



Contribution ID: 105

Type: not specified

Crystallographic and magnetic structure study in SrCo_{3-x} by high resolution x-Ray and neutron powder diffraction

Thursday, 4 February 2016 11:30 (15 minutes)

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 SrCoO_3 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 simultaneous structural and magnetic phase transitions between two topotactic phases: from a ferromagnetic perovskite phase at $\text{SrCoO}_{3.0}$ to the antiferromagnetic brownmillerite $\text{SrCoO}_{2.5}$ [1,5]. In this study we have determined their crystallographic and magnetic structures of $\text{SrCoO}_{2.50}$, $\text{SrCoO}_{2.75}$, $\text{SrCoO}_{2.875}$, and cubic $\text{SrCoO}_{3.00}$ using high resolution X-ray and neutron powder diffraction from 4 K to 600 K. The correct structure of oxygen-deficient end-member $\text{SrCoO}_{2.5}$ was determined in space group of Imma , instead of Pnma or Ima2 proposed previously, with G-type antiferromagnetic order up to $T_N = 570$ K. In $\text{SrCoO}_{2.875}$, 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 Co^{3+} and on Co^{4+} . The end member $\text{SrCoO}_{3.00}$ 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 $1.96(8)$ $\mu\text{B} / \text{Co}^{4+}$ corresponds to an intermediate spin state of Co^{4+} .

[1] H. Jeon et al., Nature Mater. 12, 1057 (2013). [2] Yang et al., Nature Mater. 8, 485 (2009). [3] J. Seidel et al., Nature Com. 3, 799 (2011). [4] T. Takeda, et al., J. Phys. Soc. Jpn. 22, 970 (1972). [5] S. J. Callori, J. Seidel, C. Ulrich et al., Phys. Rev. B 91, 140405(R) (2015).

Primary author: Ms CHANG, Fenfen (The school of physics, university of New South Wales, NSW 2052)

Co-authors: Mr ULRICH, Clemens (School of Physics, University of New South Wales, Sydney, NSW 2052, Australia); Mr XIANG, Feixiang (4Institute for Superconducting and Electronic Materials, University of Wollongong, Australia); Mr HESTER, James (3Australian Nuclear Science and Technology Organization, Lucas Heights, NSW 2234, Australia); Mr SEIDEL, Jan (5School of Materials Science and Engineering, University of New South Wales, Australia); Mr REEHUIS, Manfred (2Helmholtz-Zentrum Berlin für Materialien und Energie, D-140109 Berlin, Germany); Mr AVDEEV, Maxim (3Australian Nuclear Science and Technology Organization, Lucas Heights, NSW 2234, Australia); Mr WANG, Xiaolin (4Institute for Superconducting and Electronic Materials, University of Wollongong, Australia)

Presenter: Ms CHANG, Fenfen (The school of physics, university of New South Wales, NSW 2052)

Session Classification: Contributed talk