Preparation and physical properties in the double perovskite $Ba_2Fe_{1+x}Mo_{1-x}O_6$

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Abstract

We have prepared specimens of the double perovskite $Ba_2Fe_{1+x}Mo_{1-x}O_6$ ($x = 0.0$, 1/9, 2/9 and 1/3) from different methods and investigated their structure, magnetism, and transport behaviors. All compounds synthesized using oxides and carbonates in H_2/Ar atmosphere appear cubic structure without impurities. Those compounds show high conductivity ($\rho \sim 10^{-3}$ Ω-cm) with metallic type and reveal a ferrimagnetism $T_C \sim 340$ K and a value of $\mu_{eff} \sim 3\mu_B$ in 77 K. In contrast to those behaviors without Mo metal, the reaction of stoichiometric materials of $BaCO_3$, Fe_2O_3, MoO_3 and Mo in inert gas was found to be very dependent upon the composition x of the mixture.

Key words: double perovskite; structure; magnetism; transport

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The observation of colossal magnetoresistance (CMR) in the perovskite mixed valent manganites has led to a renewed interest in ferromagnetic oxides. It is believed that the double exchange mechanism in the presence of strong electron-phonon couplings arising from Jahn-Teller distortions is responsible for the observed properties in the manganites [1]. Recently, double perovskite Sr_2FeMoO_6 was established as a new interest material [2]. The half-metallic ferromagnets have attracted much interest as a source of fully spin-polarized charge carriers for tunneling junctions [3,4]. Kobayashi *etal.* have recently explored the so-called double perovskites, having the general formula $A(BB')O_6$, where A is a divalent alkaline earth cation (Ca, Sr and Ba), and B and B' are small ions located on octahedrally coordinated interstices of the closed-packed lattice having a simple cubic configuration [2]. The present work continues the studies of structures and physical properties of the double perovskite $Ba_2Fe_{1+x}Mo_{1-x}O_6$ (x=0.0, 1/9, 2/9, 1/3) from two different preparation methods.

Bulk samples of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ (x=0.0, 1/9, 2/9, 1/3) were prepared by standard solid state reaction in 2% H_2/Ar or pure Ar inert gas atmosphere. The stoichiometric materials of $BaCO_3$, Fe_2O_3, and MoO_3 (or MoO_3 and Mo metal) were mixed, and then calcined at 900^{o}C for 3 hours. Thereafter, these specimens were pelletized and sintered at the temperatures of 1150^{o}C. All samples were then cooled in this atmosphere to room temperature at a rate of 150^{o}C/h.

X-ray diffraction patterns of all the samples were taken with a Shimadzu XRD6000 powder X-ray diffractometer using Cu Kα radiation. Powder X-ray diffraction (XRD) shows that all oxides crystallize in ordered double perovskite structures. All samples were single-phase (not show) and exhibited a cubic (Fm3m) for x=0 and 1/9 and tetragonal (I4/m) for x=2/9 and 1/3 when preparation powders are $BaCO_3$, Fe_2O_3, MoO_3 and Mo metal. Another experimental samples preparation uses $BaCO_3$, Fe_2O_3, and MoO_3 without Mo metal.

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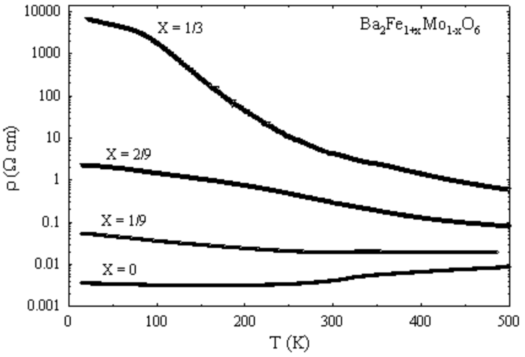

Fig. 1. Temperature dependence of resistivity of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ for preparation with appropriate amounts of $BaCO_3$, Fe_2O_3, MoO_3 and Mo metal.

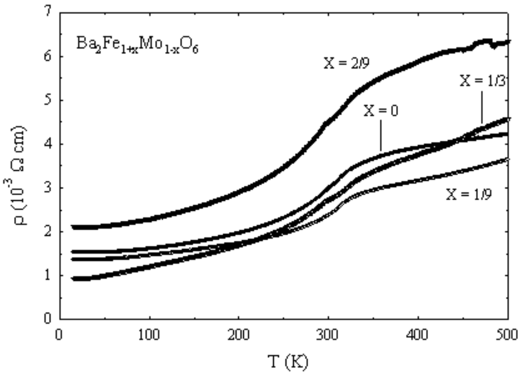

Fig. 2. Temperature dependence of resistivity of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ for preparation with appropriate amounts of $BaCO_3$, Fe_2O_3 and MoO_3.

All sample show cubic structure at room temperature (not show).

The resistance and magnetic measurement as a function of temperature, performed with the four probe technique and a vibrating sample magnetometer (Lake Shore 7307) respectively. Figure 1 exhibits the temperature dependence of resistivity showing a change from metal to insulator for preparation powders with $BaCO_3$, Fe_2O_3, MoO_3 and Mo metal. In x=0 the sample is metallic and the resistivity is of $10^{-2} \sim 10^{-3}$ Ω-cm. In the range of $1/9 \leq x \leq 1/3$ of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ is insulating. The samples remain metallic (see Fig. 2) for samples preparation using $BaCO_3$, Fe_2O_3 and MoO_3 without Mo metal. The χ-T curves (0.2 T) for preparation powders with $BaCO_3$, Fe_2O_3, MoO_3 and Mo metal exhibited in Fig. 3 shows a transition temperature T_C around 340 K and a saturation magnetization at 77 K to be $3\mu_B$/formula unit. As in Fig. 4, the χ-T curves for samples preparation using $BaCO_3$, Fe_2O_3, and MoO_3 without Mo metal give a decrease of saturation magnetization with the x increase.

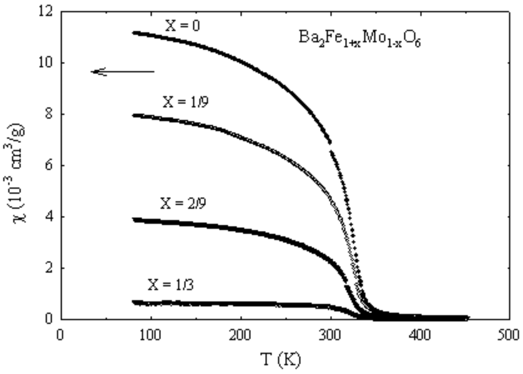

Fig. 3. Temperature dependence of magnetic susceptibility of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ for preparation with appropriate amounts of $BaCO_3$, Fe_2O_3, MoO_3 and Mo metal.

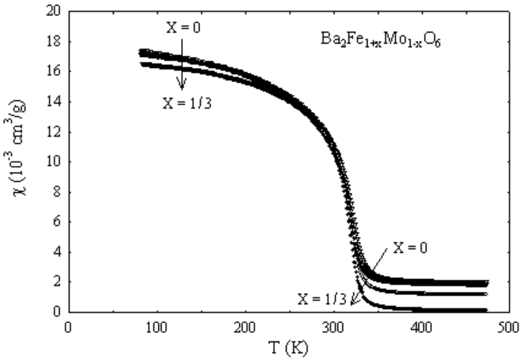

Fig. 4. Temperature dependence of magnetic susceptibility of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ for preparation with appropriate amounts of $BaCO_3$, Fe_2O_3 and MoO_3.

In summary, we have prepared a polycrystals of $Ba_2Fe_{1+x}Mo_{1-x}O_6$ in which part of Mo ions is replaced with Fe ions and used different reagent-grade chemicals in synthesized process. We have investigated the crystal structures, resistivity and magnetic susceptibility. It can be found that the cubic system have metallic, lower resistivity and high saturation magnetization.

Acknowledgements

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