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Structure and physical properties of double perovskite compounds Sr_2FeMO_6 (M = Mo, W)

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Abstract

The crystal structure and physical properties of the Sr_2FeMO_6 (M = Mo, W) double perovskite have been investigated. Analysis of the X-ray powder diffraction pattern based on Rietveld refinement indicates that Sr_2FeMoO_6 and Sr_2FeWO_6 have tetragonal cell (space group: *I*4/*m*) and orthorhombic cell (space group: *Immm*), respectively. The Curie–Weiss fit for Sr_2FeWO_6 gives Curie constant, $C = 6.08$ and Weiss temperature, $\theta = -32.6$ K. The small and negative value of θ suggests the existence of both weak ferromagnetic and antiferromagnetic interactions at low temperature. The antiferromagnetic interaction dominates over the weak ferromagnetic one.

Keywords: Double perovskite; Magnetic property; Electrical property

1. Introduction

In recent years, compounds with the general formula $A_2BB'O_6$ and double perovskite structure have been widely studied. This attention is due to the fact that many compounds of this family present remarkable magnetic and electrical properties that could be used in technological applications. Among them, Sr_2FeMoO_6 and Sr_2FeReO_6 have been known as prospective magnetoresistance compounds, which show an appreciable intrinsic tunneling-type magnetoesistance (TMR) at room temperature (RT) in the polycrystalline form [1–3]. The magnetic structure of Sr_2FeMoO_6 was attributed to an ordered arrangement of parallel Fe^{3+} ($3d^5$, $S = 5/2$) magnetic moments, antiferromagnetically coupled with Mo^{5+} ($4d^1$, $S = 1/2$) spins. Since Fe^{3+} is in the high spin state, its d orbitals are split into spin up and spin-down states. Sleight and Weiher [4] proposed that if the spin-down 3d orbitals of Fe have similar energy to the 4d orbitals of Mo, they can form a narrow band and provide the conduction mechanism. The band calculations, which show a mixing of the spin-down O 2p, Fe 3d and Mo 4d bands at the Fermi level, support this mechanism [1,5,6]. Other Fe-based ordered double perovskite A_2FeMO_6 (A = Ba, Sr, Ca; M = Mo, Re, W) have also been reported having half-metallic nature and high T_c [7–14].

In this paper, we report the synthesis and characterization of Sr_2FeMO_6 (M = Mo, W) compounds.

2. Experimental

Sr_2FeMO_6 (M = Mo, W) compounds were prepared as black polycrystalline powders by solid-state reaction in reductive atomsphere. Stoichiometric amounts of high purity (99%) $SrCO_3$, (99%) Fe_2O_3 or (99%) MoO_3 and (99%) WO_3 were ground and calcined for 12 h at 800 °C in air. The resulted powders were reground and pressed into pellets

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(15 mm in diameter and 3 mm in thickness). The pellets of Sr_2FeMoO_6 and Sr_2FeWO_6 were then sintered at 1000 °C for 38 h and 1200 °C for 18 h in a 5% H_2/N_2 gas mixture, respectively.

Phase identification and structure analysis were examined by X-ray powder diffraction (XRD) with Cu Kα radiation (Model SCINTAG X1). The GSAS program [15] was used for the Rietveld refinements in order to obtain information on the crystal structures of Sr_2FeMO_6 (M = Mo, W). The scanning electron micrograph (SEM) pictures were recorded at room temperature on a Philips XL30 SEM equipped with a secondary electron detector (SE) at 15 kV. Compositional analyses were performed by using an EDAX-DX4 energy dispersive X-ray spectrometer (EDS). Electron diffraction (ED) and high-resolution transmission

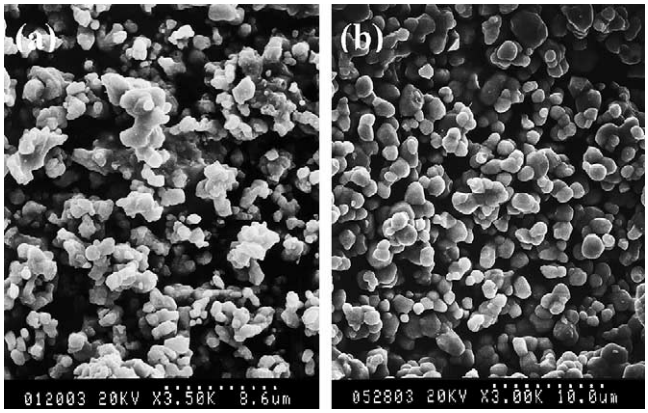

Fig. 2. Scanning electron micrograph of Sr_2FeMO_6 (M = Mo, W) with: (a) Sr_2FeMoO_6 and (b) Sr_2FeWO_6.

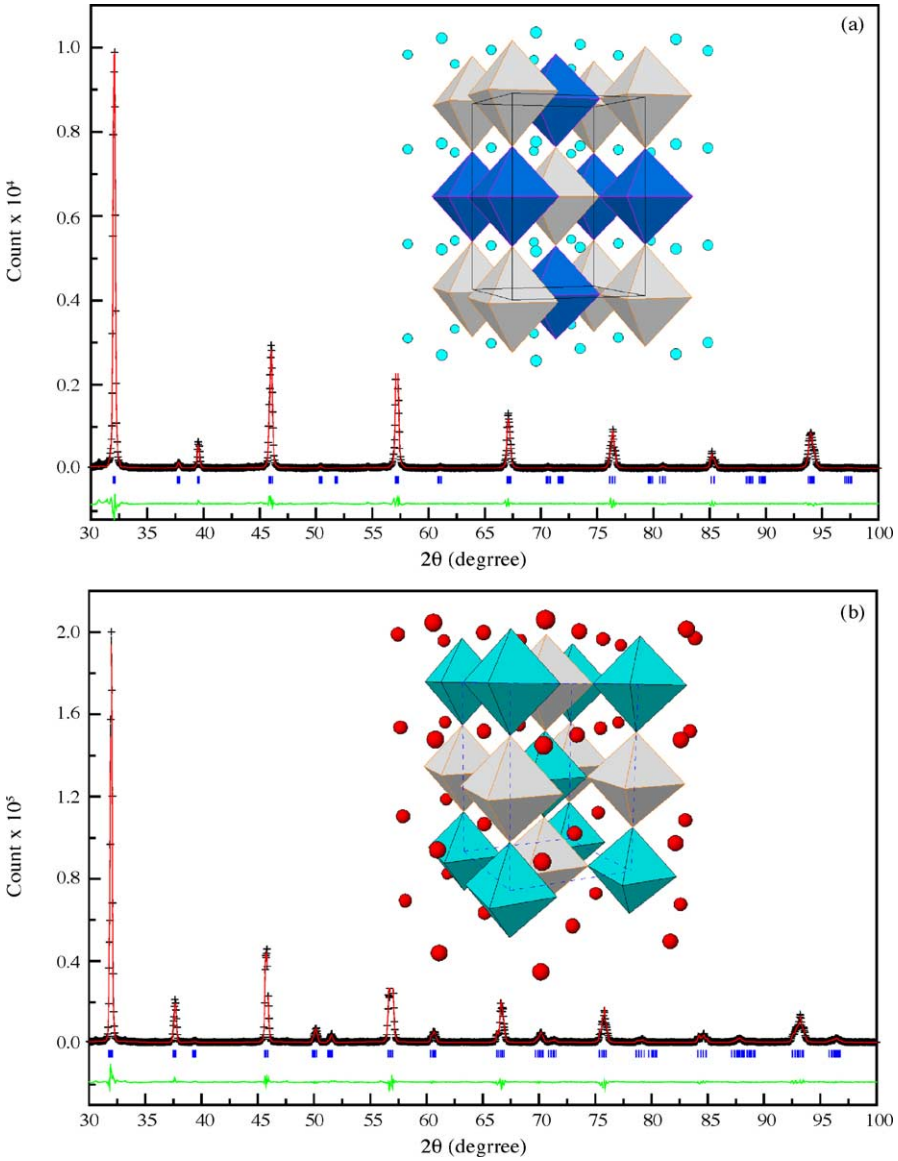

Fig. 1. Rietveld fits to powder XRD data of Sr_2FeMO_6 (M = Mo, W) with: (a) Sr_2FeMoO_6, space group *I*4/*m* and (b) Sr_2FeWO_6 space group *Immm* at 300 K. Observed (crosses) and calculated (solid line) intensities are shown with the difference at the bottom.