 3(a) is suggestive of FM ordering in this material. At 5 K, the magnetic moment μ_S = 0.05 μB/f.u at H = 70 kOe is

observed which is much lower than the effective value 0.33 μB/f.u calculated for this material with sizable SOC effect. However, below 100 K the M_{ZFC} shows decline in moment which could be related

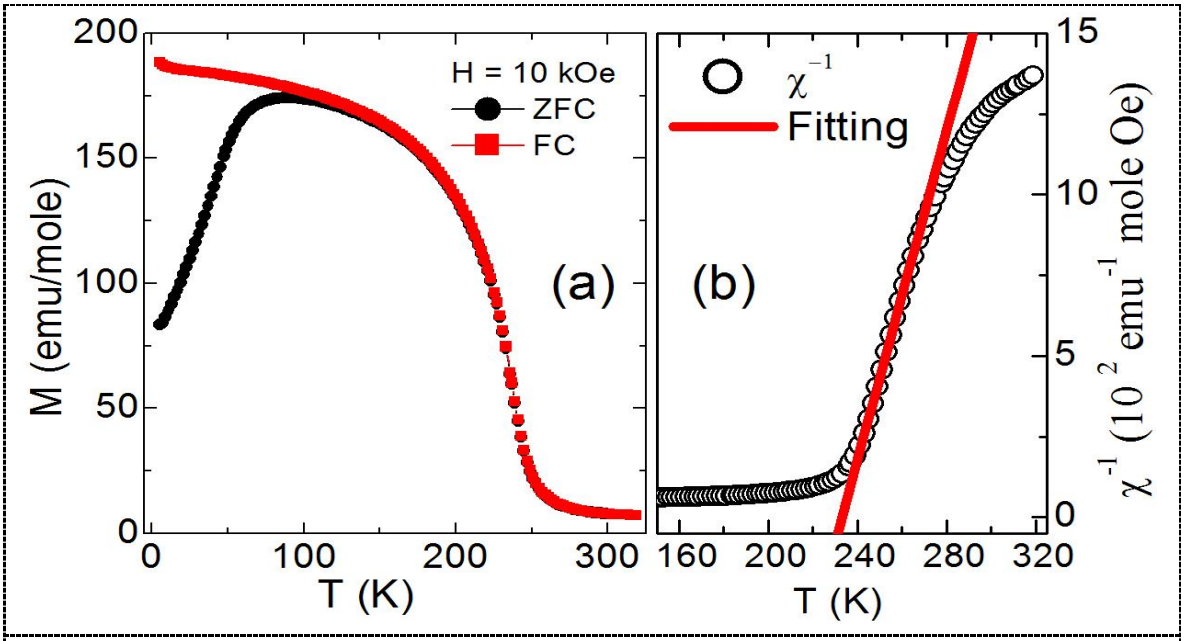

Figure 2. (a) ZFC and FC magnetization data measured in 10 kOe are plotted as a function of temperature for Sr2IrO4. (b) Inverse susceptibility (χ^{-1}) shows Curie-Weiss behaviour.

to structural distortion. The M_{FC}, however, shows gradual decrease with temperature, and we have scrutinized this thermal demagnetization behavior in terms of spin wave excitations. At low temperature the thermal effect on magnetization could be understood as [12,13]:

$$M(T) = M(0)[1 - BT^{3/2} - CT^{5/2} - \ldots.] \quad (1)$$

$$D = \frac{k_B}{\pi}\left[\frac{2.612 g\mu_B}{M(0)\rho(B)}\right]^{2/3} \quad (2)$$

where B and C are coefficients related to spin wave stiffness constant D (Eq. 2). While $T^{3/2}$ dependence signifies Bloch's law the $T^{5/2}$ term arises due to enhanced magnon-magnon interactions. In the figure 3(b) we have plotted normalized demagnetization as a function of temperature i.e.,

$$\Delta M/M(0) = [M(0) - M(T)]/M(0)$$

The spin wave demagnetization is usually observed in low T regime, and thus we have fitted the plot 3(b) with Eq. 1 up to temperature T ~ 0.4Tc. It can be mentioned that fitting with only Bloch's $T^{3/2}$ term did not yield good result. We have estimated M(0) (0.432 emu/g) by extrapolating M(T) data down to 0 K. The reasonable good fitting in Fig. 3b with coefficients B = 4.8 x 10^{-5} $K^{-3/2}$ and C = 1.8 x 10^{-5} $K^{-5/2}$ implies large number of magnons are excited with significant interaction among them. The constant D calculated using Eq. 2 (taking g = 2 and ρ = 6.728 g/cm^3) comes out 3365 meVÅ^2 which is, however, very high compared to 3d manganites i.e. ~95 meVÅ^2 for $La_{0.85}Sr_{0.15}MnO_3$ [12]. This high D can be attributed to canted spin ordering in Sr_2IrO_4 yielding very low M(0). We find D/T_c ratio, which

evaluates the range of exchange interaction, is ~14.13 meVK^{-1} implying extended range interaction in this material.

From the results of magnetization study we observed the effective magnetic moment comes out to be 0.56μ_B/f.u is quite close to the expected value of 0.57μ_B/f.u. as calculated in Bhatti etal.[9] whereas the measure μ_H is close to the reported vales in earlier reports [3,4,9] but the value is very low then the expected value which is due to the canted spin arrangement of this material. Further the thermal demagnetization shows the spin wave is excitation at low temperature and long range magnons are active in this material. High value of stiffness constant is actually result from spin canting nature and strong spins lattice coupling effect in this material. However for further detail understanding of spin wave dispersion and magnon active modes, neutron scattering measurements are required for direct estimation of D in this interesting system with SOC effect.

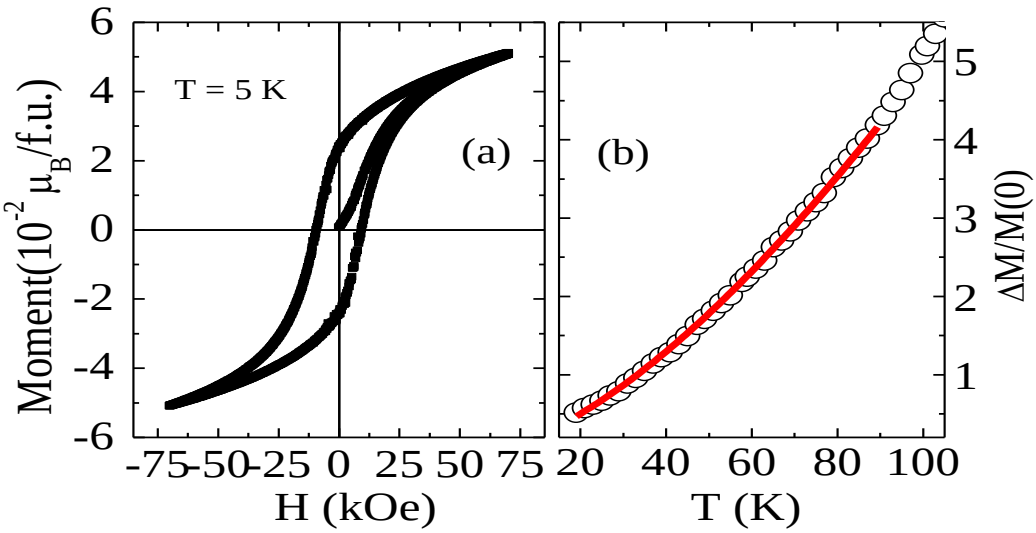

Figure 3. (a) Isothermal magnetization is shown for Sr2IrO4 at 5 K. (b) Fitting of M(T) following Eq. 1 is shown.

4. Conclusion

The *M(T)* shows a transition to weak ferromagnetic state with T_c ~225 K. The observed rotation of IrO_6 octahedra is believed to induce canted *AFM* spin ordering hence weak moment. Analysis of low-*T* magnetization in terms of spin-wave shows very high stiffness constant *D* which is significant for this canted type weak FM state.

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