The out of-plane Cu 3d O 2p holes in the Bi2212 system

Saini, N.L.; Law, D.S.L.; Menovsky, A.A.; Franse, J.J.M.; Garg, K.B.

DOI
10.1016/0921-4534(94)91733-7

Publication date
1994

Published in
Physica C

Citation for published version (APA):

General rights
It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations
If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: https://uba.uva.nl/en/contact, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.
The Out-of-plane Cu 3d and O 2p Holes in the Bi2212 System

N.L. Saini a, l, D.S-L. Law b, A. Menovsky c, J.J.M. Franse c and K.B. Garg a

a Department of Physics, University of Rajasthan, Jaipur-302004, INDIA.
b DRAL RUSTI Daresbury Laboratory, Warrington, Cheshire WA4 4AD, U.K.
c Van der Waals Zeeman Lab, Univ. van Amsterdam, THE NETHERLANDS.

The polarisation dependent X-ray absorption measurements (XAS) have been made below the transition temperature of Bi2Sr2CaCu2O8+y (Bi2212) superconducting system. The results suggest a negligible amount of Cu 3dz2-r2 symmetry holes but give a strong evidence of presence of a significant amount of pz symmetry holes. The polarisation dependent Cu L3 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 CuO2 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 Tc 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 3dx2-y2 character with 10-20% weight of 3dz2-r2 (3dx2) character. There are, however, some discrepancies have been found with a density of 3dz2 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 2pz symmetric holes in the system. However, our recent study using Fluorescence Yield (FY) technique have been able to show a negligible amount of 3dz2 holes while significant density of pz 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 CuO4 square plane at low temperature [7]. In this short communication, we report preliminary results of our polarised XAS at Cu L3 and O K-edges on a high quality Bi2212 single crystal.

2. EXPERIMENTAL

The single crystals (Tc~85K) 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 ~40K 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 L3 XAS spectra measured at different angles of incidence. The angle \( \theta = 0^\circ \) represents the case where E \( \neq X \), 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 L3 peak in the E \( \neq X \) spectrum. Both the LT and RT spectra at the 75\(^\circ\) show a very small intensity (6-8% of the E\( \neq X \) polarization). The extrapolated intensity for the E\( \neq X \) polarization 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 3dz2 symmetry either in normal or superconducting state of the Bi2212 system. This is also the case with La-51-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 3dz2 holes in the Bi2212 superconductor.

There appears to be hardly any difference between the Cu L3 spectra at LT and RT. However, we
observed small difference in the asymmetry of the main peak in the ENXab 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 px,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 ENXab spectrum. The spectra are normalised to the main edge at -2.5 eV above the pre-peak. The intensity of this pre-peak decreases in going towards the ENXc polarisation. On extrapolation, the ratio of the ENXc to ENXab case turns out to be $-10\%$ and $-13\%$ 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 ENXab polarisation at RT. Actually, it is the lower density of px,y holes which brings up the estimated ratio of p_z/px,y to a little higher value ($-13\%$) than the estimated ratio ($-10\%$) 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.

---

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 FY 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.

We are happy to acknowledge the Daresbury staff for the experimental help. One of us (NLS) is grateful to ICTP, Trieste for a fellowship.

REFERENCES

2. K.B.Garg et al (to be published) and references therein (1994).