Multi-probe study on Charge Transport Transitions of $PrBaCo_2O_{5.5+x}$

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Charge Transport Transition (CTT) is a kind of phenomenon demonstrating huge resistivity changes,, and has been widely observed in strongly correlated systems. The CTT in $RBaCo_2O_{5.5+x}$ can be induced by temperature, pressure and also hole doping. Most of the effort has been focused on the temperature induced MIT of stoichiometric $RBaCo_2O_{5.5}$, which is accompanied by an anomaly in inverse magnetic susceptibility. This anomaly is generally attributed to the spin state transition (SST) of Co^{3+} ions. The competition between crystal field (CF), on-site Coulomb correlations, and the intra-atomic exchange energies leads to three possible spin states of Co^{3+} ions: the low spin state (LS, $t_{2g}^6e_g^0$), the intermediate spin state (IS, $t_{2g}^5e_g^1$), and the high spin state (HS, $t_{2g}^4e_g^2$). However, the crystal structure phase transitions coupling with the CTTs in $RBaCo_2O_{5.5+x}$ are still in controversy and there is no consensus on the spin states below and above the transition temperature as well. Moreover, no satisfactory mechanism has been established for this system so far.

We conducted a multi-probe study $PrBaCo_2O_{5.5+x}$ polycrystalline samples with a combination of diffraction techniques (electron, X-ray and neutron) and X-ray spectroscopies (XPS and XAS). On discovering some weak super lattice peaks, the Pmma ($2a_p \times 2a_p \times 2a_p$) structure model of $PrBaCo_2O_{5.5}$ in insulating phase by single crystal X-ray diffraction study is justified, and a new Pmmm ($a_p \times 2a_p \times 2a_p$) structure model is constructed for hole doping sample, $PrBaCo_2O_{5.5+x}$ in the high-conductivity phase. Through magnetic structure analysis on neutron powder diffraction data, we directly observed the existence of low spin-state Co^{3+} in $PrBaCo_2O_{5.5}$ in low-conductivity phase and for the first time found hole doping induced spin state transition in $RBaCo_2O_{5.5+x}$ system. It was finally recognized that the CTTs in $PrBaCo_2O_{5.5+x}$, induced by both temperature and hole doping, are coupling with the *Pmma* ($2a_p \times 2a_p \times 2a_p$) structure transition to *Pmmm* ($a_p \times 2a_p \times 2a_p$), which caused by spin-state transition of Co^{3+} ions. Therefore, we propose a common scenario for the CTTs.