ESRF	Experiment title: EXAFS Study of the underdoped-overdoped transition in the single-layer superconducting cuprate $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$	**Experiment number: HE 1713**
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Report: We have measured the Cu *K* - EXAFS of underdoped (UD), optimum doped (OPT), and strongly overdoped (OD) crystals of the single-layer cuprate superconductor $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ at low temperatures (60 - 300 K). The data were recorded from a "low-T_c" (T_{cmax}= 18.5 K), and a "high-T_c" (T_{cmax} = 28 K) series of samples using the total electron yield (TEY) mode. The He exchange gas in the cryostat, coupling the sample thermally to the cold head, serves as an amplifier of the electron yield [1]. The efficiency of the detector increases with gas pressure, and tends to saturate around 1 bar (Fig. 1, *right*). At low temperatures we operated the detection systen with a pressure of typically 400 mbar. Drifts of the efficieny during low-*T* operation are very slow, and do not affect single scans. The sample position in the low-*T* runs was adjusted using the experimentally determined thermal expansion of the TEY sample rod (Fig. 1 *left*) . Thus we could safely avoid any direct illumation of the TEY collector by the x-ray beam.

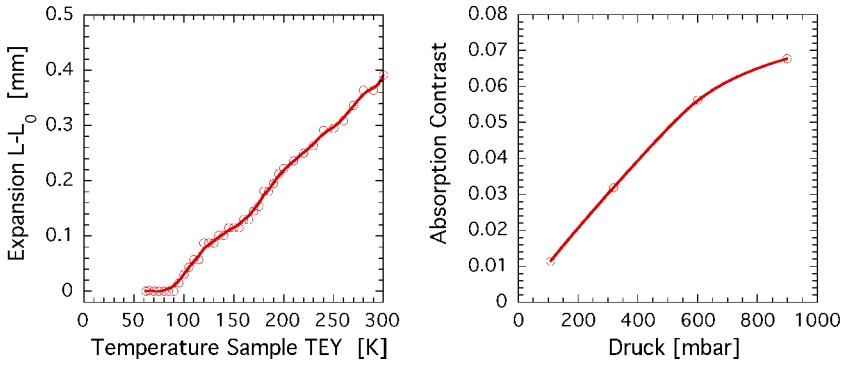

Fig. 1 *Left*: Relative thermal expansion of the TEY sample rod as determined from the transmission of a pin hole.
Right: Absorption contrast at the Cu *K*-edge of $Bi_2Sr_{2-x}La_xCuO_6$ as a function of the He exchange gas pressure in the TEY sample chamber. TEY Bias =70 V.

Fig. 2 compares with each other Fourier transform spectra of overdoped (x=0.15) $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$ recorded from the "high-", and "low-T_c" series. The radial distribution functions (RDF) of Cu-Sr/La are

found identical, not unexpected from the same La/Sr ratio in the doping layer. But the Cu-O1,2 RDF's and the peak heights of the multiple scattering paths, Cu-O1,2-Cu, differ significantly from each other suggesting a relationship between local atomic disorder in the CuO_2 sheet, and the maximum T_c of the sample series.

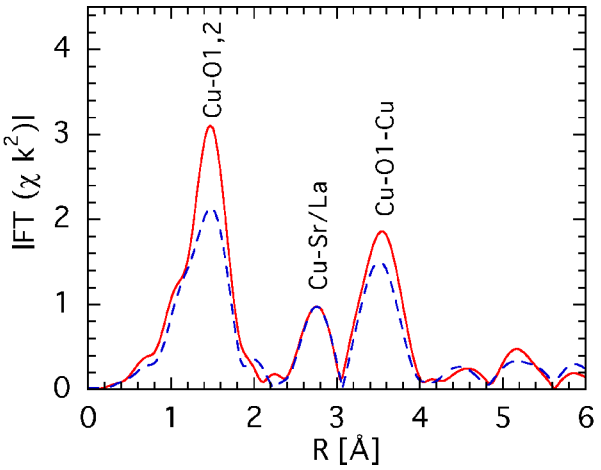

Fig. 2 Cu *K* EXAFS in overdoped $Bi_2Sr_{1.85}La_{0.15}CuO_{6+\delta}$ at $T = 300$ K: co-plotted moduli of the Fourier transforms, $|FT(\chi k^2)|$, from the "low-T_c" series of crystals (blue dashed line), and from the "high-T_c" series of crystals (red drawn out line,) at *identical* concentrations of La dopants ($x = 0.15$). Disorder in the CuO_2 plane of the "low-T_c" series dampens the *nn* radial distribution function Cu-O1,2, and the multiple scattering (MS) path Cu-O1,2-Cu. The RDF Cu-Sr/La containing the dopants is identical in the two series.

Fig. 3 summarizes results from a first analyis of the temperature dependent *nn* Cu-O1,2 EXAFS in the strongly *overdoped* regime (x=0.15), "low-T_c" series. Here we have expected no structural anomalies. The fits to the filtered Cu-O1,O2 shell are based on self-consistent calculations (FEFF 8) of the cluster potential. Self-consistency in the calculation of the cluster potential turned out to improve considerably the accuracy of E_0, which is crucial for a proper normalization of the rather critical low-*k* part of the Cu-O XAFS. Surprisingly we find a significant deviation from the usual *coth* - type temperature dependence of the harmonic vibrational contribution to the disorder $\sigma^2(T)$ in the *nn* Cu-O1,2 shell of the cuprate superconductors. Notably the mean-squared displacements $\sigma^2(T)$ start to increase below 100 K, yielding evidence for a displacive structural transformation in the CuO_2 sheet. A displacive structural transformation around $T = 100$ K is corroborated by the kink in the temperature dependence of the mean-cubic displacements, c_3 (Fig. 3, right). c_3 decribes the deviation from a symmetric Gaussian pair distribution function, and thus may be taken as a measure of anharmonicities in the vibrational contribution to the disorder. But the anharmonicty connected with the normal thermal expansion will increase c_3 at high temperatures, not decrease it. Below ≈ 100 K it is usually negligably small, or at least independent on temperature. The temperature behavior of c_3 is thus highly unusal and, independently from the anomalous $\sigma^2(T)$, it suggests a displacive structural transformation in the CuO_2 sheet.

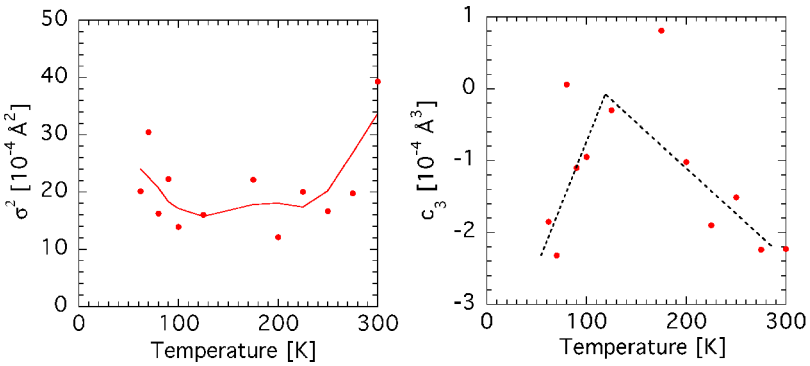

Fig. 3 Results from single shell fits to the filtered (R_{eff}=1.1-1.9 Å) Cu-O1,O2 shell of strongly overdoped $Bi_2Sr_{1.85}La_{0.15}CuO_{6+\delta}$. as a function of temperature. Dashed and drawn out lines are guides to the eye. *Left:* Mean-squared displacements, σ^2 *Right:* Mean-cubic displacements, c_3 .

Literature:

[1] J. Röhler, A. Jacobi, C. Janowitz, A. Krapf, R. Manzke, ESRF Experimental Report HE1525 (2003).