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To cite this article: L X Yang et al 2008 J. Phys.: Conf. Ser. 121 022017

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Pressure induced metallization in ACrO3 in perovskite compounds

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Abstract. We studied the electrical conductivity of ACrO3 (A=Sr, Ca) perovskites performed at various pressures up to 40 GPa using diamond anvil cell techniques. The samples were synthesized under high pressure high temperature. Pressure induced metallizations were observed in both samples. However the xray diffraction experiments with synchrotron radiation source indicated no discernable crystal structural transition up to 60 GPa. Therefore the pressure induced metallizations were ascribed to electronic type phase transitions. It possibly came from the change of electronic structure due to an orbital ordering evolution induced by pressure.

1. Introduction

The transition-metal oxides show so many interesting physical properties such as the charge-ordering system $La_{1-x}Sr_xFeO_3$ [1], $La_{1-x}Sr_xNiO_4$ [2] and the superconductive system $La_{2-x}Sr_xCuO_4$ [3] and the metal-insulator transition systems R_{1-x}A_xTiO₃[4]. The most acceptable explanations of the phenomenon just base the complexity electrical structures and the strong electron-electron interactions [5]. The most of transition-metal oxides with perovskite or a perovskite-related structure is usually very stable under high pressure and the effects of pressure of these materials just are the decrease of the volume and the transition of electrical structures. So the high pressure research of these materials can easily investigate the behavior of the electronic structures. ACrO₃ (A=Ca, Sr) perovskites are Mott solutions with tunable narrow energy gap and replacing Sr by Ca gives an increases the band gap. The x-ray diffraction shows that the crystal structures of Sr/CaCrO₃ keep stable in the pressure range 0-60 GPa at room temperature and the bulk modulus of $SrCrO_3$ (B₀ =178±5 GPa) is smaller than CaCrO₃'s $(189\pm 2$ GPa) [6] and it indicates that CaCrO₃ is more difficult to compress under pressure. The bonding instability has been confirmed by the pressure induced bond softening in SrCrO₃ [6]. So ACrO3 (A=Ca, Sr) is a perfect system to research the behavior of the electrical structures under pressure and we performed the electrical conductivity of ACrO₃ (A=Ca, Sr) performed at various pressures up to 40GPa using diamond anvil cell techniques.

2. Experiment

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Journal of Physics: Conference Series 121 (2008) 022	017 doi:10.1088/1742-6596/121/2/022017

A hardened Be-Cu DAC and a T301 stainless steel were used in our experiments. The pressure medium and the insulator layer is Al_2O_3 powder. Pressure was measured by the ruby fluorescence method. The electrical resistance was measured by a real four-probe method. All experiments were performed from 80K to 300K.

3. Results and Discussion

The pressure variation of the electrical resistance R (P) of Sr/CaCrO₃ at a special temperature (280K)



is shown in figure. 1. As can be seen a precipitous decrease of $Sr/CaCrO_3$ all occur at low pressure but it mainly come from the decrease of the grain-boundary resistance and the contact resistance under pressure. So the change is not a reliable proof for the insulator to metal transition.

Figure 1. The pressure dependence of the electrical resistance of $Sr/CaCrO_3$ under different pressure at 280K.

In order to further explore the high pressure electrical state of $Sr/CaCrO_3$ we performed the R (T) measurement at various pressures. As shown in figure. 2, the R (T, 0GPa) curve of $SrCrO_3$ is typical of





an insulator and the R (T, 10GPa) curve with a minimum value at about 260K is a characteristic of the metal-insulator transition (MIT). The temperature of MIT (T_c) also decreases under higher pressure and it reaches 240K at the highest pressure 23.1GPa. CaCrO₃ has the resembled electronic properties under pressure like SrCrO₃'s and the start pressure and temperature of MIT is about 29.3GPa and 260.4K (figure. 3). The transition temperature T_c of CaCrO₃ also decreases following the increasing of pressure and at the highest pressure 40.4GPa it reaches about 235K. Our results of T_c of SrCrO₃ and CaCrO₃ vs pressure are displayed in figure. 4. We extrapolate the T_c (P) curves of



Figure 3. The temperature dependence of renormalized resistance of CaCrO₃.



Figure 4. Pressure dependence of the metalinsulator transition temperature of Sr/CaCrO₃.

Joint 21st AIRAPT and 45th EHPRG Int. Conf. on High Pressure Science and TechnologyIOP PublishingJournal of Physics: Conference Series 121 (2008) 022017doi:10.1088/1742-6596/121/2/022017

 $SrCrO_3$ and $CaCrO_3$ to lower pressure and it would locate the $T_c=290K$ for $SrCuO_3$ and $CaCrO_3$ near 5.5GPa and 16GPa. The transition pressure of $CaCrO_3$ is much larger than $SrCrO_3$ and it indicate that $CaCrO_3$ is more difficult to metallize under pressure.

4. Conclusions

We have performed the electrical conductivity measurements of $Sr/CaCrO_3$ in DAC. The MIT of $Sr/CaCrO_3$ under pressure all occur and at room temperature (290K) the transition pressure of $SrCrO_3$ and $CaCrO_3$ is 5.5GPa and 16GPa and it belongs to an electronic type phase transition. The MIT of CaCrO3 the same as $SrCrO_3$ comes from the pressure induced bond softening and the different band gaps of $Sr/CaCrO_3$ are the reason of the difference of the metallization pressure. So all the results of $Sr/CaCrO_3$ indicate that the pressure can change the band gap continuously and these compounds undergo an electronic type phase transition under pressure.

Acknowledgements

This work was supported by NSF & MOST through the research projects.

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