



	Experiment title: Study of c-axis-polarized phonons in the model high-temperature superconductor $\text{HgBa}_2\text{CuO}_{4+\delta}$ using inelastic X-ray scattering.	Experiment number: HC3700
Beamline: Id 28	Date of experiment: from: June 13 2018 to: June 19 2018	Date of report:
Shifts: 18	Local contact(s): Alexiei Bosak	<i>Received at ESRF:</i>
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The aim of the experiment was to study the electron-phonon interaction in the high- T_c model superconductor $\text{HgBa}_2\text{CuO}_{4+\delta}$ (Hg1201), via inelastic X-ray scattering (IXS). The far-seeing motivation for these studies was to understand the mechanism of the formation of the charge-density-wave (CDW) order in the cuprates and its role on the lattice dynamics. In accordance with the proposed research plan, using the diffuse X-ray scattering, we explored the reciprocal space in search of the momenta at which the signatures of the CDW order are the strongest. The diffuse scattering was expected to provide clues regarding the strength of the interaction between the CDW and the lattice, and then subsequently, IXS measured near these points in reciprocal space where the lattice instability is identified in the diffuse scattering.

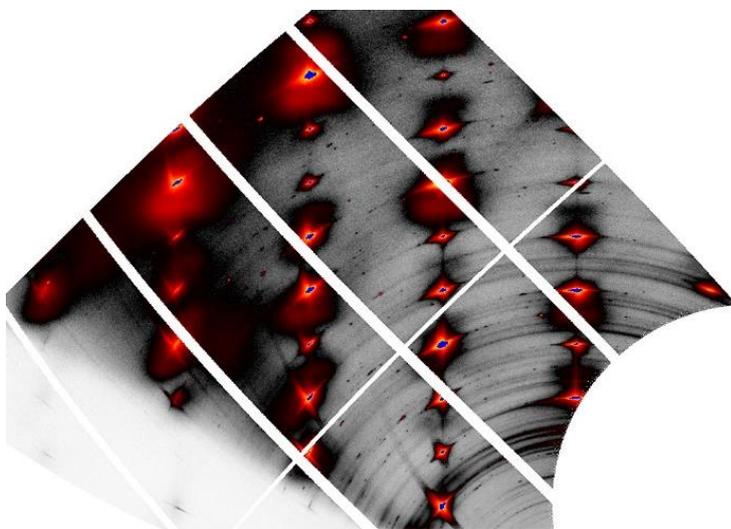


Fig. 1. The a-c plane diffuse X-ray scattering pattern of an underdoped Hg1201 sample. The data were collected at $T_c = 71\text{K}$, where the CDW order is the strongest. The Bragg peaks are very sharp, however, no signature of the CDW order was observed. The collected data showed no indication of the lattice distortion associated with the CDW instability.

The diffuse scattering performed on a single crystal of Hg1201 ($T_c = 71\text{K}$), provided no evidence of a lattice instability related to the CDW formation. This result indicates that the CDW order in Hg1201 has a very weak effect on the lattice dynamic, unlike what was observed in a sister compound $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ (YBCO).¹ Considering the negative result of the lattice instability in Hg1201, we continued research on the related topic, in the electron-doped cuprate $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO). The experiment allowed us to explore the optical-phonon anomaly discovered by us previously, during the experiment HC3124. The anomalous behavior of the optical phonon mode was observed in an underdoped sample ($x = 0.078$). In this experiment, we followed this anomaly as a function of temperature and doping, and obtained the detailed dispersion relation along [100] direction, for an optimally doped sample ($x = 0.145$), as shown in Fig. 2a.

Our high-energy resolution IXS data allows the detailed analysis of the momentum dependence of the optical phonon modes. The summary dispersion relation extracted from the data collected at various temperatures in the optimally doped sample is shown in Fig 2a. Importantly, our detailed analysis combined with the result from HC3124 demonstrates that the data collected on the samples at different doping levels, in different regimes of the phase diagram, agree within the experimental error. It furthermore shows that the phonon dispersion along the [100] direction is doping independent, at least in the studied doping range.

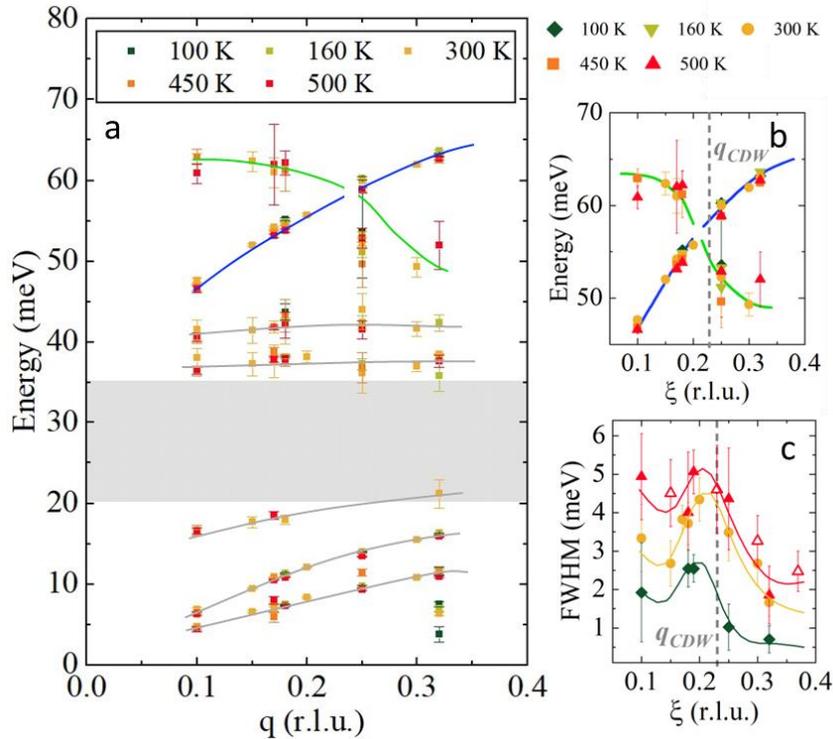


Fig. 2. (a) Phonon dispersion in NCCO ($x = 0.145$) measured at indicated temperatures. The experimental points were acquired along $q = (\xi, 0, 0)$ for ξ from 0.1 to 0.3 with a fine step of 0.05. The estimation of the q values has an error of $q = (0, 0 \pm 0.02, 0 \pm 0.06)$. The solid blue and green lines indicate the two highest-energy optical modes of our interest. (b) The close-up of the dispersion relations for optimally doped NCCO. A position of the bond-stretching mode is marked by a green line, while a blue line represents the other LO mode. (c) FWHM of the blue-marked mode at 100 K, 300 K, and 500 K. Open symbols correspond to the measurements for the underdoped sample. The lines in both panels are guides to the eye. Grey vertical line represents the wavevector of the CDW order (q_{CDW}) for the optimally doped sample.²

Figure 2(b) shows the temperature evolution of the two high-energy optical phonons. Within the experimental resolution, the dispersion of the two phonon branches is temperature independent. No evident changes in the phononic spectra are observed upon crossing various phase boundaries, e.g., AF order or CDW order. The experimentally obtained dispersions do not change with doping or temperature. We observed an anomalous broadening of the most prominent optical LO phonon mode, which contains a contribution from the Cu–O bond-stretching vibrations. The local increase of the full-width-at-half-maximum (FWHM) of the blue-marked branch, presented in Fig. 2(a,b), is observed at $\xi \approx 0.2$, which coincides with the momentum at which the two high-energy optical phonons anticross. This local increase of the width is not the effect of a superposition of two overlapping phonon peaks but it is an intrinsic feature of the LO mode, observed in the whole studied temperature range and at both doping levels.

In summary, we observed the first evidence of anomalous broadening of the phonon mode involving the bond-stretching Cu–O1 vibrations in the electron-doped cuprate. Our results indicate that there is no link between the formation of the static CDW order and the softening of the bond-stretching phonon dispersion at $q = (0.2, 0, 0)$. The experimental results may be interpreted as evidence of electron-phonon coupling in electron-doped cuprates, not influenced by the onset of the static CDW order but sensitive to dynamic correlations, reported by us recently.^{2,3}

References:

¹ Le Tacon et al., Nature Physics, 10(1), 52–58 (2013). <https://doi.org/10.1038/nphys2805>

² Da Silva Neto, E. H. et al., Physical Review B, 98(16), 161114 (2018). <https://doi.org/10.1103/PhysRevB.98.161114>

³ Yu, B., Tabis, W., Bialo, I. et al., Physical Review X, 10(2), 021059 (2020). <https://doi.org/10.1103/physrevx.10.021059>