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The Out-of-plane Cu 3d and O 2p Holes in the Bi2212 System

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The polarisation dependent X-ray absorption measurements (XAS) have been made below the transition temperature of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+y}$ (Bi2212) superconducting system. The results suggest a negligible amount of Cu $3d_{z^2-r^2}$ symmetry holes but give a strong evidence of presence of a significant amount of p_z symmetry holes. The polarisation dependent Cu L_3 and O K spectra are reported both in superconducting as well as in normal state of the Bi2212 system.

1. INTRODUCTION

The importance of the CuO_2 planes in cuprate superconductors have been established and it is known that the holes reside in these are responsible for superconductivity and due to this fact a number of polarisation dependent XAS studies have been made to obtain valuable information on the symmetry of holes in high T_c superconductors [1,2]. In particular, the Bi2212 system has attracted more attention and led to the conclusion that the unoccupied Cu 3d states are mainly of $3d_{x^2-y^2}$ character with 10-20% weight of $3d_{z^2-r^2}$ ($3d_{z^2}$) character. There are, however, some discrepancies have been found with a density of $3d_{z^2}$ holes from 5% to 20% [3,4,5,6]. On the other hand, a number of polarised O K-XAS have been published [1,3,5] but not able to give conclusive evidence for the presence of the O $2p_z$ symmetric holes in the system. However, our recent study using Fluorescence Yield (FY) technique have been able to show a negligible amount of $3d_{z^2}$ holes while significant density of p_z holes [2]. Leaving apart the controversy in the room temperature data, we have investigated the symmetry of holes in superconducting as well as in normal state of the Bi2212 system. A small change may be expected due to the observed inhomogeneous Cu site configuration in Bi2212 system which is an effect of tilting of the CuO_4 square plane at low temperature [7]. In this short communication, we report preliminary results of our polarised XAS at Cu L_3 and O K-edges on a high quality Bi2212 single crystal.

2. EXPERIMENTAL

The single crystals ($T_c \sim 85\text{K}$) were prepared by travelling- solvent floating method in a mirror furnace with two ellipsoidal reflections using the 750 W halogen lamps [2]. The polarised XAS measurements were performed on the station 1.1 of SRS at Daresbury Laboratories using a liquid He cooled UHV manipulator. The samples were at $\sim 40\text{K}$ for low temperature measurements. All these spectra have been measured by the total yield (TY) method.

3. RESULTS AND DISCUSSION

Figures 1(a) and 1(b) show the low temperature (LT) and room temperature (RT) Cu L_3 XAS spectra measured at different angles of incidence. The angle $\theta = 0^\circ$ represents the case where $E \parallel ab$ and $\theta = 75^\circ$ the case where E is nearly parallel to the c -axis. The zero of the energy scale is taken at the Cu L_3 peak in the $E \parallel ab$ spectrum. Both the LT and RT spectra at the 75° show a very small intensity (6-8% of the $E \parallel ab$ polarisation). The extrapolated intensity for the $E \parallel c$ polarisation come out to be ~ 1 -2% in two cases. This result is quite similar to our earlier measurements on the same crystal using the FY [2]. This shows that there are no holes of $3d_{z^2}$ symmetry either in normal or superconducting state of the Bi2212 system. This is also the case with La-Sr-Cu-O system reported by Chen et al [8]. The results are thus in significant disagreement with the TY spectra reported earlier [3,4,5] where they report 10-20% density of $3d_{z^2}$ holes in the Bi2212 superconductor.

There appears to be hardly any difference between the Cu L_3 spectra at LT and RT. However, we

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observed small difference in the asymmetry of the main peak in the E $\backslash$ ab case (discussed below).

Fig 1. Cu L₃ XAS at LT (a) and RT (b)

Figures 2(a) and 2(b) show the O K-XAS at LT and RT respectively. In the normal incidence ($\theta=0^\circ$), only the states of O p_{x,y} symmetry will be sampled while at grazing incidence only the p_z orbitals are accessible. The zero of the energy scale in the figures has been kept at the pre-edge peak in the E $\backslash$ ab spectrum. The spectra are normalised to the main edge at ~ 2.5 eV above the pre-peak. The pre-peak is due to the transition $3d^9 \underline{L} \rightarrow 1s 3d^9$ into the unoccupied O 2p states appearing in the correlation gap with doping holes. The intensity of this peak decreases in going towards the E $\backslash$ c polarisation. On extrapolation, the ratio of the E $\backslash$ c to E $\backslash$ ab case turns out to be $\sim 10\%$ and $\sim 13\%$ respectively. These results indicate a significant number of holes with p_z symmetry in Bi2212 system and are in support of the FY measurements [2].

There appears to be small differences in the LT and RT O K-spectra. In fact, we observe a small decrease (5-8%) in the intensity of pre-peak in the E $\backslash$ ab polarisation at RT. Actually, it is the lower density of p_{x,y} holes which brings up the estimated ratio of p_z/p_{x,y} to a little higher value ($\sim 13\%$) than the estimated ratio ($\sim 10\%$) at LT. To make sure this, we analysed the intensities of the Cu L₃ spectra by fitting with two Gaussians. The estimated ratio of shoulder to the main peak turns out to be 24% and 19% respectively in two cases. This qualitative

decrease in the intensity of the shoulder confirms the small change observed in the O K-XAS spectra

Fig. 2. O K-XAS at LT (a) and RT (b).

In summary, we have reported polarisation dependent XAS spectra in superconducting as well as in the normal state of the Bi2212 system. To the best of our knowledge, this is the first polarisation XAS study in the superconducting state. The TY XAS data are quite similar to our FY XAS measurements on the same crystal. More discussion and further details on the temperature dependent changes observed in the polarised XAS will be reported elsewhere.

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