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Crystallographic and magnetic structure study in SrCo3-x by high resolution x-Ray and neutron powder diffraction

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Transition metal oxides (TMOs) represent a wide set of materials with a broad range of functionalities, including superconductivity, magnetism, and ferroelectricity, which can be tuned by careful choice of parameters such as strain, oxygen content, and applied electric and magnetic fields [1-4]. This tunability makes TMO's ideal candidate materials for use in developing novel information and energy technologies and SrCoO3 provides a particularly interesting system for investigation due to its propensity to form oxygen-vacancy-ordered structures as the oxygen content is decreased. The ties between structural and functional properties of this material are obvious as it undergoes simultaneousy structural and magnetic phase transitions between two topotactic phases: from a ferromagnetic perovskite phase at SrCoO3.0 to the antiferromagnetic brownmillerite SrCoO2.5 [1,5].

In this study we have determined their crystallographic and magnetic structures of SrCoO2.50, SrCoO2.75, SrCoO2.875, and cubic SrCoO3.00 using high resolution X-ray and neutron powder diffraction from 4 K to 600 K. The correct structure of oxygen-deficient end-member SrCoO2.5 was determined in space group of Imma, instead of Pnma or Ima2 proposed previously, with G-type antiferromagnetic order up to TN = 570 K. In SrCoO2.875, clear peak splitting was observed from (200) in cubic phase to (004) and (440) in tetragonal phase, indicating that the precise structure is I4/mmm with a = b = 10.829(9) Å and c = 7.684(2) Å at 95 K. the corresponding magnetic structure is ferromagnetic with 1.86(4) μB per formula, in accordance to a spin configuration of cobalt ions with an intermediate spin state of both on Co3+ and on Co4+. The end member SrCoO3.00 possesses a simple cubic crystal structure with a = 3.817(2) Å at 95 K, and ferromagnetic order up to 280 K. The magnetic moment of 1.96(8) μB /Co4+ corresponds to an intermediate spin state of Co4+.

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