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## Temperature Dependent Local Instability of the Hg1212 Structure by Polarized EXAFS

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**Abstract.** The local structure of the  $\text{Hg}_1\text{Ba}_2\text{CaCu}_2\text{O}_{6+\delta}$  (Hg1212) crystal has been investigated by temperature dependent polarized Cu K-edge extended x-ray absorption fine structure (EXAFS). We have observed an anomalous behavior of the local structure showing anomaly at around the superconducting transition temperature  $T_C$  in the temperature dependence of the Cu-O(planar) distance. The result suggests similarity of the temperature dependent local instability in the superconducting cuprates.

### 1. INTRODUCTION

One of the main debates in the high  $T_C$  field is the instability of the local structure, diverging from the average one, due to the fact that the structural properties appear to be highly correlated with the (still unknown) electronic mechanism of superconductivity in these ceramics. This instability of the electronic properties in most of the cuprates has been seen by the experiments sensitive to the local structure showing temperature dependent anomalies around the superconducting critical temperature  $T_C$  and above  $T_C$  at a temperature  $T^*$  [1].

Cu K-edge Extended X-ray Absorption Fine Structure (EXAFS) has proved its ability to probe the instable structure at the mesoscopic scale in various families of cuprate superconductors. Cu K-edge EXAFS studies with polarized x-rays and oriented single crystal samples have been used to characterize the lattice distortions by the direct measurement of distribution of the Cu-O bond distances in these complex structures. Recently, exploiting the ability of the polarized EXAFS, we have determined the structure of the inhomogeneous  $\text{CuO}_2$  plane in the  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) [2-4] and  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  (Bi2212) [5-6].

The Hg-based high temperature superconductors have highest  $T_C$  among the cuprate family and longest average Cu-O distances indicating strong correlation between the superconductivity and the structural properties. To have further insight into the local structure of the potentially important  $\text{CuO}_2$  plane, we have made polarized Cu K-edge EXAFS measurements as a function of temperature on single crystal of  $\text{Hg}_1\text{Ba}_2\text{CaCu}_2\text{O}_{6+\delta}$  (Hg1212). The aim of this short report is to present the preliminary EXAFS results. We have been able to measure polarized EXAFS spectra on a very small crystal ( $\sim 200\mu\text{m}$ ). The polarized EXAFS allowed us to separate the contribution of in plane backscatter from that of the out of plane. The temperature dependence of the in plane polarized (E//ab) EXAFS is reported. The results suggest that the local structure of the Hg1212 system goes under anomalous structural changes at around  $T_C$ . The observation of the anomaly at  $T_C$  suggests the general nature of the local structural distortions in the  $\text{CuO}_2$  plane of the high  $T_C$  superconductors.

### 2. EXPERIMENTAL

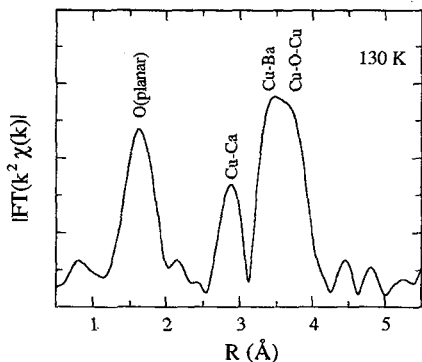
The single crystal of Hg1212 was grown by high gas pressure technique [7]. The temperature dependent polarized Cu K-edge absorption measurements were performed on the beam-line CRG-IF, equipped with bent conically shaped Si(111) double crystal monochromator and sagittal focusing, at the European Synchrotron Radiation Facility (ESRF) at Grenoble. The crystal of size  $200 \times 200 \mu\text{m}^2$  showing  $T_C = 110$  K (onset) was mounted in a closed-cycle He refrigerator and the temperature was monitored with an accuracy of  $\pm 1$  K. The spectra were recorded in the fluorescence yield mode using a 5-element Ge detector system. The spectra were repeated for the reproducibility. The EXAFS signal  $\chi = (\alpha - \alpha_0)/\alpha_0$ , where  $\alpha$  is the absorption coefficient and  $\alpha_0$  is the so called atomic absorption, was extracted from the absorption spectrum using standard procedure [8] and corrected for fluorescence self absorption [9].

### 3. RESULTS AND DISCUSSION

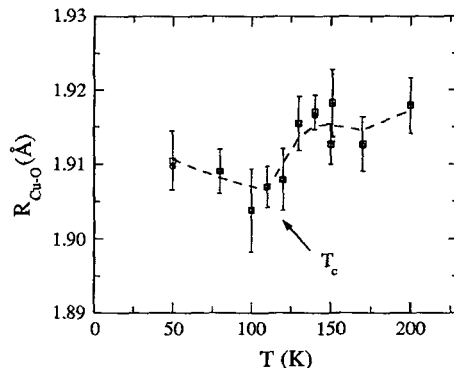
The Fourier transform (FT) of the extracted EXAFS signal (multiplied by  $k^2$ ) from the E//ab polarized Cu K-edge absorption of the Hg1212 single crystal, at a representative temperature (130 K) is shown in Fig. 1. The Fourier transform has been performed in the  $k$  range between  $k_{\text{min}} = 3 \text{ \AA}^{-1}$  to  $k_{\text{max}} = 16 \text{ \AA}^{-1}$  using a Gaussian window. The main peaks in the Fourier

transform (FT) reflect the distribution of atoms in the E//ab direction. The position corresponding to the FT peaks in Fig. 1 do not give measure of the real inter atomic distances as the FT is not corrected for the phase shifts. The strong contribution from the Cu-O(planar) pair (at 1.9 Å distance) is reflected by a FT peak at ~1.6 Å effective distance.

The Cu-O(planar) EXAFS of the first shell was isolated by Fourier filtering and corrected by theoretically calculated phase shifts. The EXAFS was modelled using curved wave theory. The number of parameters determined by the EXAFS analysis is limited by  $N=(2\Delta R\Delta k)/\pi$ . In the present case, the  $\Delta R=0.8\text{\AA}$ ,  $\Delta k=10\text{\AA}^{-1}$  ( $3-13\text{\AA}^{-1}$ ) and hence the number of parameters to be fitted is limited by about 5. In the analysis all the parameters including the effective coordination number (which agrees well with the parameters reported earlier [2, 4-5, 10] for Cu-O pairs in different systems) were fixed while the radial distance (R) and the Debye Waller factor ( $\sigma^2$ ) for the Cu-O(planar) pair were allowed to vary. Thus the present analysis is essentially a two parameter fit.



**Figure 1:** Fourier transform of the experimental E//ab distance EXAFS spectrum at 130 K



**Figure 2:** Temperature dependence of the Cu-O(planar) measured by EXAFS.

The temperature dependence of the Cu-O(planar) distance is shown in the Fig. 2. The Cu-O(planar) distance is temperature dependent and there appears to be anomalous change at  $T_c$ . This anomalous behavior is similar to one observed in the other cuprate superconductors [3-6]. The result suggests that inhomogeneity of the  $\text{CuO}_2$  plane, responsible for the anomalous behaviour, is a common feature for high  $T_c$  superconductivity.

The similarity in the structural anomalies at around the superconducting transition temperature  $T_c$  merely highlights the importance of the correlation between the charge and the lattice distortions for the superconductivity in the high  $T_c$  cuprate superconductors. The local lattice instability at low temperature has been associated with charge localization in a distorted local lattice i.e., polarons that coexist with itinerant charge carriers in the metallic undistorted  $\text{CuO}_2$  plane [11].

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