ESRF	**Experiment title:** ***The 2-hole state of superconducting cuprates studied by Cu L_3 resonant photoemission and resonant inelastic x-ray scattering***	**Experiment number**: HE1435
Beamline: ID08	**Date of experiment**: from: 5/3/2003 to: 11/3/2003	**Date of report**: 1/3/2004
Shifts: 18	**Local contact(s)**: Nick. B. Brookes	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Giacomo GHIRINGHELLI*, INFM & Politecnico di Milano, Italy

Nicholas BROOKES*, ESRF

Lucio BRAICOVICH*, INFM & Politecnico di Milano, Italy

Claudia DALLERA*, INFM & Politecnico di Milano, Italy

Alberto TAGLIAFERRI*, INFM & Politecnico di Milano, Italy

Matteo Ciucci*, INFM & Politecnico di Milano, Italy

Report:

The proposed experiment aimed at studying the double hole occupancy in a family of cuprates as a function of the doping. We chose $La_{2-x}Sr_xCuO_4$ (LSCO) where the hole doping in the CuO_2 planes can be controlled by the Sr content, while the main structural properties remain the same. We wanted to measure both the resonant photoemission spectra and the resonant x-ray inelastic scattering (RIXS) at the L_3 edge of Cu on the same samples, in order to compare the evolution of the spectral shape and position in the two cases. In fact in the two processes the first step is the same ($3d^9;3d^9\underline{L}$)→($2p^5 3d^{10};2p^5 3d^{10}\underline{L}$) whereas the final state is different: in resonant photoemission one further hole is present in the Cu site ($3d^8$; $3d^8\underline{L}$; $3d^9\underline{L}$), in RIXS the occupation number is unchanged with respect to the ground state ($3d^9;3d^9\underline{L}$). The starting point was the fact that in the absorption spectrum at Cu L_3 the main peak (very strong resonance) presents a tail on the high energy side, tail that grows with the doping level (see figure 1). What type of evolution of the spectral shape and position do we see in the different sample when the excitation energy is chosen to correspond to the $3d^9\underline{L}$ tail?

We have recorded the full set of photoemission and RIXS spectra on three samples across the Cu L_3 absorption edge: LSCO with x=0.13 (under-doped, figure 2) , x=0.15 (optimally doped, figure 3), x=0.27 (over-doped, figure 4). The samples were cleaved *in situ* for photoemission measurements and in air for RIXS (which is a much less surface sensitive technique). The excitation energy was chosen from –4 eV to +4 eV with respect to the absorption peak. The energy resolution was better than 150 meV and 0.8 eV combined for photoemission and RIXS respectively. The figures 2, 3 and 4 show the sets of spectra measured above L_3 for the three samples. The RIXS data on the undoped LSCO were measured as well, during a run belonging to the long term proposal HE1088. The analysis is not complete yet, but even the raw data show that upon doping the double hole configuration leads to a delocalisation of the Cu states: the spectra get broader and above the absorption threshold the fluorescence like behaviour becomes dominant, as a consequence of the non-local nature of the scattering process. Indeed the $3d^9\underline{L}$ state implies a stronger Cu-O hybridisation, i.e. the appearance of a Cu "character" in the O 2p band.

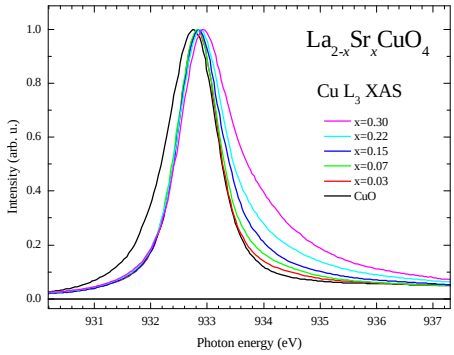

FIGURE 1. Absorption specta at the Cu L_3 edge in LSCO as a function of the doping.

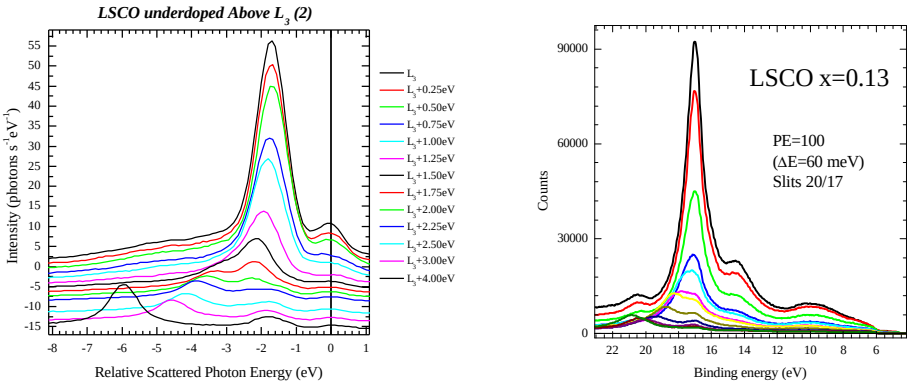

FIGURE 2. RIXS and photoemission spectra fot the x=0.13 LSCO sample, excited just above the Cu L_3 absortion peak.

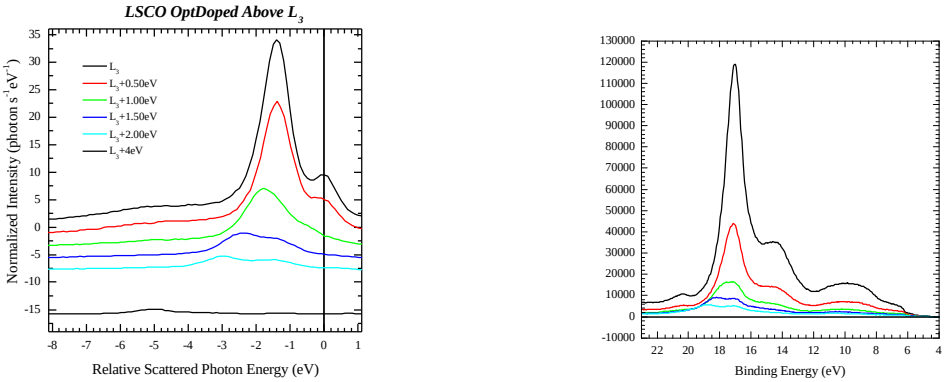

FIGURE 3. RIXS spectra fot the x=0.15 LSCO sample, excited just above the Cu L_3 absortion peak.

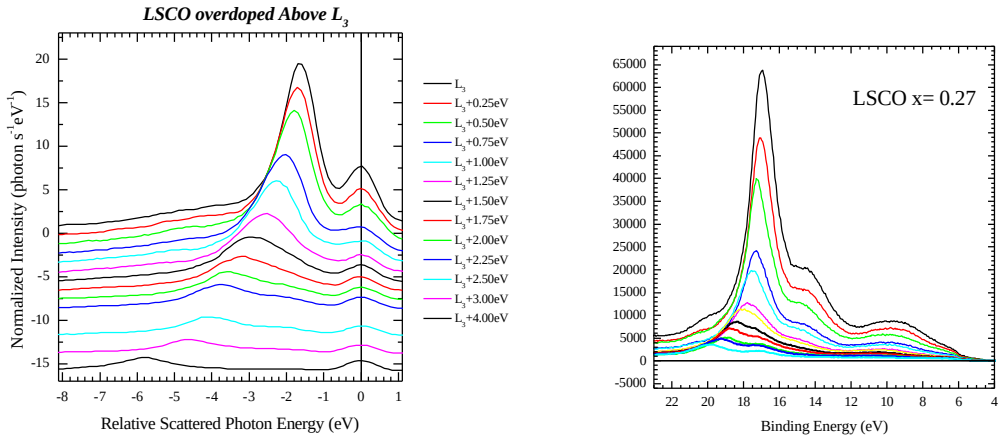

FIGURE 4. RIXS spectra fot the x=0.27 LSCO sample, excited just above the Cu L_3 absortion peak.

ADDENDUM

The RIXS measurements of this report are closely related to other RIXS spectra measured on various cuprates in the same months of 2003 (LTP HE1088). The instrumentation was the same and we concentrated on the spectral shape when exciting at the maximum of the Cu L_3 resonance. The analysis can be made in a rather simple way within a crystal field atomic model. These results are presented in a paper, accepted for publication on Physical Review Letters: G. Ghiringhelli, N.B. Brookes et al., Phys. Rev. Lett, In press (2004). We attach below the abstract and one figure taken from the accepted manuscript.

Low energy electronic excitations in layered cuprates studied by copper L_3 resonant inelastic x-ray scattering

G. Ghiringhelli,[1] N.B. Brookes,[2] E. Annese,[3] H. Berger,[4] C. Dallera,[1] M. Grioni,[5] L. Perfetti,[5] A. Tagliaferri,[1] and L. Braicovich[1]

[1] *INFM - Dip. di Fisica, Politecnico di Milano, p. Leonardo da Vinci 32, 20133 Milano, Italy*
[2] *European Synchrotron Radiation Facility, B.P. 220, 38043 Grenoble Cédex, France*
[3] *INFM - Dip. di Fisica, Università di Modena e Reggio Emilia, via Campi 213/A, 41100 Modena, Italy*
[4] *IPN, Ecole Polytechnique Fédérale (EPFL), CH-1015 Lausanne, Switzerland*
[5] *Ecole Polytechnique Fédérale (EPFL), CH-1015 Lausanne, Switzerland*

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We have measured the resonant inelastic x-ray scattering (RIXS) spectra at the Cu L_3 edge in a variety of cuprates. Exploiting a considerably improved energy resolution (0.8 eV) we recorded significant dependencies on the sample composition and orientation, on the scattering geometry and on the incident photon polarization. The RIXS final states correspond to two families of electronic excitations, having local (*dd*-excitations) and non-local (charge transfer) character. The *dd* energy splitting can be estimated with a simple crystal field model. The RIXS at the L_3 edge demonstrates here a great potential, thanks to the resonance strength and to the large $2p$ spin-orbit splitting.

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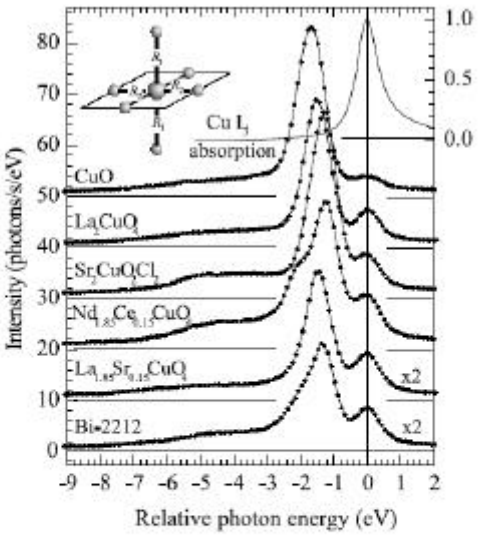

FIG. 1: The RIXS spectra measured at the Cu L_3 peak on three insulating and three superconducting cuprates at grazing incidence and V polarization [GI,V]. The energy scale is given in relative scattered photon energy, having aligned the highest energy peak to zero, by implicitly assigning it to an elastic peak. All the spectra are as measured. The topmost curve shows the Cu L_3 absorption peak of $La_{1.85}Sr_{0.15}CuO_4$. Inset: the local D_{4h} crystal field symmetry used in the calculations.