ESRF	**Experiment title:** X-ray absorption study of superconducting $YBa_2Cu_3O_{6.6}$ under high pressure	**Experiment number**: HC-3915
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Report:

Recent experiments in superconducting cuprates have revealed the ubiquitous presence of charge-ordered electronic states strongly competing with high temperature superconductivity [1]. Our recent x-ray scattering experiments on $YBa_2Cu_3O_{6+x}$ have shown the complete suppression of all signatures of the charge density wave (CDW) state below the modest pressure of ~1 GPa [2]. The purpose of the current experiment was to explore local structural changes related to the suppression of the CDW order and the previously reported simultaneous increase of the superconducting T_c in underdoped $YBa_2Cu_3O_{6.67}$ [3]. To this end, we have used x-ray absorption spectroscopy (XAS) under combined high pressure and low temperature conditions.

XAS measurements were performed in transmission geometry at the Cu K edge. The experiment was performed at the BM23 beamline at the ESRF, with a double crystal Si (111) monochromator and Kirkpatrick−Baez mirrors to focus the monochromatic x-ray beam (5x5 μm spot size). The samples were loaded in a nano-polycrystalline diamond anvil cell (DAC) in order to avoid glitches from the anvils. The DAC was then inserted in the dedicated continuous flow He-cryostat available in BM23. Although, our initial plan was to measure detwinned single crystals of $YBa_2Cu_3O_{6+x}$, soon after the first test scans we had to switch to powder samples because the obtained signal from the single crystals was severely distorted by strong Bragg peaks. Combined transmission and fluorescence geometry should be considered for future investigations on single crystals of this system.

After measuring x=0.48, 0.67 and 0.75 powders at ambient conditions as a reference for the doping dependence of the edge structure in the XANES part of the spectrum, we moved to the high pressure measurements on x=0.67 samples. Pressure dependent datasets were collected above and below T_c and a temperature dependent dataset was collected at the maximum pressure (10 GPa). The experimental data that we recorded at 50 K, therefore below T_c, around the critical pressure of ~1 GPa are shown in Figure 1. The extended X-ray absorption fine structure (EXAFS) signal, $\chi(k)$, was obtained after removing the background signal. The

Fourier Transform (FT) curves of the k^2-weighted EXAFS signal were obtained for the k-range 1.5 – 13 $Å^{-1}$ using a sinus window with the Athena software of the Demeter package. The EXAFS structural analysis is still ongoing. However, already at this stage an inspection of the EXAFS signal indicates that there are clear changes on the material under pressure, as the high k oscillations are changing both their intensity and their frequency. In addition, noticeable changes are expected on the 1st shell, which are reflected on the first intense peak around 1.5 Å in the FT signals. The intensity of this peak clearly increases at 1.6 GPa, therefore above the pressure were we see all CDW effects disappearing. In our ongoing data analysis, we are considering possible origins of the effect, such as a pressure evolution towards a more regular local environment around the Cu ions.

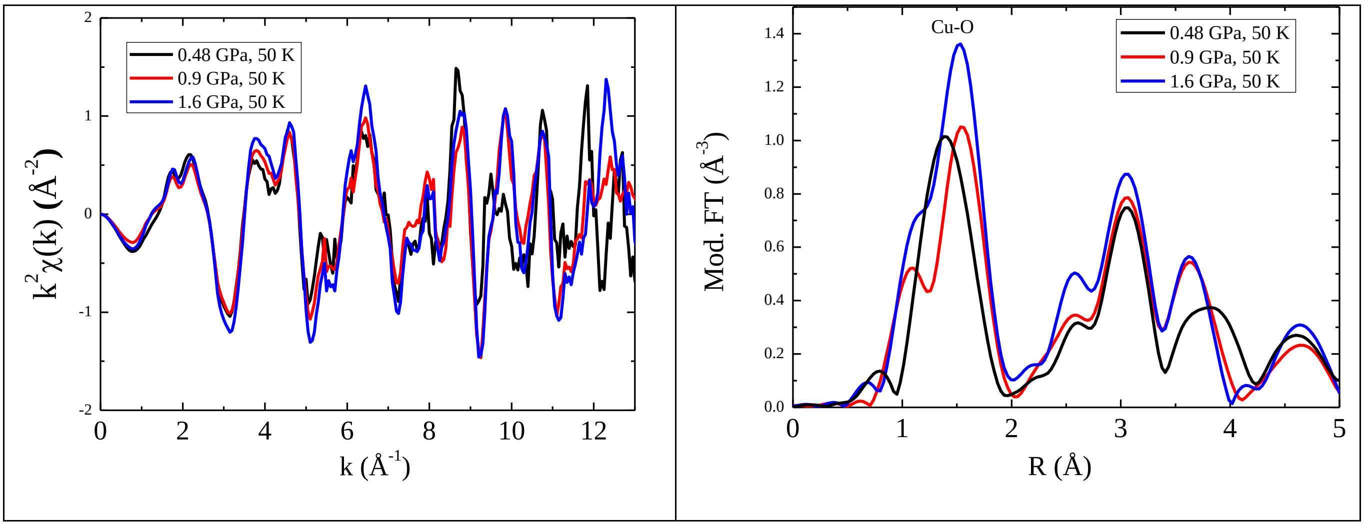

Figure 1: Left: EXAFS signal of $YBa_2Cu_3O_{6.67}$ weighted in k^2 for selected pressures at 50 K. Right: Modulus of the Fourier Transformed EXAFS signal along the whole pressure range, considering a sinus window k: [2,12.5] $Å^{-1}$, Δk = 0.5 $Å^{-1}$.

References:

[1] Comin, R. and A. Damascelli, Annu. Rev. Condens. Matter Phys. **7** (1), 369-405 (2016)

[2] Souliou S.M. et al., PRB 97, 020503(R) (2018)

[3] Sadewasser S. et al., PRB, 61, 741 (2000), Cyr-Choinière O. et al., PRB 98, 064513 (2018)