ESRF	**Experiment title:** Charge or orbital ordering in $Nd_{0.5}Sr_{0.5}MnO_3$?	**Experiment number**: HS 1622
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Report:

A resonant X-ray scattering study at the Mn K-edge of the charge-ordered perovskite $Nd_{0.5}Sr_{0.5}MnO_3$ was performed to prove the main goals of our structural model [1] proposed to explain the charge-orbital ordering transition in manganites with Mn^{3+}/Mn^{4+} ratio equal to 1.

(0 3 0) charge-order and (0 5/2 0) orbital order reflections, in the *Pbnm* setting, were observed in a single-crystal cut in the $[001]_{cubic}$ plane at T=70 K, well below the charge-ordering transition temperature T_{co} ~150 K. Twin mosaic was inevitable in the crystal so both, (0 2 0) and (2 0 0) domains, were detected. The characteristic dependence of the intensity of these superlattice reflections on the azimuthal angle and on the polarization of the incident beam (by means of a Cu (220) analyzer) were investigated in detail at fixed temperature.

Figure 1 shows the intensity of the (0 5/2 0) orbital ordering reflection as a function of the photon energy for the π-polarized scattering beam. A maximum is shown at 6552 eV, within 1 eV respect to the Mn K-absorption edge. A π periodicity of the intensity on the azimuthal angle ϕ has been found at the resonance and no σ-polarized scattered intensity has been detected. Moreover, no (5/2 0 0) peak was observed in agreement with a previous study of Nakamura *et al*. [2]. On the other hand, for charge-ordering (3 0 0) scattering, either σ-σ or σ-π contributions have been detected, as it is shown in figure 2(a) and 2(b), respectively, for two ϕ values corresponding to the maximum and minimum resonant intensity.

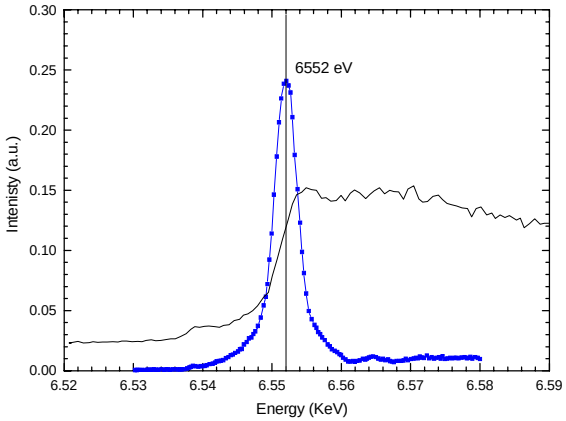

Figure 1. Polarization-resolved (σ→π) scan of intensity plotted versus incident photon energy of the orbital (0 5/2 0) reflection of $Nd_{0.5}Sr_{0.5}MnO_3$ sample near the Mn K absorption edge at T=70 K. The value of the azimuthal angle corresponds to the maximum resonant intensity in the σ→π geometry.

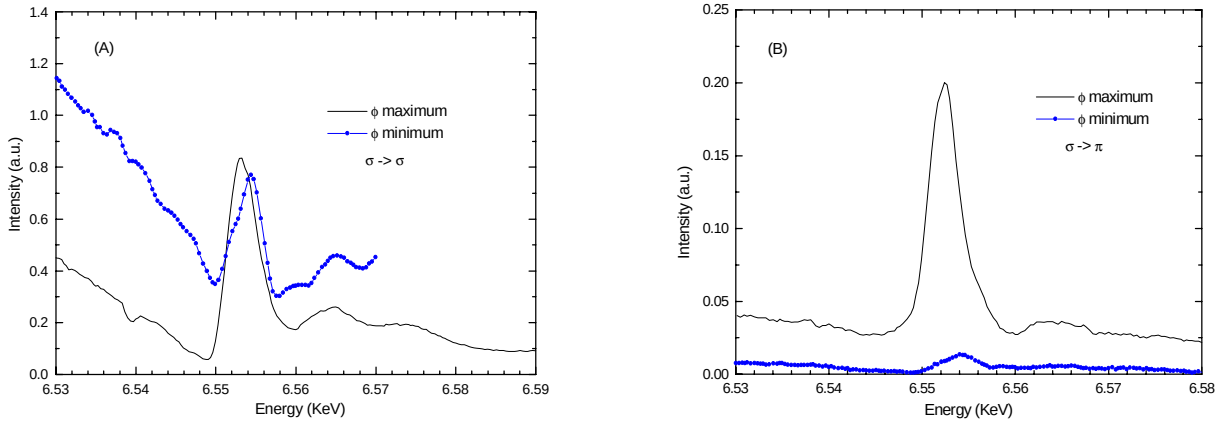

Figure 2. Polarization-resolved scans of intensity plotted versus incident photon energy of the charge (3 0 0) reflection of $Nd_{0.5}Sr_{0.5}MnO_3$ sample near the Mn K absorption edge at T=70 K. The two values of the azimuthal angle corresponds to the maximum and minimum resonant intensity in both polarization geometries.

The σ-polarized scattered intensity shows ϕ dependence with π periodicity for both, (3 0 0) and (0 3 0) reflections, which also agrees with that previously reported by Nakamura *et al*. [2] for the (0 3 0) one. Besides, the energy dependence of the intensity of (3 0 0) (or (0 3 0)) resonant reflection has been found to strongly depend on the azimuthal angle value and a shift of ~1.5 eV is observed for the energy resonance between the ϕ values correspondent to the maximum and minimum intensity. For the π-polarization, instead, only the (3 0 0) resonant reflection was detected but the same dependence on the photon energy as for the σ-polarization was observed. However, a π/2 periodicity is found for the scattering intensity in this case. A very remarkable feature was the fact that the intensity of the (3 0 0) resonant reflection is different from zero for off-resonance photon energies in the σ-π channel. This characteristic is usually related to the presence of resonant magnetic scattering reflections, although in this particular case, it seems to be a much more complex effect.

The main experimental results of this study are perfectly described within the framework of our structural model [1] based on the presence of two Mn atoms with different local geometrical structure (a tetragonal distorted and a regular MnO_6 octahedral environments, respectively) without taking into account any charge or orbital ordering. However, more detailed resonant X-ray scattering experiments are necessary to give a complete description of this system, above all, regarding the presence of non-resonant σ-π intensity for the charge-order reflection and the possibility of some charge disproportionate (δ).

[1] J. García *et al*., *J. Phys.: Condens. Matter* **13** (2001) 3243-3256
[2] K. Nakamura *et al*., *Phys. Rev. B* **60**(4) (1999) 2425-2428