| ESRF | **Experiment title:** Determination of the static and dynamic Jahn-Teller distortions of the $MnO_6$ octahedra at Tc in giant magnetoresistive $A_{1-x}A'_xMnO_6$ manganites | **Experiment number:** HS-44 |
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| **Shifts:** | **Local contact(s):** Filipponi Adriano | *Received at ESRF:* |

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**Report:**

Manganese perovskites with general formula $A_{1-x}A'_xMnO_6$ have been the subject of renewed interest due to magnetoresistance (MR) exhibited near ferromagnetic (FM) spin ordering temperature $T_c$.

Neutron powder diffraction data on orthorhombic $A_{1-x}A'_xMnO_6$ as a function of temperature through the metal-insulator transition have indicated that significant anomalies of bond distances, bond angles and Debye-Waller factors occur at $T_c$ [Radaelli *et* al. Phys. Rev.Lett. 75, 24 (1996)]. It is apparent that the behaviour of Mn-O bond length at Tc can be interpreted as a sudden reduction of the static Jahn-Teller (JT) distortion of the Mn octahedra.

The x-my absorption measurement were made on a powder sample of $La_{0.75}Ca_{0.25}MnO_3$, Tc - 220 K, and on a high quality $Nd_{0.7}Sr_{0.3}MnO_3$ single crystal, Tc - 220 K, have been recorded and compared with a pure $LaMnO_3$ sample. We have collected spectra of Mn K-edge high resolution x-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS) spectra in fluorescence mode using our 13 elements Ge detector of Rome University.;

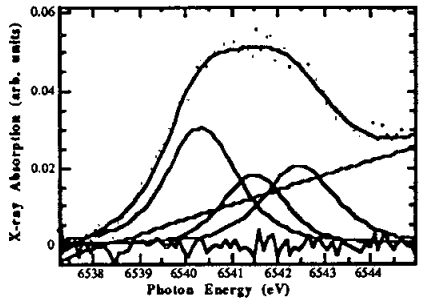


**Fig. 1:** Mn K-edge x-ray absorption spectra of $Nd_{0.7}Sr_{0.3}MnO_3$ in the pre-edge region probing the final states in the Mn 3d derived molecular orbitals

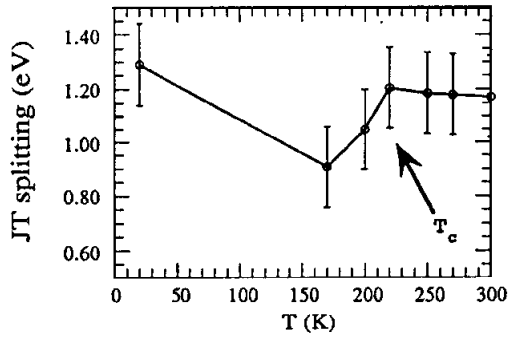


**Fig. 2:** Jahn -Teller splitting in $La_{0.75}Ca_{0.25}MnO_3$

The Mn K-edge XANES and EXAFS spectra have been recorded in the temperature range (20÷300 K). We have been able to detect only the partial absorption cross section by selecting only the Mn x-ray emission line as a function of the incident photon energy.

In fact the tails of the absorption due to other elements, La, Ca, Sr and Nd partially overlap with the Mn partial cross section.

The results of the analysis of the EXAFS spectra of $La_{0.75}Ca_{0.25}MnO_3$ as a function of temperature show a large Debey-Waller factor for the two longer Mn-0 distances in agreement with a dynamical Jahn Teller $MnO_6$ distortion with an anomalous behaviour at $T_c$.

We have isolated the pre-peaks in pre-edge region of XANES spectra on $La_{0.75}Ca_{0.25}MnO_3$ and $Nd_{0.7}Sr_{0.3}MnO_3$ (fig.1). The XANES multiple scattering calculations have been used for the assignment of the electronic transitions and we have identified the peaks to the t2g orbitals and the JT splitting of the $e_g$ orbitals. Therefore we have observed the temperature dependent JT splitting shown in Fig. 2 that is in agreement with the lattice distortions.