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Polarized Cu L_3 X-ray Absorption Edge of $Bi_2Ca_2Sr_2Cu_3O_{10+\delta}$ Superconductors

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Abstract

The symmetry of the itinerant $\underline{d}^*$ holes in the narrow conduction band of the 110K superconducting $Bi_2Ca_2Sr_2Cu_3O_{10+\delta}$ system has been studied by polarized Cu L_3 x-ray absorption spectroscopy using synchrotron radiation. The integral of the 2p->3d white line of the E//c polarized spectra probes the probability of $\underline{d}$ holes with $m_\ell=0$ ($3d_{3Z^2-r^2}$) and/or $m_\ell=1$ ($3d_{xz}$ or $3d_{yz}$) orbital momentum. We have found that the weight of the orbital momentum with a component in the c direction, $m_\ell=0$ ($3d_{3Z^2-r^2}$) is in the range of 34% and it decreases with decreasing T_c.

Introduction

The analysis of the electronic configuration of the Cu ions in metallic cuprate perovskites, investigated by Cu L_3 x-ray absorption spectroscopy, has shown that the probability of the Cu $3d^8$ configuration in doped superconductors cannot not be detected experimentally within the experimental noise and an upper limit of 5% was given [1,2]. It was pointed out [1,2] that the Cu(III) formal valence state was associated with new itinerant states $3d^9\underline{L}^*$ ($\underline{L}$ indicates holes with oxygen 2p character) where the * was used to indicate that the character of the itinerant $\underline{d}^*$ and $\underline{L}^*$ holes was different from the excited states $3d^9\underline{L}$

of the parent antiferromagnetic insulating system. The notation $3d^9$ for the density of states of d holes is used to indicate that number of d holes per unit cell n_d remains $n_d \leq 1$ because of the lack of Cu $3d^8$ configuration in the experimental data.

Results and Discussion

In this work we have studied the class of high T_c superconductors $Bi_2Sr_2Ca_2Cu_3O_{\sim 10}$ (Bi2223) discovered by Maeda et al. [3,4] which are quite stable in vacuum and therefore can be studied by electron spectroscopies.

X-ray absorption spectroscopy probes the local (projected on the site of the absorption atom) and partial (only the holes with angular momentum $\ell = \ell' \pm 1$, where ℓ' is the angular momentum of the core electron selected by the dipole matrix element) density of states.

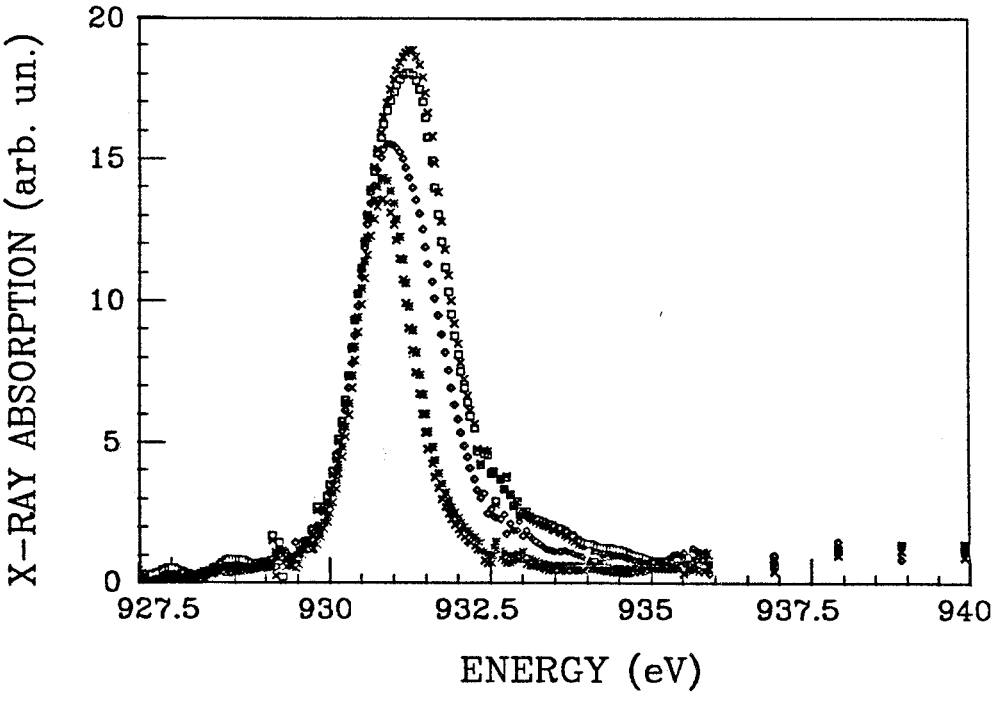

Fig.1 Polarized Cu L_3-edge XAS of the Bi2223 measured with photon incidence angle 10°, 75° and at the magic angle 35° and the two extrapolated E//c and E//ab (crosses) polarized curves. The absorption coefficient has been normalized to one at the level of the continuum absorption above 936 eV.

The Cu 3d partial density of states of the band crossing the Fermi level can be studied by Cu 2p XAS. Moreover the polarized Cu L_3 XAS spectra allows the determination of the angular momentum of the d hole, in fact the E//c spectra probe only d holes with m_ℓ=0, $3d_{3z^2-r^2}$, and the m_ℓ=1, $3d_{xz}$, $3d_{yz}$, orbital momentum.

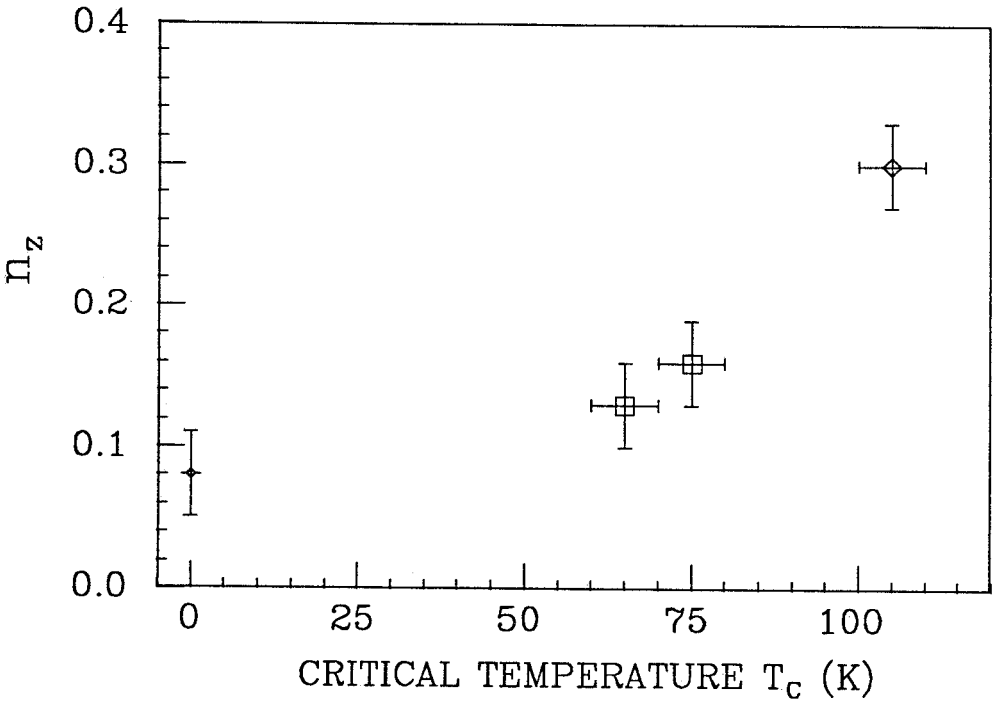

Fig.2 Plot of the relative number n_z of $3d_{3z^2-r^2}$ holes on the total number of d holes versus T_c of different samples. n_z is obtained as one half of the ratio between the integral I(E//c) of the E//c white line and the sum 1/3 ·[2·I(E⊥c)+I(E//c)] polarized white line spectrum.

In this work we address the question: is the percentage of $3d_{3z^2-r^2}$ holes increasing with doping? In fact the partial density of hole states in the conduction band crossing the Fermi level has a partial Cu $3d_{x^2-y^2}$, n=3 ℓ=2 m_ℓ=2, character, $3d_{3z^2-r^2}$, n=3 ℓ=2 m_ℓ=0, and oxygen $2p_x$, ℓ=1 m_ℓ=1. Therefore there are non integer numbers n_x of Cu $3d_{x^2-y^2}$ holes, n_z holes of Cu $3d_{3z^2-r^2}$ and n_p holes of $2p_x$, $2p_y$. The number n_p goes to zero with decreasing T_c. The open problem is how the ratio n_z/n_x is modified by the hole doping, in

fact the total number of d holes n_z+n_x is expected to change slowly by keeping $n_z+n_x \leq 1$, because the Cu $3d^8$ configuration is not observed experimentally.

In order to face this problem we have undertaken a long term research project investigating a large number of well characterized $Bi_2(Ca_{1-x}Sr_{2-x})Cu_2O_8$, $Bi_{2-y}Pb_yCa_2Sr_2Cu_3O_{10+\delta}$ samples by polarized Cu L_3 XAS using synchrotron radiation.

In Fig.1 we report the polarized Cu 2p XAS spectra of a single phase T_c=105K Bi2223 100% oriented pellet with a single phase.

The integral of the E//c spectrum in the range 925 -936 eV (I_z) of the white line associated to 2p→ 3d transitions is determined by the number of d holes n_z assuming a negligible contribution from the $3d_{xz}$ component. One half of the ratio I_z/I_n of the integral I_z over the integral of the white line non-polarized I_n, measured at the magic angle gives the percentage of the n_z holes over the total number of d holes. In Fig.2 are reported the values of n_z for the insulating and Bi2212 and Bi2223 superconductors with different T_c. The data in Fig. 2 show that the orbital momentum of the d holes is modulated by doping and it is in the range of 20-30% in the normal metallic phase of this class of high T_c superconductors. These results are in agreement with the theoretical results for a renormalized electronic structure of doped CuO_2 planes [5] showing and additional $3d_{3z^2-r^2}$ band close to the Fermi level.

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