ESRF	**Experiment title:** **EXAFS and XANES study of the $La(Mn_{1-x}Ga_x)O_3$ perovskites: analysis of the Jahn-Teller transition.**	**Experiment number**: HS-1511
Beamline: BM29	**Date of experiment**: from: 5-04-2001 to: 10-04-2001	**Date of report**: 28-02-2003
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Names and affiliations of applicants (* indicates experimentalists):

G. Subías*(1), J. García*(2), M.C. Sánchez*(2), J. Blasco(2) and M.G. Proietti(2)

(1) E.S.R.F., BP-220, F-38043 Grenoble-Cedex (France)
(2) Instituto de Ciencia de Materiales de Aragón, CSIC-Univ. de Zaragoza, Plaza San Francisco n.9, 50009-Zaragoza (Spain).

Report:

A comparative study on the local structure around the Mn atom across the Jahn-Teller transition (T_{JT}=750K) has been carried out in Ga-doped perovskites $LaMn_{1-x}Ga_xO_{3+y}$ ($0 \leq x \leq 1$). EXAFS and XANES spectra were recorded at both, Mn and Ga K-edges, at the beamline BM29 at ESRF as a function of temperature (T=20K-920K) in transmission mode, using a Si(311) monochromator with an energy resolution of about $7x10^{-5}$.

$LaMnO_3$ presents an orthorhombic structure (*Pbnm*) at room temperature characterized by an antiferrodistortive ordering of static local distortions due to a cooperative Jahn-Teller effect. At T_{JT}, a structural phase transition occurs and the orbital ordering disappears, accompained by a discontinuous change in the electrical conductivity. However, the driving mechanism for this orbital ordering is still not well known. Regarding this point, our x-ray absorption study at the Mn K-edge of the Jahn-Teller transition at 750 K shows the following results [1]:

(a) The temperature evolution of XANES spectra do not show significant changes above and below T_{JT} (see figure 1), indicating a similar electronic local structure for the Mn atom across the transition.
(b) Dynamical tetragonal Jahn-Teller distortions of the MnO_6 octahedron are also present above T_{JT} so the structural transition is produced by the orientationally ordering of tetragonally distorted ocathedra.

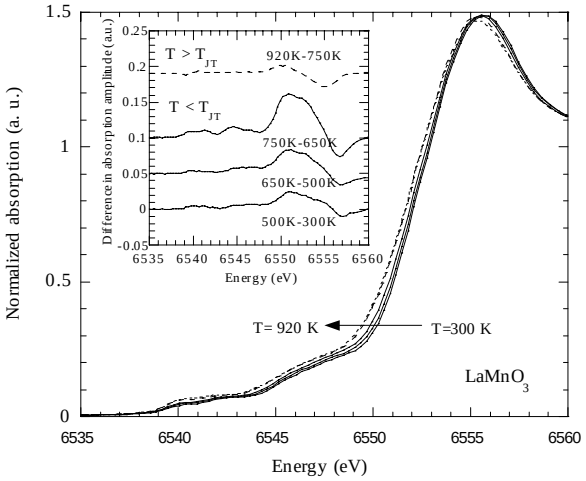

Figure 1.- Normalized XANES spectra of $LaMnO_3$ as a function of temperature. The inset shows the difference between spectra taken at successive temperatures, being the largest difference at T_{JT}.

On the other hand, the replacement of Mn^{3+} by Ga^{3+} in $LaMnO_3$ reduces the orthorhombic distortion which disappears above 50% substitution and induces a spontaneous magnetization. XANES and EXAFS analysis (Ga K-edge) of the local electronic and geometrical structure around Ga^{3+} do not appreciably change along the $LaMn_{1-x}Ga_xO_3$ series so Ga^{3+} only acts as a constructive element of the crystal structure. At the Mn K-edge, instead, the local geometrical structure around the Mn^{3+} ion transforms from the static tetragonal distortion of the MnO_6 octahedron in $LaMnO_3$ into a dynamical distortion (see figure 2).

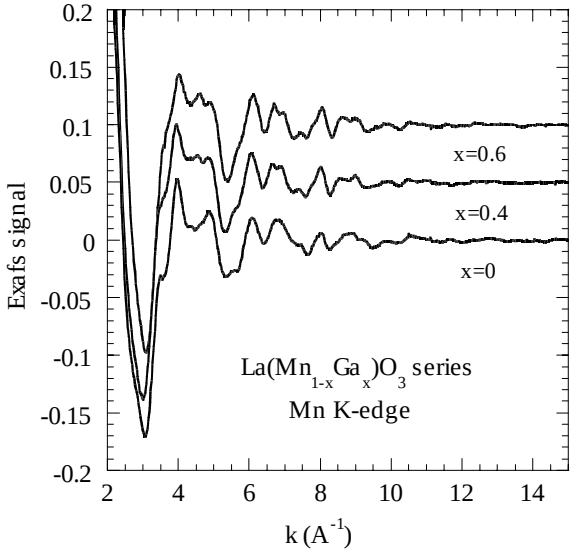

Figure 2. EXAFS spectra at the Mn K-edge of $LaMn_{1-x}Ga_xO_3$ (x=0, 0.4 and 0.6) samples at room temperature.

In terms of Jahn-Teller coupling, the Mn^{3+} ion varies from a static and cooperative Jahn-Teller regime, typical of $LaMnO_3$, to a non-correlated dynamic Jahn-Teller regime, pointed out to a lack of tetragonal distortion for isolated Mn^{3+} ions.

References

[1] M.C. Sánchez, G. Subías, J. García and J. Blasco, *Phys. Rev. Lett.* **90**(4), 045503-1 (2003).