ESRF	**Experiment title:** Study of Charge, Orbital, and Cooperative Jahn-Teller ordering in the Bi-Layer manganite $LaSr_2Mn_2O_7$	**Experiment number:** 28-01-113
Beamline: BM28	**Date of experiment:** from: 23/01/02 to: 29/01/02	**Date of report:** 19/09/02
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Report:

The charge, spin and orbital degrees of freedom play an important role in the electrical and magnetic properties of the transition-metal oxides.[1] The perovskite manganites have been of great interest recently due to their extraordinary physical properties, especially colossal magnetoresistance (CMR)[2]. The bi-layer manganite system with the general formula $La_{2-2x}Sr_{1+2x}Mn_2O_7$ has shown huge values of Colossal Magnetoresistance (CMR) for the $x = 0.4$ doped system compared to the cubic perovskite manganites, and it requires a much smaller magnetic field to produce these CMR values.[3] In the $x = 0.5$ doped system there are equal numbers of Mn^{3+} and Mn^{4+} ions which makes it a candidate to exhibit the checkerboard charge order shown by the cubic half doped manganites. Studies carried out on the $x = 0.5$ doped system show that it charge orders at 220 K and increases in intensity reaching a maximum at 180 K. At this temperature the system magnetically orders into the A-type antiferromagnetic pattern and this causes the charge ordered state to collapse and decrease in intensity before reaching a minima at 100 K[4].

We have carried out resonant X-ray scattering studies around the Mn *K*-edge at BM28 on a high quality single crystal sample of $La_{1.05}Sr_{1.95}MnO_7$ grown at Oxford University. The incident x-ray energy was tuned to the Mn *K*-edge and the X-ray beam was plane polarised in the σ plane. Using a copper (220) polarisation analyser crystal it was possible to observe the scattered signal in both the σ and π channels. Superlattice reflections were located at (2.25, -0.25, 10), (0.5, 0.5, 10) and (0.25, 0.25, 10) and energy scans were carried out on these reflections. The (2.25, -0.25, 10) and (0.5, 0.5, 10) reflections were found to be primarily σ polarised and the energy scans for these reflections are shown in Figure 1 and Figure 2 respectively whereas the (0.25, 0.25, 10) was observed in the π channel corresponding to a rotation in the plane of polarisation by 90°. The behavior of the (2.25, -0.25, 10) reflection is shown in Figure 1. It shows the behavior expected of a structural modulation associated with the motion of the Mn^{4+} species only. The intensity decreased as it was scanned through the Mn *K* edge corresponding to the decreased sample volume probed as the absorption increased.

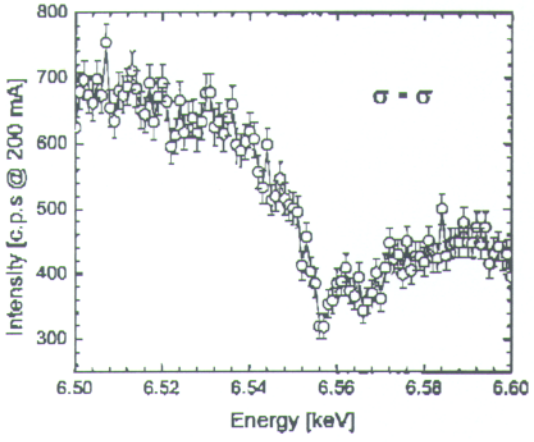

Fig. 1 Energy Scan on the (2.25, -0.25, 10) JTO peak

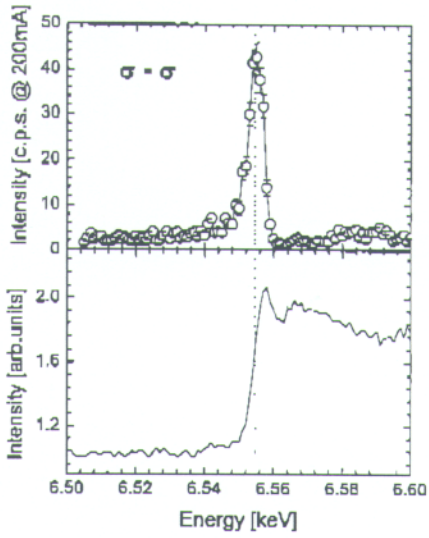

Fig. 2 Energy Scan on the (0.5, 0.5, 10) CO peak

The resonance in the (0.5, 0.5, 10) reflection is caused by the difference in the anomalous scattering factors of the Mn^{3+} and Mn^{4+} ions. Due to the chemical shift the edge positions of Mn^{3+} and Mn^{4+} are slightly different and at the Mn *K* edge there is an increase in contrast between the Mn^{3+} and Mn^{4+} resulting in a resonance. The resonance shown in Figure 2 is consistent with this model and it occurs at the *K* edge position of 6.556 keV as indicated by the fluorescence spectrum shown in the lower panel of Figure 2. The polarization was found to be unrotated which is consistent with that expected of charge order.

The (0.25, 0.25, 10) reflection was observed to have appreciable intensity at the *K* edge only and the energy is shown in Figure 3 with a resonance at 6.556 keV. However in addition a rotation in the plane of polarization by an angle of $\pi/2$ from the incident beam was observed. This is consistent with the origin of the orbital order being from the splitting of the 4*p* energy levels caused by the the ordering of the 3*d* orbitals.

From this study we have confirmed that the position of the wavevectors of the Jahn-Teller, charge and orbital order are $\boldsymbol{Q}$ = (0.25, 0.25, 0), $\boldsymbol{Q}$ = (0.5, 0.5, 0) and $\boldsymbol{Q}$ = (0.25, 0.25, 0) respectively. The origin of these 3 reflections has been confirmed by the polarisation analysis and the energy scans carried out at the Mn *K* edge.

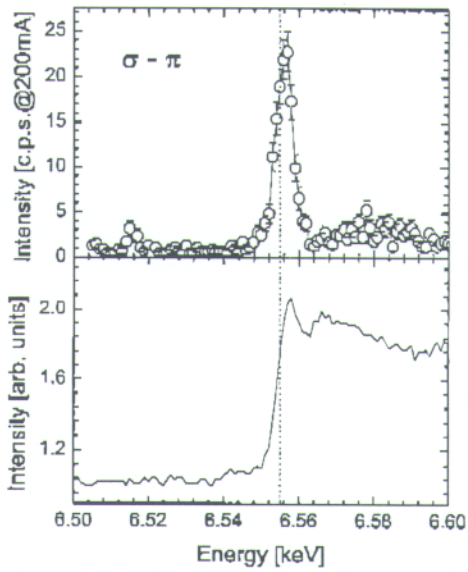

Fig. 2 Energy Scan on the (0.25, 0.25, 10) OO peak

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