	Experiment title: An XRS study of structural and orbital ordering reflections in LaMnO₃	Experiment number: HS - 2708
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Names and affiliations of applicants (* indicates experimentalists): J. Blasco ¹ , J. Herrero-Martín ^{1*} , J.García ^{1*} , G.Subías ^{1*} , M.C.Sánchez ¹ and C. Mazzoli ^{2*} ¹ Instituto de Ciencias de Materiales de Aragón. CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain ² European Synchrotron Facility, B.P. 220, 38043 Grenoble, France		

Report:

LaMnO₃ is a paramagnetic insulator with an orthorhombic unit cell (Pbnm) at room temperature. Below T_C~ 750 K the cubic MnO₆ octahedra suffer a tetragonal distortion and order in the cell following zigzag chains [1]. Short and long Mn-O bonds thus alternate in the ab plane. As a consequence, this system has been traditionally associated to a cooperative Jahn-Teller distortion producing an orbital ordering in the ab plane. However, we support the idea that the structural distortion produces an anisotropy in the atomic scattering tensors that is enough to account for the observed phenomenology as we have already argued by means of X- ray absorption experiments on this material [3] and similarly on other Mn based mixed valence compounds that we have previously studied [4, 5].

Below T_N=140 K, the randomly oriented magnetic domains collapse into an antiferromagnetic (AF) ordering between successive ab planes along the c direction. This interaction has been said to produce the appearance of resonant reflections of the type (00l) l=odd at very low temperatures and to enhance the intensity of the so-called orbital ordering reflections like (030) and (050) due to a coupling of the orbital and magnetic orderings [2].

In this experiment we have tried to check the validity of these commonly accepted orbital and magnetic ordering models through the study of some interesting resonant Bragg reflections at different temperatures and azimuthal angles.

The single crystals used were grown by the floating zone method at the University of Zaragoza. They were fully structural and magnetically characterized and they were cut and polished perpendicularly to the [100/ 010] and [001] directions.

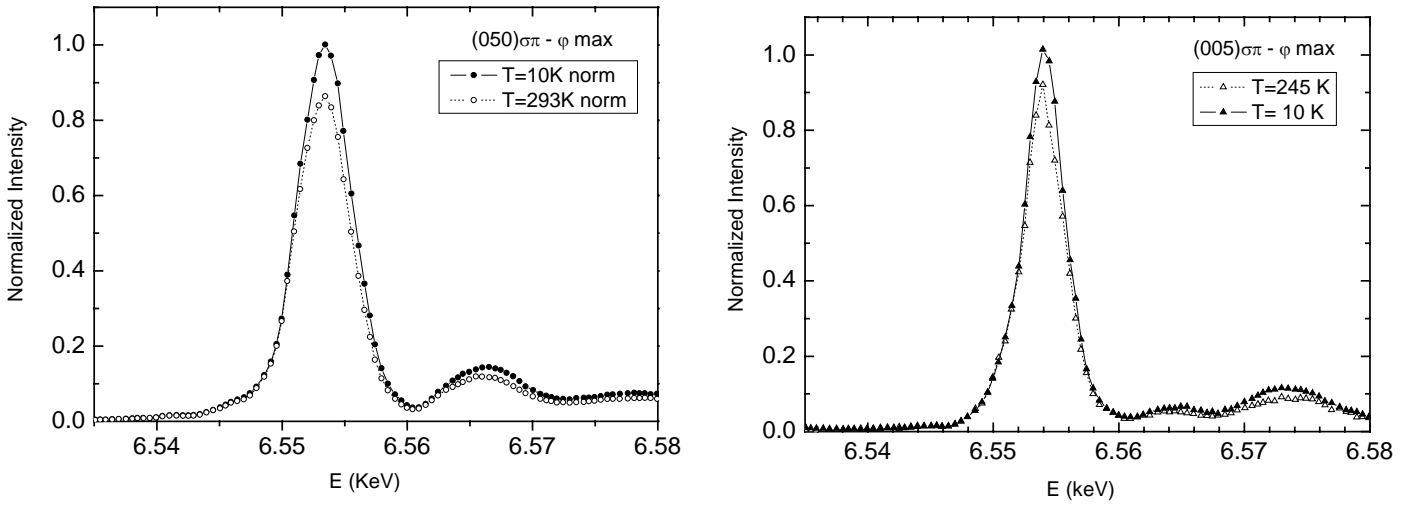


Figure 1. DAFS spectra measured of the (050) and (005) reflections at different temperatures in the σ - π' channel. Measurements were taken at $\phi = \phi(\text{max})$.

We measured the (300), (500), (030), (050), (003) and (005) reflections in the σ - π' channel at the Mn K-edge. No intensity was found in the σ - σ' channel. The (h00) and (0k0), h, k= odd, reflections are identical. On the contrary, resonances are slightly different in the case of the (00l) l= odd, reflections. Despite the main peaks are located at the same energy (6553.5 eV), they slightly narrow in this latter case (FWHM varying from 5 to 3.5 eV).

The study of the forbidden (00l) l=odd resonances as a function of temperature, usually associated to the AF ordering at low temperatures, revealed not only that they are present above T_N but that minor changes in their intensity within the range $10 \text{ K} < T < 290 \text{ K}$ (see Figure 1) were seen. The azimuthal study shows a sinusoidal dependence of period π . A very similar thermal dependence is found for the (h00) and (0k0), k=odd, reflections, with slight variations in the same studied range. The azimuthal evolution is also sinusoidal with a period π .

Our most recent theoretical analysis of these experimental data has revealed important results. For example, we have seen that having into account an anisotropic tensor of scattering with three different components (in accordance to the three different Mn-O bonds in the MnO_6 octahedra) for the Mn atoms we reproduce reasonably well the shape and azimuthal behaviour of every reflection. This means that the hypothesis of a Jahn-Teller driven orbital ordering within the ab plane is not needed in order to explain the phenomenology here observed in LaMnO_3 . Instead, the electronic charge modulation produced by the structural distortion at T_C is the responsible for it. In the same way, (00l) reflections cannot be a consequence of the AF ordering below T_N (as they do not disappear above this temperature) and the influence of this interaction seems to be very weak on the (h00) and (0k0) resonances.

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