<b>ESRF</b>	<b>Experiment title:</b> Probing the Cu-O Bond stretching phonon by inelas- tic X-ray scattering in the underdoped (x 0.1) Ca2- xCuO2Cl2 cuprate	Experiment number: HC-4310
Beamline: ID28	Date of experiment: from: 20 Jan 2021 to: 26 Jan 2021	Date of report: September 6, 2022
Shifts: 18	Local contact(s):	Received at ESRF:

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## Report:

The results of this experiment have been recently published in Ref. [1], of which we show Fig. 1 (from Fig. 5 of the same publication), in order to summarise the most relevant results to this report. In Ref. [1], we could compare the results obtained by IXS on ID28 on the experiment we report here, to the ones, obtained by high energy resolution RIXS, also at ESRF, on ID32 (Exp. HC 3884), which directly probe electron-phonon coupling, and allowed to unveil the bulk Charge-Density-Wave (CDW) in the same compound (samples from the same batch, and with the same doping). The main results can be summarised as follow:

- the wave-vector of the phonon anomaly,  $Q_A$ , is slightly shifted compared to the and propagation vector of the CDW,  $Q_{CDW}$ ;
- $Q_A$  appear at the intersection between the Cu-O bond-stretching phonon mode and a novel dispersive excitation emanating from the CDW (not shown in this report, see Fig. 2 of Ref. [1]);
- the maximum of the phonon width, as measured from IXS, corresponds to the maximum of the additional, anomalous electron phonon coupling measured by RIXS.

Further details, as well as that full, raw spectra from ESRF experiment HC-4310, are given in the above mentioned Ref. [1]. We plan to extend further these results both as a function of doping and temperature, in order to understand the exciting, new physics that we just unveiled.



Figure 1: From Ref. [1] (see Fig. 5 of the reference). (a) RIXS BS phonon dispersion at 25 K, with density functional theory calculations, extracted from ref. [2], are shown with a grey solid line. (b) RIXS intensity map at 25 K, with subtracted elastic and paramagnon peaks. (a). (c), (d) IXS BS phonon dispersion (c) and width purple(d) at 25 K. IXS spectra have been measured at both BL35XU (SPring-8) and ID28 (ESRF) beamlines. Note that in contrast to the peak position, the fitted FWHM at  $q = (0.5 \ 0 \ 0)$  was a parameter not stable in the fit (with very large error bars), which strongly depends on the model used (either pseudo-Voigt or damped harmonic-oscillator). (e) Momentum-dependence of the RIXS integrated intensity of the elastic/paramagnon-subtracted data at 25 K with  $\sin^2(\pi Q_{\parallel})$  curve (black solid line). The integrated energy window corresponds to the white dashed lines in (b). The bottom panel represents the difference between the integrated intensity and the  $\sin^2(\pi Q_{\parallel})$  curve, with Lorentzian fit (solid line).  $Q_{\rm CDW}$ and  $Q_{\rm A}$  are indicated with a dashed line and arrow respectively.

## References

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- [2] B. W. Lebert, H. Yamamoto, M. Azuma, R. Heid, S. Tsutsui, H. Uchiyama, A. Q. R. Baron, B. Baptiste, and M. dAstuto, "Doping-induced in-plane anisotropy of bond-stretching phonon softening in oxychloride Ca<sub>2-x</sub>CuO<sub>2</sub>Cl<sub>2</sub> compounds", Phys. Rev. B **101**, 020506(R) (2020).