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Non-Homogeneity of the CuO₂ Plane of the Oxygen Doped La₂CuO_{4.1} System by Polarized EXAFS

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Abstract. Temperature dependent in-plane polarized Cu K-edge extended x-ray absorption fine structure (EXAFS) study has been carried out on a high quality single crystal of oxygen doped La₂CuO_{4.1} (LCO) system to investigate the local structure around Cu. The EXAFS data recorded with high degree of plane polarization and up to high momentum transfer ($Q=40 \text{ \AA}^{-1} = 2k$) allowed the quantitative determination of the distorted and undistorted Cu planes. The determination of the Cu-O(planar) distances shows presence of minority Cu sites characterized by two longer Cu-O(planar) bonds and a tilting of 15° with the average crystallographic structure at $T < T_g \sim 150 \text{ K}$. The data show the coexistence of localized and itinerant charges trapped into stripes of distorted and undistorted domains within the CuO₂ plane.

1. INTRODUCTION

The electronic and structural inhomogeneities within the superconducting CuO₂ plane at a mesoscopic scale length is a point of intense interest [1-2]. Cu K-edge Extended X-ray Absorption Fine Structure (EXAFS) is a fast and local probe of the structure of the CuO₂ plane and it has been used to study various families of cuprate superconductors [3-6]. The resulting inhomogeneous CuO₂ lattice, characterised by distribution of Cu-O bond distances, has been assigned to an anharmonic 1D charge modulation [6] and the results were confirmed recently by solving the CuO₂ superstructure using anomalous diffraction in Bi₂Sr₂CaCu₂O₈ (Bi2212) [7]. A recent letter on the subject has shown that the 1D lattice modulation involves in plane lattice distortions, that directly modulate the electronic structure of the superconducting planes of La_{1.85}Sr_{0.15}CuO₄ (LSCO) [8], where the PDF of the in plane Cu O(planar) atoms show the formation of the stripe structure below $T_g \sim 100 \text{ K}$ [8].

The oxygen doped La₂CuO_{4.8} system is a superconducting cuprate where the doping is realized by introducing interstitial oxygen in the rocksalt layers [9]. Phase separation is known to occur for $0.01 < \delta < 0.06$ and $T < 260 \text{ K}$ with the formation of oxygen poor (insulating La₂CuO_{4.01}) and oxygen rich (superconducting La₂CuO_{4.06}) phases. The system is superconducting below $T_C \sim 40 \text{ K}$ for $\delta > 0.06$. Superstructure reflections with a wavelength of the order of 25 \AA have been observed by neutron and electron diffraction at low temperature [10] in the superconducting phase at high doping indicating a lattice modulation. The presence of different Cu sites and the distribution of tilts of the CuO₆ octahedra in the CuO₂ plane is detected by nuclear magnetic resonance (NMR) and has been assigned to the coexistence of tilted and untilted octahedra forming striped domains [11].

The aim of the present work is to probe the inhomogeneity and to determine the temperature dependent amplitude of the modulation of the CuO₂ plane in the oxygen-doped La₂CuO_{4.8} system by polarized Cu K-edge EXAFS. We have investigated a crystal with high oxygen doping and free from the macroscopic phase separation and near the optimum doping for high T_C superconductivity [11,12]. For the purpose we have taken advantage of high brilliance x-ray source provided by the 6 GeV European synchrotron radiation facility (ESRF) allowing to collect the EXAFS data with high signal to noise ratio up to high momentum transfer.

2. EXPERIMENTAL

The single crystal of La₂CuO_{4.1} was processed as La₂CuO₄ by flux method and doped by electrochemical oxidation [12]. The measurements were made on a crystal of size $3 \times 2 \times 0.5 \text{ mm}^3$ showing a sharp superconducting transition at $T_C = 38 \text{ K}$. The temperature dependent in plane (E//ab) polarized Cu K-edge absorption measurements were performed on the beam-line CRG-IF at the ESRF at Grenoble. The crystal was mounted in a closed-cycle He refrigerator and the temperature was monitored with an accuracy of 1 K . The X-ray beam was monochromatized by a bent conically shaped Si(111) double crystal monochromator, and sagittally focused on the sample. The spectra were recorded by detecting the fluorescence yield. Twelve scans were recorded at each temperature. The EXAFS signal $\chi = (\alpha - \alpha_0)/\alpha_0$, where α is the absorption coefficient and α_0 is the so called atomic absorption, was extracted from the absorption spectrum using standard procedure [13] and corrected for fluorescence self absorption [14].

3. RESULTS AND DISCUSSION

The Cu K-edge EXAFS using polarized synchrotron light with the E vector parallel to the crystal surface ($E//ab$) and recording the spectra up to high momentum transfer allows to detect selected information about the CuO_2 plane of the superconducting $\text{La}_2\text{CuO}_{4.1}$ crystal and its temperature dependent behaviour.

Fig. 1 shows the Fourier transform of the phase corrected EXAFS spectra (multiplied by k^2) extracted from the $E//ab$ polarized Cu K-edge absorption measured on the $\text{La}_2\text{CuO}_{4.1}$ single crystal, at a representative temperature (35K). The Fourier transform has been performed from $k_{\min}=3 \text{ \AA}^{-1}$ to $k_{\max}=19 \text{ \AA}^{-1}$ using a Gaussian window. The main peaks denote the distribution of the atomic sites with respect to the Cu. It is evident from the Fourier transform spectra that the O(planar) backscattering appears at the real Cu-O(planar) distance $\sim 1.9 \text{ \AA}$ while the backscattering of La can be seen $\sim 3.2 \text{ \AA}$. The peak at around 3.8 \AA represents the Cu-O-Cu multiple scattering. As expected, the contribution of the Cu-O(apical) is suppressed and the contribution of the Cu-O(planar) is well separated from the other shells of neighboring atoms and can be easily extracted by the standard Fourier filtering.

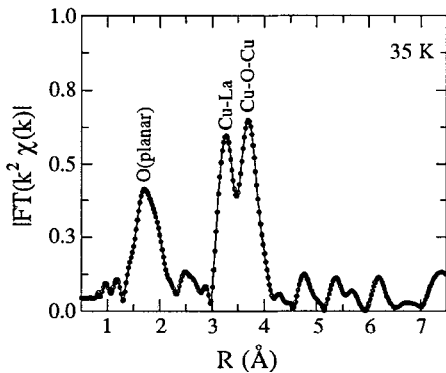


Figure 1: Fourier transform of the experimental spectrum $E//ab$ EXAFS at 35 K performed between $k_{\min}=3 \text{ \AA}^{-1}$ to $k_{\max}=19 \text{ \AA}^{-1}$ using a Gaussian window.

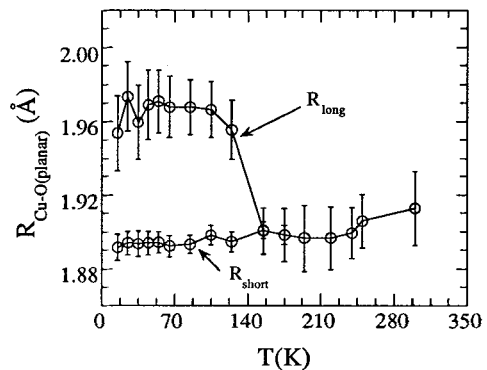


Figure 2: Temperature dependence of two Cu-O(planar) distances (R_{short} and R_{long}) measured by EXAFS. The R_{long} is the anomalous distance.

The Fourier filtered Cu-O(planar) EXAFS was modelled using curved wave theory to get information about the inhomogeneous CuO_2 plane. The number of parameters determined by the EXAFS analysis is limited by $N=(2\Delta R\Delta k)/\pi$ where Δk and ΔR are respectively the ranges in k and R space over which the data are fitted. In the present case, the $\Delta R=0.8 \text{ \AA}$, $\Delta k=16 \text{ \AA}^{-1}$ ($3-19 \text{ \AA}^{-1}$) and hence the number of parameters to be fitted is about 8.

The fitting was performed with two Cu-O(planar) distances using the same approach as described for $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ (LSCO) [8]. The value of E_0 and the reduction factor due to multi-electrons excitations, S_0^2 was fixed to the value obtained by analyzing EXAFS of other copper oxide superconductors [8] and found to be similar to the values reported for other related copper oxides [15]. The two distance fit was performed first by using five parameters: R_{long} , R_{short} and N_{long} ($N_{\text{short}} = N_{\text{tot}} - N_{\text{long}}$, where N_{tot} is the fixed coordination number) and two Debye Waller factors. The two Debye Waller factors were fixed to the values corresponding to the correlated Debye model with $\theta_D = 600 \text{ K}$ to obtain the R_{long} , R_{short} and N_{long} parameters.

Fig. 2. shows the temperature dependence of the two Cu-O(planar) distances. The results show that there are two different Cu sites at $T < 150 \text{ K}$ characterized by two Cu-O(planar) distances separated by $\Delta R \sim 0.08 \text{ \AA}$. The separation is out of estimated uncertainties. The two distances converge into a single distance at $T > 150 \text{ K}$.

It can be seen that R_{short} is independent of temperature and close to the crystallographically measured distance while the long distance can be considered the anomalous one. Following the same line of thinking [8] the short distance is attributed to the LTO (low temperature orthorhombic) phase, while the long Cu-O(planar) distance is attributed to the local LTT (low temperature tetragonal) one.

The pictorial view of the two types of Cu sites having LTT and LTO tilts is shown in Fig. 3. We have obtained the tilting angle θ of the CuO_4 square plane using $\cos\theta=R_{\text{short}}/R_{\text{long}}$. The tilting is in the range of 15 degrees which is of the same order of magnitude as the tilting angle observed in the local LTT kind of domains in LSCO [8]. Such a large tilting has been observed by NMR [11] and neutron diffraction [9] in the LCO system and by EXAFS [6] in the Bi2212 system. From the relative number of anomalous long bonds we deduce the probability of presence of $(40 \pm 2\%)$ anomalous CuO_4 square planes with rhombic distortion having two long bonds per Cu site, forming LTT like domains. The distorted and undistorted domains of the CuO_4 plane will get disposed spatially in stripes (of width W) made of distorted lattice alternating with stripes (of width L) of undistorted lattice in the presence of the modulation due to ordering of the extra oxygen [9, 10]. The width W (L) of the

LTT (LTO) like stripe is measured by joint EXAFS (measuring the pair distribution) and diffraction (giving the modulation period, $\lambda_p \sim 24.3 \text{ \AA} = L+W$). The width of the stripe made of distorted (undistorted) is found to be $W = 0.4 \cdot 24.3 \sim 9.7 \text{ \AA}$ ($L \sim 14.5 \text{ \AA}$).

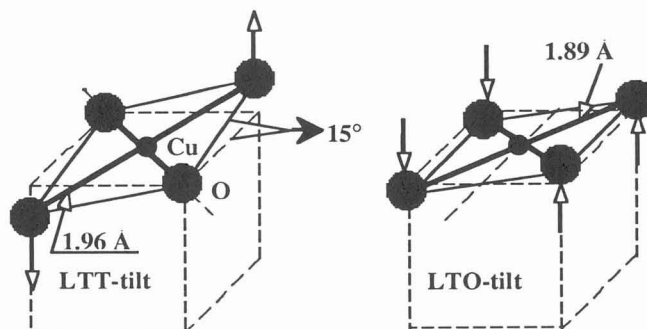


Figure 3: Pictorial view of the LTT and LTO tilts.

In conclusion, we have shown the coexistence of two different kinds of domains with the LTT and LTO types of structure in the $\text{La}_2\text{CuO}_{4.1}$ compound. These domains are spatially distributed in stripes of distorted and undistorted structure. The same kind of distortions have been seen in the isostructural LSCO compound and in the Bi2212 system, suggesting that inhomogeneity of the CuO_2 plane is a common feature for high T_C superconductivity. This result gives further support to the two component model based on stripes of localized and itinerant charges within the CuO_2 plane [16].

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