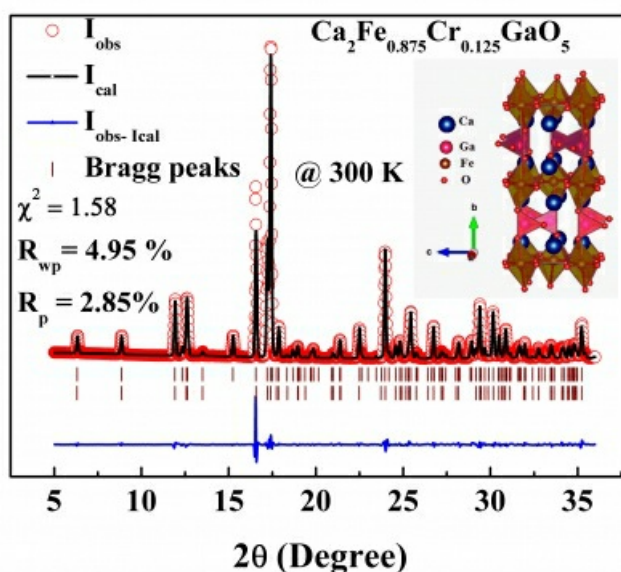


Structure and magnetic property correlation in a novel brownmillerite, $\text{Ca}_2\text{Fe}_{0.875}\text{Cr}_{0.125}\text{GaO}_5$ Ramchandra Dhal¹, Manvendra Singh², A K Sinha², Santhosh P N¹¹Department Of Physics, IIT Madras, Chennai, Chennai, India, ²Raja Ramanna Centre for Advanced Technology, Indore, India
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Brownmillerite (A₂B₂O₅/ABO_{2.5}) structure can be obtained by taking 16% of oxygen off from a cubic perovskite structure along (110) direction in an ordered manner [1]. Brownmillerites have attracted a substantial amount of attention for interesting structure and properties such as complex magnetic structure and magneto transport properties and enhanced electrochemical properties useful for solid oxide fuel cell. SrCaMnGaO_{5+δ} (δ = 0.035) exhibits magnetoresistance of 85% in 6 T and 90% in 13 T [2]. Recently, giant room temperature magnetodielectric coefficient of about -23% was observed in Ca₂FeAlO_{5+δ} at 50 MHz frequency [3]. In our present work, structural and magnetic properties of a novel brownmillerite Ca₂Fe_{0.875}Cr_{0.125}GaO₅ were studied. Crystal structure at room temperature was studied using lab X-Ray source (Rigaku SmartLab High Resolution X-ray diffractometer) as well as Synchrotron X-ray source. Temperature dependent structure was investigated with synchrotron X-Ray source from 300 K down to 35 K. Rietveld refinement of X-ray diffraction pattern collected at 300 K using lab X-Ray suggested that the compound crystallizes in orthorhombic structure with Pnma space group but synchrotron data reveals that the structure could be described better if a second structural phase with space group Im₂ (Wt. Frac. 48%) was added to Pnma (Wt. Frac. 52%). It was observed that these two different structural symmetry were coexisting till 230 K even though the Wt. Fraction for the secondary phase was reducing as the temperature was decreasing and below 200 K structural model with Pnma space group was found to be sufficient for describing the structure. Magnetic data were collected using VSM based SQUID magnetometer. M vs T data obtained at 100 Oe show a thermal hysteresis between FCC and FCW curves in the temperature range 310 K to 90 K which may be attributed to first order transition. Even though there was no sharp structural phase transition observed but there were slope changes in the temperature variation of bond lengths and bond angle curves below 250 K and below 150 K which could be a reason for the presence of the thermal hysteresis in the M Vs T data. Nonetheless, the loop area of thermal hysteresis was found to reduce at 5000 Oe and at 1 T, FCC and FCW are merging. M vs H data at 300 K show a paramagnetic behaviour. M vs H data at 200 K show a minor hysteresis loop and the hysteresis loop area increased for the data collected at 75 K and 5 K probably due to weak ferromagnetism. This increase in hysteresis and deviation from linear behaviour of M vs H curves can be qualitatively explained by GKA rule. According to GKA rule, superexchange interaction between Fe³⁺ and Cr³⁺ gives rise to weak ferromagnetism only when Fe-O-Cr bond angle is 180°. It is seen that Fe1-O1-Cr1 bond angle below 200 K is around 172°. However, all the magnetic isotherms showed a non-saturating behaviour even after application of 7 T magnetic field suggesting a dominant antiferromagnetic interaction present in the material. Authors acknowledge DST for financial support.

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