Experimental Report

Proposal: **5-31-2277** **Council:** 10/2012

Title: Neutron powder diffraction study of structural and magnetic ground state of the double perovskite seriesLa2-xSrxCuRuO6 (0 <= x <= 1)

This proposal is a new proposal

Researh Area: Physics

Main proposer: **DAS SARMA Dipankar**

Experimental Team: PURI Anil Kumar
MUKHERJEE Sumanta
PAL Banabir

Local Contact: RITTER Clemens

Samples: La1.2Sr0.8CuRuO6
La2CuRuO6
La1.8Sr0.2CuRuO6
LaSrCuRuO6

Instrument	Req. Days	All. Days	From	To
D2B	4	2	06/03/2013	08/03/2013
D20	4	2	04/03/2013	06/03/2013

Abstract:

The series of double perovskite oxides La2-xSrxCuRuO6 (0 <= x <= 1) have been reported to have interesting magnetic properties owing to the competing nearest neighbour and next nearest neighbour interactions in combination with the disordered occupancy of Cu and Ru atoms at B/B' sites. Full profile refinement of x-ray diffraction patterns predicted a monoclinic structure for the end members while the intermediate members displayed triclinic structure. On the other hand, the parent compound La2CuRuO6 is a short range ferrimagnet while the Sr doped samples clearly display antiferromagnetic ordering at low temperature. The antiferromagnetic ground state of members with lower Sr doping was related to the existence of ferrimagnetic clusters which are antiferromagnetically coupled. In the proposed neutron diffraction experiment we plan to determine the composition dependence of magnetic structure, nature of magnetic interactions and the range of magnetic ordering besides improving the structural information of these fundamentally interesting series of oxides.

Neutron powder diffraction study of structural and magnetic ground state of the double perovskite series $La_{2-x}Sr_xCuRuO_6$ ($0 \leq x \leq 1$)

The proposal aimed to determine the detailed structure and magnetic ground of a series of double perovskite oxides $La_{2-x}Sr_xCuRuO_6$ ($0 \leq x \leq 1$) using neutron powder diffraction. The low temperature diffraction patterns collected at D20 diffractometer did not show any change compared to the room temperature patterns, except for minor lattice contraction. Therefore, it was concluded that these oxides does not have long range magnetic ordering that can be detected by neutron diffraction. The time on D20 was then utilized for probing the magnetic structure of another material NiS (whose results appear on the last page). The double perovskite oxides were then investigated on D2B diffractometer for determining the room temperature crystal structure. The diffraction patterns were refined by Rietveld method using fullprof software program. These refinements established clearly the fact that the end members La_2CuRuO_6 and $LaSrCuRuO_6$ form in monoclinic structure whereas the members with intermediate Sr doping stabilize in triclinic structure. As expected, the refinement of oxygen positions was possible with neutron diffraction while it could not be performed using x-ray diffraction patterns. In Figure 1, we show the results of refinement for two compounds $La_{1.8}Sr_{0.2}CuRuO_6$ and $LaSrCuRuO_6$ while in Table 1 the structural parameters obtained from the refinement are given. We are attempting to determine the cation ratios from the energy dispersive x-ray spectroscopy (EDS) for these samples which will help in further improvements of the structural determination.

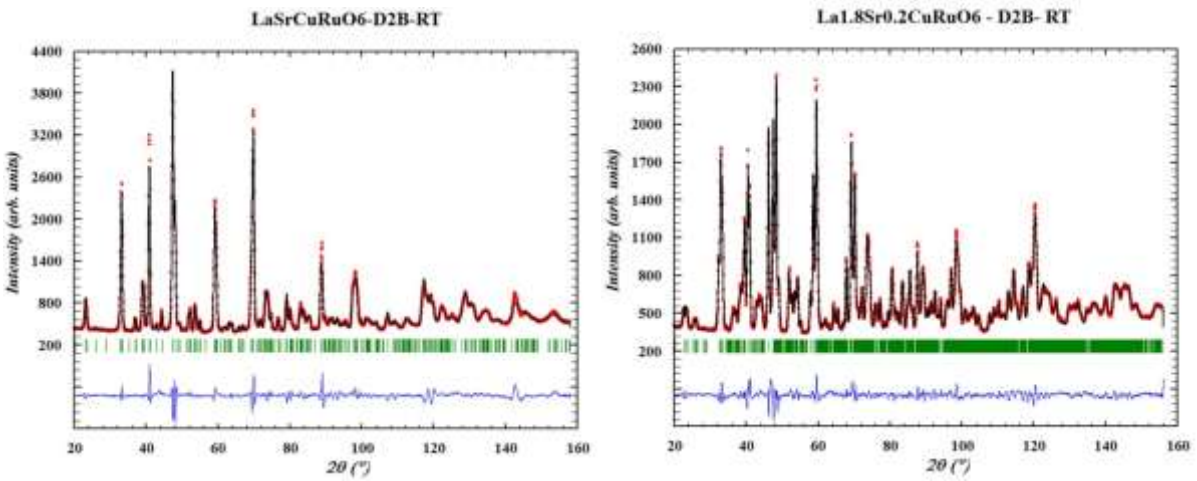

Figure 1: Graphs showing the result of Rietveld refinement on the neutron diffraction patterns of the two samples, $LaSrCuRuO_6$ (left) and $La_{1.8}Sr_{0.2}CuRuO_6$ (right).

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
LaSrCuRuO6	5.6120 (4)	5.5886 (4)	7.8232 (5)	90	90.02 (1)	90
La1.8Sr0.2CuRuO6	7.7675 (3)	7.8931 (3)	8.1085 (3)	88.916 (2)	90.151 (4)	89.992 (5)
La1.2Sr0.8CuRuO6	7.7513 (6)	7.7747 (6)	8.1640 (6)	90.00 (1)	89.82 (1)	90.04 (2)

Table 1: Room temperature lattice parameters determined from the Rietveld refinement for the double perovskite oxides. The numbers in the paranthesis are the error on the last significant decimal.

Results on NiS

At room temperature the hexagonal phase of NiS is a conducting Pauli paramagnetic metal with a characteristic metallic dependence of resistivity on temperature. Near 263 K [1], the system undergoes a first order phase transition, with an abrupt change in resistivity. The system becomes antiferromagnetic below the transition temperature, showing a significant changes in the lattice parameter without any change in crystal symmetry ($P6_3/m\ m\ c$).

To probe the magnetic ground states of NiS across the transitions, neutron diffraction experiment was performed in D20 Powder diffractometer in ILL, Grenoble, France across the transition temperature (263 K) starting from 285 K to 232 K. Both high temperature and low temperature diffraction patterns in NiS can be indexed as the NiAs type structure. In the analysis it has been seen that across the transition there are abrupt changes in the lattice parameters as shown in the figures given below

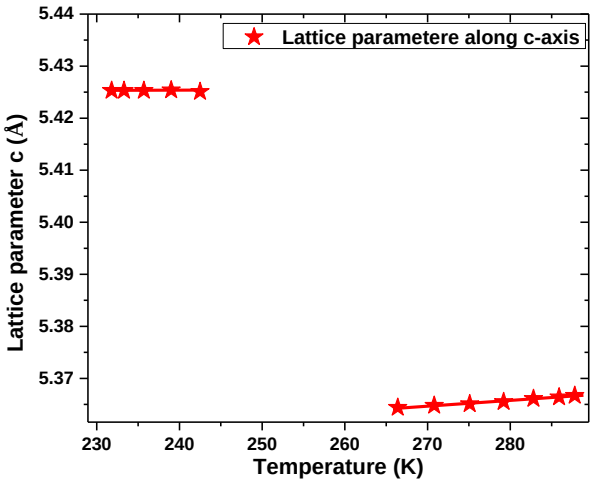

Figure 1a: Variation of lattice parameter along c-axis

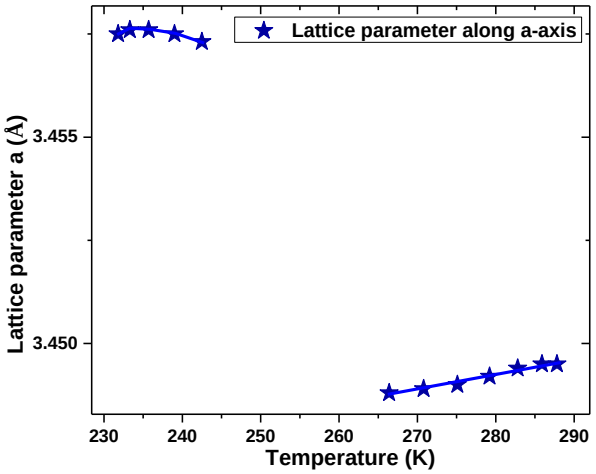

Figure 1b: Variation of lattice parameter along a-axis

During the cooling across the transition temperature (263 K) lattice parameter along c-axis changes from 5.3644Å to 5.4251Å and along a-axis changes from 3.4488 Å to 3.4573 Å.

The low temperature phase is A- type antiferromagnetic in nature. In the antiferromagnetic state the moments in a hexagonal layer are coupled ferromagnetically along ab-plane and the coupling between adjacent hexagonal planes are antiferromagnetic. In the neutron diffraction data the (101) reflection peak intensity increases very abruptly in the neighborhood of 263 K. The moment at around 230 K comes out to be $1.286\mu_B$ which significantly lower compared the previously reported value [1].

Reference:

1. Joseph T. Sparks and Ted Komoto, J. Appl. Phys. **34**, 1191 (1963).