Spintronics-Oriented Magnetism and Structural Insights of Yb_2FeCrO_6 Double Perovskite

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Summary: Yb_2FeCrO_6 (YBFCO) double perovskite, synthesized via the sol-gel method, exhibits an orthorhombic (*Pbnm*) structure, a semiconductor band gap of 1.92 eV, and dual magnetic transitions canted antiferromagnetism at 247 K and spin reorientation (T_{SR}) at 39 K. The material shows an exchange bias effect at the T_{SR} transition and coexisting ferromagnetic-antiferromagnetic behavior, making it a strong candidate for spintronics applications.

Keywords: Spin Reorientation, Double Perovskite, *Exchange Bias*

1. Introduction

Spintronics, an emerging field that harnesses electron spin for data storage and processing, relies on materials with strong magnetic interactions, high spin polarization, and tunable electronic structures. Double perovskite oxides (R_2FeCrO_6) have attracted significant attention due to their ability to host two distinct transition metal ions at the B-site, enabling robust superexchange interactions that give rise to novel magnetic phenomena [1-3]. Among them, R_2FeCrO_6 compounds exhibit dominant 180° Fe^{3+}–O–Cr^{3+} interactions, leading to intriguing effects such as spin reorientation, exchange bias, and significant magnetocaloric behavior [1]. These properties make them promising candidates for spintronic devices and cryogenic magnetic refrigeration. However, the Yb-based double perovskite family remains largely unexplored despite its potential for enhanced spin-lattice coupling and unconventional magnetic phases.

In this study, we report the synthesis and comprehensive characterization of Yb_2FeCrO_6 (YBFCO) using the sol-gel method, ensuring nanostructured morphology and high phase purity. Structural and vibrational properties were analyzed using XRD, Raman, and FTIR spectroscopy, while FESEM and EDX confirmed morphology and elemental composition. Optical band transitions were explored using UV-Vis-NIR spectroscopy, and detailed magnetic measurements via VSM were conducted to evaluate its spintronic and magnetocaloric potential.

2. Results and discussion

The polycrystalline double perovskite Yb_2FeCrO_6 (YBFCO) was successfully synthesized using the sol-gel method. Rietveld refinement of XRD data confirmed a single-phase orthorhombic *Pbnm* structure, indicating a well-ordered Fe^{3+}/Cr^{3+} sublattice with lattice parameters a = 5.213(1) Å, b = 5.528(1) Å, c = 7.525(2) Å, and unit cell volume V = 216.92 Å^3. The refinement parameters (R_p = 15.3%, R_{wp} = 13.5%, R_{exp} = 11.39%, χ^2 = 1.41) indicate good fitting quality. The average crystallite size (D) ~57.06 nm, calculated using the Scherrer equation, and a Goldschmidt tolerance factor of ~0.8, along with an orthorhombic strain of 0.050, suggest structural stability with moderate distortion. FTIR analysis confirmed Fe/Cr–O stretching vibrations between 400-650 cm^{-1}, validating metal-oxygen bonding. FESEM images exhibit a homogeneous grain distribution with an average grain size of ~450 nm, while EDX confirmed the presence of Yb, Fe, Cr, and O in stoichiometric proportions. UV-Vis-NIR spectroscopy revealed a direct bandgap of 1.93 eV, indicating potential optoelectronic applications.

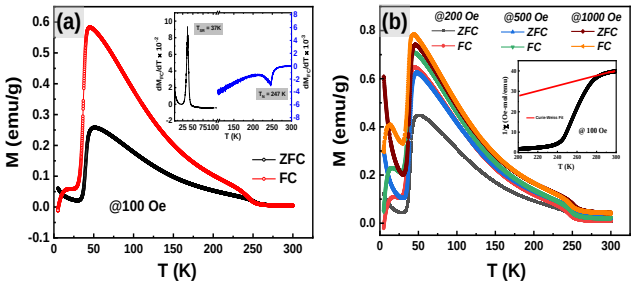

Figure 1: (a-b) ZFC-FC M-T curves at 100 Oe 100 Oe, 200 Oe, 500 Oe, and 1 kOe (5–300 K) with inset of show the first derivative of FC magnetization and χ^{-1} vs. temperature at 100 Oe for YBFCO compound.

Fig. 1 (a-b) M-T measurements show a G-type antiferromagnetic ordering of Fe^{3+}/Cr^{3+} sublattices at T_N ~ 247 K. Upon further cooling, a spin reorientation (SR) transition was observed at T_{SR} ~ 39 K, attributed Fe/Cr anisotropy and interactions with Yb^{3+} ions, leading to a shift from Γ_4(GxAyFz) to Γ_2(FxCyGz). The Curie-Weiss fit yields θ_{CW} = -167 K, confirming AFM interactions.

M-H curves, recorded up to ±9T, confirm the coexistence of antiferromagnetic (AFM) and weak ferromagnetic (FM) interactions below T_N, with the absence of saturation, even at high fields, suggesting a canted AFM structure. Additionally, the coercive field (H_C) and remanent magnetization (M_R) increase with decreasing temperature, peaking around T_{SR}, before decreasing due to spin reorientation. Notably, an exchange bias anomaly was observed near T_{SR}, highlighting the influence of AFM-FM interactions, which could be useful in spintronic applications.

References

[1] A. Banerjee *et al.*, *Phys. Rev. B* **98**, (2018), 104414.
[2] K. Yadav *et al.*, *Phys. Lett. A* **384**, (2020), 126638.
[3] M.A. Islam *et al.*, *J. Alloy and Compd*. **944**, (2023),169066.

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