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Crystal Growth and Magnetic Properties of Pyrochlore Iridate Bi2Ir2O⁷

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Abstract. We report the single crystal growth of pyrochlore iridate $Bi_2Ir_2O_7$ and its magnetic properties. The single crystals of Bi2Ir2O⁷ have been grown at 1150°C through the self-flux method. The crystals are found in octahedron-type shape with a typical size of \sim 340 µm. The Laue diffraction pattern suggests that the crystals of Bi2Ir2O7 are in a unique crystalline domain. Temperature-dependent zero-field and field-cooled magnetization data do not exhibit magnetic bifurcation down to 2 K and isothermal magnetization at 2K show a low moment 0.019 *µB/f.u*.

INTRODUCTION

In recent times, 5*d* transition metal oxides (TMOs), mainly pyrochlore iridates $A_2Ir_2O_6O'$ ($A =$ rare earth elements), have received a lot of interest due to the presence of iridium, magnetic frustration, and unique electronic and magnetic properties [1-3]. The 5*d* Ir exhibits a large spin-orbit coupling (SOC) and weak electronic correlation (*U*) due to heavy Ir ($Z = 77$) and the extended nature of 5*d* orbitals, respectively. In iridates, SOC, *U* and crystal field effect (CFE) exhibit a comparable energy scale. The dedicated interplay between these energies provides an ideal platform to study the many interesting novel phases (quantum spin liquid, Weyl semimetal, topological Mott insulator, etc.) in this class of materials [1, 2]. Apart from the novel phases, geometrical frustration is an inherent feature in pyrochlore materials due to the corner-shared network of tetrahedra, where the A and Ir magnetic ions sit on the vertices of the octahedra. This frustration is found to give rise to novel and complex magnetic ground states such as spin glass, spin ice, quantum spin liquid, etc.

In pyrochlore iridates, the A-cation plays a unique role to decide their electronic and magnetic properties, i.e., from magnetic insulator to nonmagnetic metallic phases [3]. Furthermore, if the $A³⁺$ ion is magnetic, then it introduces a complex magnetic nature due to possible *f-d* exchange interaction between localized 4*f* A-ions and itinerant 5*d* Ir [4, 5]. In the pyrochlore iridate family, $Bi_2Ir_2O_7$, $Eu_2Ir_2O_7$ and $Y_2Ir_2O_7$ are important members due to their nonmagnetic nature of A-ion [6-8]. Among these members, $Bi_2Ir_2O_7$ has a particular interest due to the nonmagnetic Bi-cation $(Bi³⁺-6p⁰)$ and comparatively large A-site. The $Bi₂Ir₂O₇$ show paramagnetic metallic behavior down to low temperature [6]. Moreover, Bismuth acts as a flux in the single crystal growth of $Bi₂Ir₂O₇$.

In this work, we have grown single crystals of $Bi_2Ir_2O_7$ by the self-flux method. The chemical composition and crystallinity of the $Bi_2Ir_2O_7$ crystals are confirmed by Laue diffraction and energy dispersive x-ray spectroscopy (EDX). Temperature-dependent magnetic data suggest the paramagnetic nature for $Bi₂Ir₂O₇$, and field-dependent magnetization at 2 K and measured in an applied field $H = 70$ kOe reveals a low magnetic moment.

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EXPERIMENTAL METHODS

Single crystals of $Bi_2Ir_2O_7$ have been grown by the self-flux method. For the crystal growth, ingredient powder materials $Bi₂O₃$ and IrO₂ with phase purity > 99.99% are taken in a molar ratio of 46:54 and ground well. The ground powder mixture is placed in a Pt crucible with a lid and heated from room temperature to 850°C with a heating rate of 1.5°C/min, then to 1150°C with a heating rate of 2°C/hour. The mixture is slowly cooled down to 850°C with the same cooling rate of 2°C/hour and then the crucible is decanted at 850°C after which the furnace is allowed to cool to room temperature. A bunch of octahedron-type crystals is found at the bottom of the Pt-crucible. Crystals are extracted from the crucible and are found with a typical size of \sim 340 μ m and its picture is shown in Fig. 1a. More detail on crystal growth is described elsewhere [6,9,10]. The quantitative analysis of chemical composition has been done with energy dispersive x-ray analysis (EDX) using a ZEISS Crossbeam 550/550L scanning electron microscope with an Oxford detector. X-ray Laue diffraction has been performed to check the single crystallinity of the grown crystal as shown in Fig. 1b which implies that $Bi_2Ir_2O_7$ single crystal is in a unique crystalline domain. DC Magnetization (*M*) data have been collected using a superconducting quantum interference device (SQUID, Quantum Design) magnetometer MPMS.

FIGURE 1. (a) and (b) show the crystal image and Laue diffraction pattern of the $Bi_2Ir_2O_7$ single crystal, respectively.

RESULT AND DISCUSSIONS

Fig. 2 shows temperature-dependent magnetization $M(T)$ of Bi₂Ir₂O₇ measured along the magnetic field direction H ǀǀ <001> at 5 kOe with the following zero field cooling (ZFC) and field cooling (FC) procedure. The magnetic moment (M) increases with decreasing the temperature down to 2 K and below around \sim 30 K the magnetization increases sharply which is consistent with the previously reported studies [6]. The ZFC and FC magnetization does not exhibit any bifurcation down to the lowest measured temperature which implies a paramagnetic nature for $Bi_2Ir_2O_7$ while in the pyrochlore iridate family, the other nonmagnetic rare-earth pyrochlore iridates $A_2Ir_2O_7$ $A = Y$ and Eu exhibits a clear magnetic bifurcation around 160 K and 120K [5, 8, 11]. However, a similar type of magnetic behavior with temperature is seen in the previous studies of $Bi_2Ir_2O_7$ [6]. The inset of Fig. 2 depicts the temperaturedependent inverse magnetic susceptibility $(\chi^1 = H/M)$ data, which is deduced from the M_{ZFC} data measured at 5 kOe field. As evident in the figure, the $\chi^1(T)$ data shows a linear behavior for T < 50 K and it has been fitted with modified Curie-Weiss behavior (Eq. 1.):

$$
\chi = \frac{M}{H} = \chi_0 + \frac{C}{T - \theta_P} \tag{1}
$$

FIGURE 2. Temperature dependence of the magnetization (M_{ZFC} and M_{FC}) measured in 5 kOe for Bi₂Ir₂O₇. The inset shows temperature dependent inverse susceptibility (Line is fitted by Eq. 1.) with modified Curie-Weiss fitting.

where χ_0 , *C* and θ_P are the temperature-independent susceptibility, Curie constant and Curie temperature, respectively. From the straight-line fitting of $\Delta \chi^1$ (= $\chi(T)$ - χ_0)⁻¹ data, we have found θ_P = - 2.7 K which implies very weak AFM interactions. Moreover, the obtained value of *θ^P* is close to the reported value [6].

Fig. 3 shows the magnetic field-dependent magnetization $M(H)$ collected at 2 K along the H \parallel <001> and in the field range of \pm 70 kOe. The isothermal magnetization data at 2 K increases with increasing the field and does not show any sign of saturation up to 70 kOe. At 2 K and the highest applied field of 70 kOe, the moment is found to be 0.019 $\mu_B/f.u.$ which is significantly lower than the expected spin-only value (gS μ_B) i.e., 1 μ_B/Ir for S = 1/2 system. This low value of magnetization matches the reported value [6].

FIGURE 3. shows magnetic field dependent magnetization for Bi2Ir2O⁷ at 2 K.

CONCLUSION

In summary, single crystals of pyrochlore iridate Bi₂Ir₂O₇ were grown through the self-flux method and their magnetic properties were studied. The obtained octahedron-type single crystals were characterized by Laue diffraction, which confirms the high crystallinity in the crystals. This material does not exhibit any magnetic bifurcation between M_{ZFC} and M_{FC} down to 2 K, which suggests a paramagnetic-type behavior for Bi₂Ir₂O₇.

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