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Local Structure EXAFS Study of Nd_2CuO_4 and $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ Using Multiple-Scattering Data-Analysis

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Abstract. High-quality Cu K-edge EXAFS spectra of Nd_2CuO_4 and $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ are analyzed as a function of temperature in the range $T=5-70\text{ K}$ using the "GNXAS" method based on the multiple-scattering theory. The Cu-Nd and Cu-O-Cu in-plane quasi-linear distributions are studied as a function of temperature. Structural differences between doped and undoped compound are discussed.

1. INTRODUCTION

In this brief report we show the main results of the multiple-scattering (MS) EXAFS data-analysis at the Cu K-edge of Nd_2CuO_4 (NCO) and $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ (NCCO) for $T = 5, 30, 70\text{ K}$. A few EXAFS studies have been performed on those n-doped cuprates so far, in spite of the importance of this class of materials. The present results follow a similar study performed on lanthanum cuprates.[1] EXAFS spectra of layered cuprates have been found to be particularly sensitive to in-plane quasi-linear configurations Cu-O-Cu and have been used to study the angle distribution.[1,2] Details about suitable sample preparation methods and specific treatment of the raw data including appropriate background modelling can be found in ref. [1]. Data-analysis was performed using the GNXAS method.[3,4]

2. RESULTS AND DISCUSSION

In Fig. 1 we compare the EXAFS $k^2\chi(k)$ signals of NCO and NCCO at $T = 5\text{ K}$ (below T_c). Strong EXAFS oscillations are observed up to the limit of the present measurements (18.5 Å^{-1}), due to the strong backscattering of eight Nd atoms at about 3.32 Å and to the collinear Cu-O-Cu multiple-scattering signal at about 3.95 Å (according to the published T' unit cell [5]). The four in-plane oxygens at about 1.97 Å (first shell) give a weaker contribution mainly at low wave-vector values. There are evident differences between the spectra of the doped and undoped compounds, especially above 10 Å^{-1} . These differences are mainly due to variations of the strong high-frequency Cu-Nd and Cu-O-Cu components and reflect changes of the local structure in the two compounds. The dashed curves in Fig. 1 are the best-fit calculated signals including all of the main multiple-scattering contributions within a 4 Å cut-off distance. The overall agreement is very good. The discrepancy at about 4.5 Å^{-1} is due to the $[1s3p]$ double-electron excitation.[1] Other unexplained weaker features are related to further higher frequency components not included in present calculations (mainly Cu-Nd second-shell).

Figure 1. Experimental (solid) and calculated (dashed) EXAFS of NCO and NCCO at $T=5\text{ K}$.

Figure 2. Angle distribution function for the in-plane quasi-linear configuration Cu-O-Cu at 5 K .

Table 1: Best-fit local structural parameters as a function of temperature (statistical errors in brackets).

	$T(K)$	$R_{Cu-O} (\text{\AA})$	$\sigma_{Cu-O}^2 (\text{\AA}^2)$	$R_{Cu-Nd} (\text{\AA})$	$\sigma_{Cu-Nd}^2 (\text{\AA}^2)$	$R_{Cu-Cu} (\text{\AA})$	$\sigma_{Cu-Cu}^2 (\text{\AA}^2)$
NCCO	5	1.964(4)	0.0022(7)	3.319(5)	0.0030(5)	3.925(8)	0.0031
	30	1.965(4)	0.0025(7)	3.320(5)	0.0027(5)	3.926(8)	0.0029
	70	1.964(4)	0.0023(7)	3.321(5)	0.0029(5)	3.926(8)	0.0030
NCO	5	1.961(4)	0.0024(7)	3.334(5)	0.0028(5)	3.921(8)	0.0030
	30	1.961(4)	0.0025(7)	3.334(5)	0.0027(5)	3.922(8)	0.0031
	70	1.963(4)	0.0026(7)	3.335(5)	0.0032(5)	3.923(8)	0.0032

Best-fit average interatomic distances and variances for $Cu - O$, $Cu - Nd$, and $Cu - Cu$ distributions are reported in Tab. 1 as a function of temperature. The only visible difference between the two compounds is the change of the average $Cu - Nd/Ce$ (around to 0.015 Å in the entire range of temperatures). A recent work on the local structure of NCCO [6] pointed out the existence of small displacements of Nd/Ce atoms from their crystallographic positions, although still comparable with thermal motion of atoms. Our EXAFS study clarifies that Ce doping leads to a well-defined shift of the mean value of the $Cu - Nd/Ce$ distance distribution, while variance is practically unchanged. This result suggests that a displacement of Nd/Ce ion of about 0.02 Å above and below the CuO_2 plane, along the c axis (according to the T' unit cell), occurs in the doped compound. On the other hand, the other measured distances and variances reported in Tab. 1 coincide within the error in the doped and undoped compounds, confirming the different behaviour between this family of cuprates and the p-doped lanthanum ones (see tab.1 of ref.[1]).

Tab. 1 reports only results related to two-atom distributions. Previous works on layered superconductors showed that important multiple-scattering contributions associated with the $Cu - O - Cu$ linear configurations in the CuO_2 planes can be successfully used to study the angular distribution.[1,2] In those cases, the $Cu - O - Cu$ configurations were not found exactly collinear, showing mean angle values of about 170°. In the present case, exactly linear $Cu - O - Cu$ configurations are instead to be used. Significant shifts of the mean angle value from $\theta = 180^\circ$ leads to unacceptable poor agreement between experimental and calculated EXAFS signals. The actual distribution to be used for exactly linear configurations needs some clarification. Distance and angular distributions are factorized in such extremal conditions and a second-order expansion is needed to account for angle fluctuations in the multiple-scattering signal.[4] In a real vibrating system composed by three aligned atoms (average positions of the in-plane $Cu - O - Cu$ configuration in NCO and NCCO) the angular probability distribution vanishes at $\theta = 180^\circ$ (angle measured at the oxygen site). A suitable model for the angle distribution function can be written as:[4]

$$f(\theta) = \frac{(180 - \theta)}{\delta_\theta^2} \exp\left(-\frac{(\theta - 180)^2}{2\delta_\theta^2}\right); \quad 0 \leq \theta \leq 180.$$

In absence of the linear $(180 - \theta)$ term, δ_θ^2 would be the angle variance around $\theta = 180^\circ$. The condition of vanishing probability at $\theta = 180^\circ$ implies a change in the shape of the distribution which has a maximum at $\theta_M = 180^\circ - \delta_\theta$. Therefore, due to vibrations, the most probable angle value is always different from $\theta = 180^\circ$. For large angular fluctuations δ_θ , a disordered linear configuration can be easily confused with the case of a bent average configuration, but in the present case small values in the range $\delta_\theta = 2 - 5^\circ$ have been found. In Fig. 2 the best-fit angle distributions $f(\theta)$ for NCO and NCCO compounds at $T = 5$ K are shown. A clear difference between NCO and NCCO is found, although error bars (not shown) turn out to be quite large. The most probable angle value resulted to be $\theta_M = (180 - 2)^\circ$ and $\theta_M = (180 - 3)^\circ$ for NCO and NCCO respectively. Present evaluation of the angular distortion of the CuO_2 planes is in agreement with other structural studies.[6,7] The difference in the angle distribution between doped and undoped compounds is found only below T_c and could be connected with the onset of superconducting phase. The broadening of the angle distribution induced by doping could be due both to different vibrational amplitudes and to static structural distortion.

In conclusion our MS-EXAFS data-analysis of neodymium cuprates shows a clear difference in the $Cu - Nd$ distance distribution between the doped and undoped compound. Furthermore well below T_c a broadening of the angular distribution of the $Cu - O - Cu$ in-plane linear configurations is found in the doped compound. Although there are no doubts about the existence of CuO_2 plane distortions in neodymium cuprates, a large debate about the nature of these distortions [8] is still open. Present and further detailed EXAFS[9] investigations could be important to shed some light about this point.

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