Experimental Report

12/12/2013

Proposal: **5-24-526** **Council:** 10/2012

Title: The reason for giant magnetoresistance in La0.5Ba0.5Co1-xFexO3

This proposal is a new proposal

Researh Area: Physics

Main proposer: **SIKOLENKO Vadim V.**

Experimental Team: SIKOLENKO Vadim V.
EFIMOV Vadim

Local Contact: RITTER Clemens

Samples: La0.5Ba0.5Co1-xFexO3
La0.47Ba0.53CoO3

Instrument	Req. Days	All. Days	From	To
D2B	2	2	26/06/2013	28/06/2013
D1B	2	2	27/02/2013	01/03/2013

Abstract:

The main goal of this proposal is a detailed neutron powder diffraction (NPD) study of the La0.5Ba0.5Co1-xFexO3 compounds to clarify the crystal and magnetic structure transformations. The results of this study are supposed to find most probable model explaining the nature of the phase separation, small structural distortions and magnetic structure changes in the range of unusual phase transitions.
The combination of neutron with X-ray powder diffraction data, magnetization studies and XAFS-spectroscopy results at the Co and Fe K-edges (ESRF, BM23 beamline) will give us an opportunity to analyze the crystal and magnetic structure changes of lattice parameters and local atomic (EXAFS Debye-Waller factor of Co-O bond) and electronic(valence & spin-state change of cobalt ions) structure distortions near Co ions in order to establish the most probable model explaining the correlation of the crystal and magnetic structure transformations as well as magnetic and transport properties in a wide temperature range.

The reason for giant magnetoresistance in $La_{0.5}Ba_{0.5}Co_{1-x}Fe_xO_3$

Hole-doped cobaltites $La_{1-x}M_xCoO_3$ (M=Ca, Sr, Ba) exhibit ferromagnetism likely arising from the double exchange interaction between Co^{3+} and Co^{4+}ions, and the ferromagnetic state establishes with increasing alkaline earth doping above x=0.18 (M=Sr). However, in the case M=Ba the antiferromagnetic long range ordering in very narrow range (x=0.17 and 0.18) develops earlier than the ferromagnetic state [1]. The hole-doping effects on the transport and magnetic properties because the FM interactions are depend on Co spin state, and therefore on lattice parameters and crystal symmetry. The intermediate state (IS) of Co ions with a partial filled e_g level which is a Jan-Teller (JT) active state plays an important role in the FM state in cobaltites. The JT effect seems to be most pronounced for Ba-doped cobaltites [2]. This finding correlates well with the observation of the unique long-range tetragonal phase in $La_{0.5}Ba_{0.5}CoO_3$ compatible with static JT distortion of CoO_6 octahedra [2] and anomalous magnetization behavior [3]. Relatively small decrease of the oxygen content in this compound leads to unique low temperature structural phase separation into antiferromagnetic and ferromagnetic cubic phases with different unit cell volumes [4].
It is well known that the ferromagnetic ordering favors stabilization of the conductive state as it was observed in manganites, magnetic semiconductors and many other compounds. However we observed that the ferromagnetic state in the $La_{0.5}Ba_{0.5}Co_{1-x}Fe_xO_3$ leads to stabilization of the insulating ferromagnetic state despite the metallic paramagnetic ground state . The metal-insulator and paramagnetic-ferromagnetic transitions occur at the same temperature. It worth to be noted that the all compounds in the range $0<x<0.2$ have the very close spontaneous magnetization corresponding approximately of 1.9 Bohr magnetons for unit formula.
We have performed neutron diffraction experiment using high resolution D2B (λ = 1.594 Å) and high-intensity D1B (λ = 2.52 Å) diffractometers. Below 140K a ferromagnetic ordering has been observed. Calculated magnetic moment is slightly less, than expected. The crystal structure remains cubic (space group $Pm\bar{3}m$) by cooling down to 4.1 K.

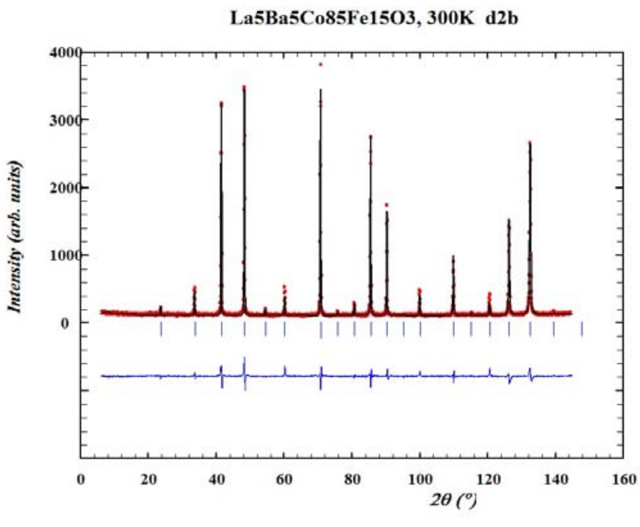

Fig.1. *Observed, calculated and difference patterns for the* $La_{0.5}Ba_{0.5}Co_{0.85}Fe_{0.15}O_3$ *at T=300K. Data from D2B high resolution diffractometer. The structure is cubic,* $Pm\bar{3}m$ *space group, a= 3.89283(3)Å*

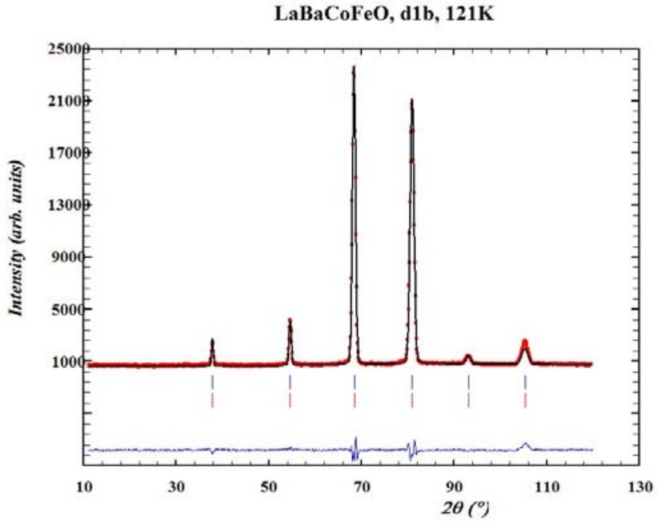

Fig.2. *Observed, calculated and difference patterns for the $La_{0.5}Ba_{0.5}Co_{0.85}Fe_{0.15}O_3$ at T=121K. Data from D1B high resolution diffractometer. The magnetic structure is ferromagnetic, the magnetic moment of Co ions is 1.2(2)μ_B*

References

1. P. Tong, J. Yu, Q. Huang, K. Yamada, D. Louca Phys. Rev.Lett.106, 156407 (2011).
2. F. Fauth, E. Suard, V. Caignaert, Phys. Rev. B **65**, 060401 (2001).
3. I. Fita, R. Szymczak, I. Troyanchuck, D. Karpinsky, A. Wisniewski, V. Markovich, H. Szymczak, Phys. Rev. B **83**, 064414 (2011).
4. I.O. Troyanchuk, D.V. Karpinsky, M.V. Bushinsky, V. Sikolenko, V. Efimov, A. Cervellino, JETP Letters **93,** 149 (2011).