| ESRF | **Experiment title:**<br>Anisotropic softening of the CuO2 planes buckling modes in $YBa_2Cu_3O_{6+y}$. | **Experiment number**:<br>HS-4801 |
|---|---|---|
| **Beamline**:<br>ID28 | **Date of experiment**:<br>from: 30 Jan. 2013 to: 05 Feb. 2013 | **Date of report**:<br>28 Feb. 2013 |
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**Report:**

The buckling mode of the oxygen ions in the $CuO_2$ planes of $YBa_2Cu_3O_{6+\delta}$ (YBCO) shows an anomaly [1] which is anisotropic in the plane. On one of the high symmetry direction, $b^*$, Inelastic Neutron Scattering (INS) data shows a broadening that it is interpreted as an anomalous dispersion, similar to a Kohn anomaly, close to the *in-plane* propagation wave-vector (0, 0.3). This can be attributed to an effect originating from the otherwise elusive charge stripe, which has been possibly observed only recently [2]. However the INS Q-resolution does not allow to follow this anomalous dispersion, which was deduced from changes in the width on the energy scan of the mode. We would like to use the higher Q-resolution of Inelastic X-ray Scattering (IXS) [3] in order to experimentally observe such dispersion.

The data we managed to collect during the experiment showed an intensity of the buckling mode much weaker than foreseen by our DFT calculations, while lower energy modes matched quite well for both the intensities and the frequencies. In the Figure, we show the most illuminating example: the IXS intensity is measured at two different *in-plane* wave-vector : for (0, 0.1) and (0, 0.3). The data are compared at two different energy resolution set-up : with Si( 9 9 9) reflection (res. ~ 3 meV) and Si( 11 11 11) reflection (res. ~ 1.5 meV). Note that the two set-up measurement where taken in different Brillouin Zone, with a wave-vector (0 -$q_k$ 10) for the 3 meV set-up and (0 -$q_k$ 14) for the 1.5 meV one, this because of angular limits of the spectrometers and scattering geometry, depending on the X-ray wavelength.

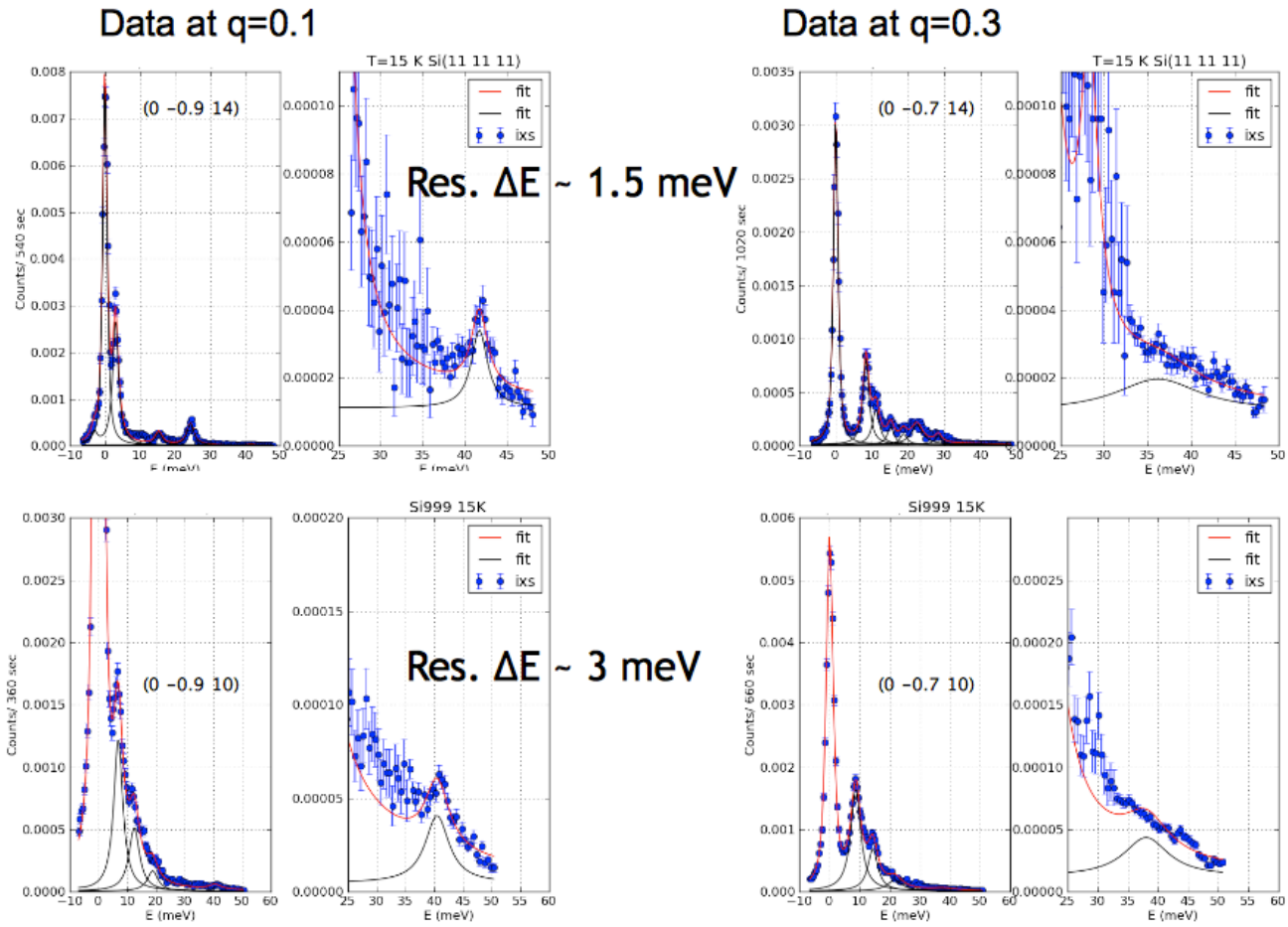


*Illustration 1: Fig. 1: Example of phonon spectra on YBa2Cu3O7-y measured by IXS (circles with error bars), at RT 15 K, fitted with a sum of harmonic modes convoluted with the resolution (lines). The modes at about 41 meV is the buckling of the in plane oxygen around the copper.*

The two BZ are equivalent for the dynamical structure factor of the buckling mode, for which the intensity is maximum (but not necessarily for the other modes, so the low energy part of the spectrum could appear different). Other scans, taken with res. ~ 3 meV with different $q_k$ are not shown. The buckling mode was almost dispersionless and well resolved from $q_k$=0.1 to 0.2 (not shown) and again with a similar energy and lifetime at $q_k$=0.5, but its intensity was too weak for any determination of position and width close to (0 0.3 *L*). This point indeed to some anomalous effect at (0 0.3 *L*), as no such difference in intensity is expected from calculations and previous data. We note that a possible explanation would be a broadening of the mode itself, in contradiction with the INS results, but this will need a much higher statistics on that point, and the ones close to it, in order to be demonstrated. The proposed experiment was planned using only one energy set-up, and more intensity on the buckling mode, but the test made in a low resolution configuration, in order to gain flux, and the additional counting time needed to sort out a signal made the accomplishment of the experiment impossible. We think, however, that we have enough data to reformulate the experimental strategy and complete the experiment with a reasonable complement of shifts. In particular, the complete set of data, indicate that the initial choice, with Si( 11 11 11) reflection (res. ~ 1.5 meV) was the better adapted, despite the low flux, provided that data are collected with longer counting time are, in particular close to (0 0.3 *L*), to achieve enough statistics.

## References

1) M. Raichle, *et al., Phys. Rev. Lett.* **107** (2011) 177004; 2) G. Ghiringhelli, *et al., Science* **337** (2012) 821; 3) M. d'Astuto, *et al., Phys. Rev. B* **78** (2008) 140511(R).