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Band structures, and magnetic and transport properties of La doped two dimensional Sr2Co04

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Qiwen Yao, Xiaolin Wang, Z. X. Cheng, Germanas Peleckis, S. X. Dou, R. Nigam, and G. P. Zhao
Band structures, and magnetic and transport properties of La doped two dimensional Sr$_2$CoO$_4$


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In this work, we report on our studies on the band structure calculations, structures, transport, and magnetic properties in two dimensional layer structured perovskite compounds Sr$_{2-x}$La$_x$CoO$_4$. Structure refinement results reveal that these compounds crystallized in K$_2$NiF$_4$-type structures with space group $I4/mmm$. The temperature dependence of resistivity shows a semiconductor-like behavior over a wide range of temperatures, a metal-insulator transition at 240 K, and an upturn at 160 K for the $x=1$, 1.25, and 0.75 samples. A coercive field is about 1 T for the sample with $x=0.75$, while it is about 0.05 T for $x=0.75$ and 0.1 T for the $x=1.25$ samples. A negative field hysteresis magnetoresistance in close correlation with the coercive field has been observed and can be explained by the grain boundary tunneling effect. The first-principles band structure calculations were carried out for Sr$_{1.5}$La$_{0.5}$CoO$_4$ and the results indicate that the system is metallic with a high spin polarization which is responsible for the observed large magnetoresistance. © 2007 American Institute of Physics. [DOI: 10.1063/1.2714196]

I. INTRODUCTION

The discovery of high temperature superconductivity and colossal magnetoresistance has aroused extensive interest in the magnetic and electrical properties of perovskite transition metal oxides. The layered-type perovskite oxides $A_2$BO$_4$ with a K$_2$NiF$_4$-type structure are characterized by two dimensional confinement of the B-O-B network, which significantly reduces the one-electron band width of the $e_g$ electrons, thus inducing strong electron correlation, and alters the degrees of freedom (charge, spin, orbital, and lattice) of the material. It has been reported that Sr$_2$CoO$_4$ single-crystalline thin films prepared by pulsed laser deposition and polycrystalline samples prepared by high temperature and high pressure (6 GPa) are metallic ferromagnets with the fairly high Curie temperature ($T_C$) of 255 K, large magnetic anisotropy, and quasi-two-dimensional electrical transport properties. Y doping of Sr$_2$CoO$_4$ polycrystalline samples fabricated under high pressure was found to change the system from ferromagnetic metal to antiferromagnetic semiconductor. Ferromagnetic semiconducting states have been observed in La$_{1-x}$Sr$_x$CoO$_4$ compounds made under ambient pressure in O$_2$. With increasing Sr contents, the system changed from antiferromagnetic insulator to ferromagnetic semiconductor. The Curie temperature is about 200 K for $x=1.25$, as estimated from magnetization versus temperature dependence, but the LaSrCoO$_4$ seemed to be a paramagnetic semiconductor. In this work, we report on our investigations into the structures, and the magnetic and magnetotransport properties of the La doped Sr$_2$CoO$_4$ using the conventional solid-state reaction and compare our results with what has been previously reported.

II. EXPERIMENT

Polycrystalline samples Sr$_{2-x}$La$_x$CoO$_4$ ($x=0.5, 0.75, 1, 1.25$) were synthesized by conventional solid-state reaction. Highly pure powders of La$_2$O$_3$, SrCO$_3$, and Co$_3$O$_4$ were mixed according to appropriate atomic ratios, pelleted, and then sintered in air at 1000 °C for 12 h with several intermediate grindings. The resultant phases and structures were studied using the powder x-ray diffraction (XRD). Structure refinements were carried out by the Rietveld method using the Rietica program. Magnetic and electrical transport properties were investigated using a commercial Quantum Design magnetic property measurement system (MPMS) and physical property measurement system (PPMS) system between 5 and 330 K in magnetic fields up to 8 T. A first-principles band structure calculation was performed using the CASTEP package. We adopted the standard generalized gradient approximation (GGA), with the Perdew-Burke-Ernzerhof functional.

III. RESULTS AND DISCUSSIONS

From XRD experiments, we found that samples with $x=0.75, 1, 1.25$ are close to single Sr$_2$CoO$_4$ phase, while the $x=0.5$ sample contains the Sr$_2$CoO$_4$ as the main phase, but with Sr$_2$Co$_2$O$_7$ phases as a secondary phase. However, the single phase with $x=0.5$ can be successfully obtained by using different starting materials. Figure 1 shows a typical powder XRD pattern of a SrLaCoO$_4$ sample. It can be seen...
that the calculated pattern is in good agreement with the observed one. The lattice parameters and unit volumes increase with increasing La content, in agreement with the fact that the size of La$^{3+}$ is greater than that of Sr$^{2+}$. Our refinement data are in accordance with what was determined from La doped Sr$_2$CoO$_4$ prepared using a solution method. 4,7

The temperature dependence of the resistivity for the samples with $x=0.75$, 1, and 1.25 is shown in Fig. 2. The $x=1$ sample exhibits a semiconductorlike behavior over a wide range of temperatures below 350 K, in agreement with what has been reported in Ref. 4. A metal-insulator transition is seen around 255 K for the $x=1.25$ sample. However, the $x=0.75$ sample reveals an increase in resistivity at $T=150$ K. The room temperature resistivity of these samples increases with decreasing $x$. The resistivity for the $x=1$ and 1.25 samples has approximately the same value, which is about 10 $\Omega$ cm, while the resistivity of the $x=0.75$ sample is about one order of magnitude larger than the other two samples. In the lower temperature range (below 150 K), the rapid increase in resistivity with decreasing temperature for the $x=1$ sample indicates more electron localization than with the $x=0.75$ and 1.25 samples. This means that the $x=1$ sample looks more insulating at low temperature than the $x=0.75$ and $x=1.25$ samples. This is a possibility that because the valence of Co is 3$^+$ in SrLaCoO$_4$ ($x=1$), however, it is $<3+$ or $>3+$ in the $x=1.25$ and $x=0.75$ samples. The introduction of La$^{3+}$ can bring more electrons (for $x=1.25$) or holes ($x=0.75$) and lead to better conductivity than the $x=1$ sample.

The $\rho$ below 120 K for all the three samples can be well fitted by the equation $\rho=\rho_0 \exp(T_0/T)^{1/4}$, as shown in Fig. 3. This suggests that the three dimensional (3D) variable-range hopping (VRH) mechanism that has been proposed by Mott and the validity of which has been confirmed in manganite compounds can be used to account for the conducting mechanism at the low temperatures for the La doped Sr$_2$CoO$_4$ compounds.

Figure 4 shows the temperature dependence of the magnetization measured in a magnetic field of 0.2 T. All samples exhibit a paramagnetic to ferromagnetic transition at temperatures of about 250, 230, and 220 K (estimated by extrapolating the moment in the middle of the transition to the temperature axis) for the $x=1.25$, 1, and 0.75 samples, respectively. The kink at about 160 K for the $x=0.75$ sample may be related to the upturn at 160 K in the resistivity versus temperature dependence.

The magnetic hysteresis (MH) loops for these three samples are shown in Fig. 5. The $x=0.75$ sample shows a large coercive field of 1 T. This implies a large crystal an-
isotropic energy. For the other two samples, their coercive fields are 0.05 T for $x=1$ and 0.1 T for $x=1.25$, respectively. The magnetoresistance (MR) effect is observed for all three samples. The MR values (defined as $[\rho(H)-\rho(0)]/\rho(0)$) are 1%, 2%, and 3% at 150 K for the $x=1$, 0.75, and 1.25 samples, respectively, as shown in Fig. 6(a). The MR is enhanced to 7% at 5 K for the $x=1.25$ sample. A further study on the $x=1.25$ sample, it can explain the magnetism and metalliclike properties in the Sr$_{2}$CoO$_{4}$ compound. The band structure results indicate that the planar oxygen are responsible for the high spin polarization in this compound. The band structure calculations is needed for the Sr$_{2}$CoO$_{4}$ with other La doping levels.

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