ESRF	**Experiment title:** Determinaition of local lattice structure of the oxygen deficient perovskite $La_{8-x}Sr_xCu_8O_{20}$ system by EXAFS	**Experiment number:** HS-377
Beamline: BM29	**Date of experiment:** from: 01 July 1997 to: 05 July. 1997	**Date of report:** 15.02.00
Shifts: 12	**Local contact(s):** Dr. Michael BOROWSKI	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*N.L. Saini, Università di Roma "La Sapienza", Roma
A. Bianconi, Università di Roma "La Sapienza", Roma
*A. Lanzara, Università di Roma "La Sapienza", Roma
*F. Natali,Università di Roma "La Sapienza", Roma

Report:

The aim of the experiment was to study the local CuO_2 lattice of the oxygen deficient perovskites, $La_{8-x}Sr_xCu_8O_{20}$ (8-8-20), which has captured attention of the researchers working in the field of perovskites due to anomalous transport properties. In addition, the system contains Cu and O networks, having one-dimensional CuO chain shadowed by a complex three-dimensional network of CuO_5 pyramids and CuO_6 octahedra, forming a tetragonal unit-cell. Therefore the system constructs a good example of existing 1D insulating electronic component with a 3D itinerant electronic component. The study was also motivated by the charge ordering phenomena in the perovskites which has been a point of recent interest.

During the allocated beamtime we had measured temperature dependence of the local structure by Cu K-edge x-ray absorption measurements to explore correlation between the anomalous behaviour of the transport properties and the local atomic displacements. Several dopings in the range of in the composition range of x~1.5 to ~2.2 were studied to investigate the doping dependence. Availability of high quality single crystals of the system, grown by the travelling-solvent floating-zone method, allowed us to exploit the polarization dependence of the absorption cross section to discreminate in-plane and out-of-plane local displacements. High resolution polarized XANES study was combined with EXAFS measurements up to high momentum transfer. Geometrical constraints ristricted us to study a small number of temperature in case of EXAFS as most of the EXAFS spectra were obtained in the E//c geometry to have access to the Cu-O chains which are found to be a controlling factor for the anomalous transport properties. The local structure was found to show a strong change across the anomalous temperature where the system shows anomalies in the resistivity and Hall effect data. The EXAFS analysis clearly revealed change in the pair distribution of Cu-O networks, ven though a quantitative estimate of these lattice displacements still invites more studies due to complexity of the system. On the other hand the high resolution XANES clearly shown role of lattice displacements in the partial localization of electrons in the 1D networks, appears to be due to charge ordering.

As a representative example, here we show a comparative study of the the local structure around the Cu-site of at two doping, x=1.56 and x=2.24. We have choosen the single crystals of x=1.56 and x=2.24 to represent two extremes of the doping versus anomalous temperature phase diagram, showing respectively with a transition from paramagnetic to antiferromagnetic metal (x=1.56) and with no transition (x=2.24). We have found significant change in the XANES multiple scattering resonances across the anomalous temperature providing a direct evidence for an important role of atomic displacements to the transport anomalies and paramagnetic-antiferromagnetic transition in the three dimensional perovskite system. The results of the polarized XANES suggests that the out-of-plane Cu-O displacements are anomalous indicating their correlation with the lattice ordering in this direction.

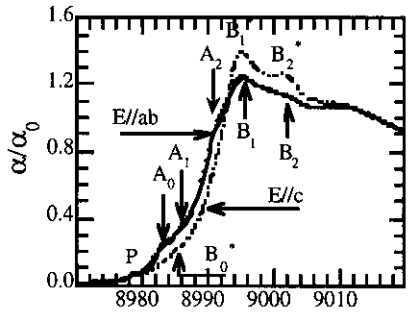

Fig. 1. Polarized Cu K-edge XANES spectra of the $La_{6.44}Sr_{1.56}Cu_8O_{20+\delta}$ crystal measured with the **E//ab** and **E//c** at 30 K. Different absorption features have been identified by second derivative of the absorption spectra and denoted as P, A_0, A_1, A_2, B_1 and B_2 in the **E//ab** spectrum while as P, B_0^*, B_1^* and B_2^* in the **E//ab** spectrum.

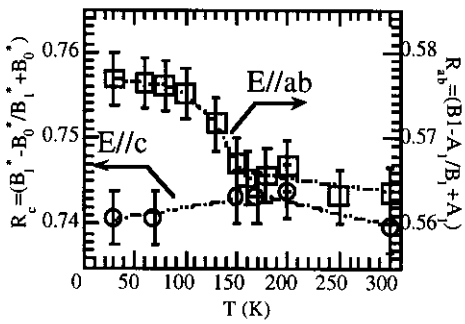

Fig. 2. Temperature dependence of the **E//ab** and **E//c** XANES peaks of the anomalous sample. The normalized main peak intensities for the two polarizations are shown. We have shown the average noise as uncertainties in the peak intensities. The dotted lines represent smooth curves to guide the eyes.

In summary, we have conducted local structural study of the (8-8-20) system for the first time. We have made local structural investigations by high resolution Cu K-edge XANES and EXAFS. In view of the complex Cu-O networks, we have used **E//ab** and **E//c** polarized spectra (Fig. 1) and made an attempt to distinguish the lattice displacements in the system. The doping dependence of the absorption spectra reveals that the average Cu-O distance decreases with increasing Sr doping in the system. The doping dependence is found to be larger for the **E//c** spectra. We have observed clear lattice anomalies around 150 K where the transport properties show anomalous behaviour (Fig. 2). The significant local lattice displacements across the anomalous temperature revealed by the present results provide an evidence for the important role of electron-lattice interactions in the anomalous transport and paramagnetic-antiferromagnetic transition in this three dimensional perovskite system. The present findings suggest that the local atomic structure of the vertically aligned CuO_4 square planes might be playing vital role in the anomalous transport and magnetism in the (8-8-20) system. Indications of these lattice displacements are clear even though we need further studies for a quantitative distinctions of the lattice displacements across the anomalous temperature.

Nevertheless, the present results appear to show that the square planes are getting collinearly aligned forming linear chains running in the c-axis direction. This alignment helps antiferromagnetic ordering, with increased magnetic susceptibility and a small resistivity upturn indicating localization. This antiferromagnetic insulating phase resides in a sea of itinerant electrons that keeps the system metallic, i.e., there are two components active to characterize the electronic properties of the system, where the itinerant electrons are related with the Cu-O networks containing CuO_6 octahedra and CuO_5 pyramids while the localized part is related with the one-dimensional chains formed by the CuO_4 square planes. Since the antiferromagnetic phase with enhanced magnetism appears with local geometrical changes, we think that the (8-8-20) is another candidate where a charge/orbital ordering might occur and the anomalous transport could be governed by charge instability in addition with a spin density wave like instability.