



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.

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High- T_c model superconductor $\text{HgBa}_2\text{CuO}_{4+\delta}$ (Hg1201) was studied via inelastic X-ray scattering (IXS). The far-seeing motivation for our experiment was to study the origin of the still not well understood pseudogap phenomenon observed in all the high- T_c superconductors. In our recent inelastic neutron scattering experiments [Li] the presence of magnetic excitations, distinctly different from the well-known spin fluctuations near the antiferromagnetic wave vector $\mathbf{q}_{\text{AF}} = (1/2, 1/2)$, was revealed in the pseudogap phase. These new modes, for the optimally doped sample OP96 (the same as measured here), were centered at the zone center ($q=0$), and the related excitations were observed at energy transfers 35 and 53 meV. They were weakly dispersive across the Brillouin zone and first appeared well above T_c as the system was cooled below the pseudogap temperature T^* . While spin-flip neutron scattering experiments suggested magnetic origin of these modes, phononic origin could not be decisively rejected. This experiment was aimed to rule out, or accept, the phononic origin or contribution to the anomalies and also to further characterize the phononic spectra of Hg1201.

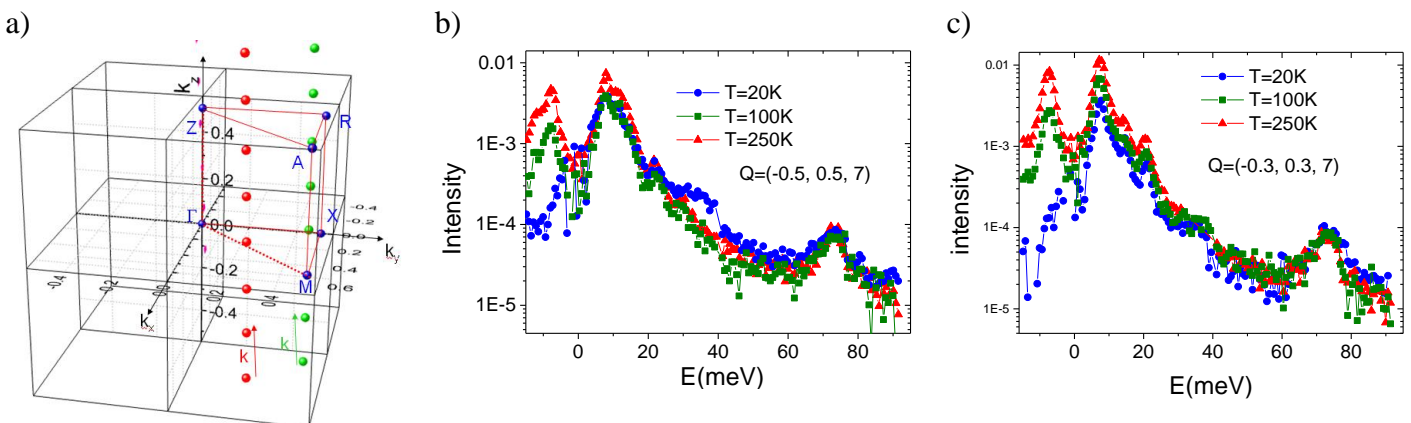


Fig. 1 **a.** \mathbf{q} vectors in the reduced Brillouin zone at which the phonons were studied. **b,c** the energy scans at two representative momentum transfers at various temperatures. Note the anomaly at $\sim 35\text{meV}$, enhanced at $T=20\text{K}$, for $Q=(-0.5, 0.5, 7)$ may be caused by the spin fluctuations; apart from that, the spectra nearly overlap.

The single crystal of optimally doped Hg1201 (OP96) of ca $2 \times 2 \text{ mm}^2$ had its a-b plane parallel to the surface. Due to rapid sample deterioration with moisture, the sample was handled in a controlled nitrogen gas environment.

c-axis-polarized phonons in the -15 – 90 meV energy transfer range were measured simultaneously at 9 distinct momenta and the data were collected by means of 9 analysers (marked as A1-A9). The positions of the analysers in the corresponding reduced Brillouin zone are shown in Fig. 1a. The measurements were performed below and above the various characteristic temperatures (at 20K, i.e. at $T \ll T_C=96\text{K}$, at $T=100\text{K}$, i.e. in the range $T_C < T < T^* \approx 220\text{K}$, and at $T=200\text{K}$ and, partially, 290K, i.e. at $T > T^*$).

The phonon spectra for two momentum transfer vectors are shown in Fig. 1b,c (the data are labeled after A2-analyser's momentum transfer). Note that apart from the well-known spin fluctuations near the antiferromagnetic wave vector $\mathbf{q}_{\text{AF}} = (1/2, 1/2, 0)$ the spectra nearly overlap. In order to seek for the subtle effects in the experimental data at different temperatures the following procedure is applied. First, the apparent four phonon peaks were fitted in the energy region below $E=25\text{meV}$. The results, in the form of dispersion relation along the nearly straight lines (formed by red and green points in Fig. 1a) are plotted along *K* and presented in Fig. 2a,b. A softening of $\sim 11\text{meV}$ phonon is observed at $K \approx 0.3\text{r.l.u.}$, see Fig. 2a. Some anomaly is also visible in the vicinity of $K \approx 0.42\text{r.l.u.}$ at $T=20\text{K}$ presented in Fig. 2b. The two *K*-values correspond to *L* values of 7 and 7.5 r.l.u., respectively.

Second, the high-energy background was estimated by subtracting the fitted four peaks from the whole experimental spectra. The results, not presented here, show a clear difference in the energy region around 35meV (for $\mathbf{Q}=(-0.5\ 0.5\ 7)$) between 20K and higher temperatures, the fact already presented in Fig. 1b and attributed to spin fluctuations. The high-energy part of this background, for momentum transfer $\mathbf{Q}=(-0.3\ 0.3\ 7)$ is shown on Fig. 2c. No phonon is seen in the expected region of 53meV, while there is a slight increase in the intensity at $T=20\text{K}$, in comparison to the spectra at higher temperatures, for the bunch of phonons in ca. 75meV region.

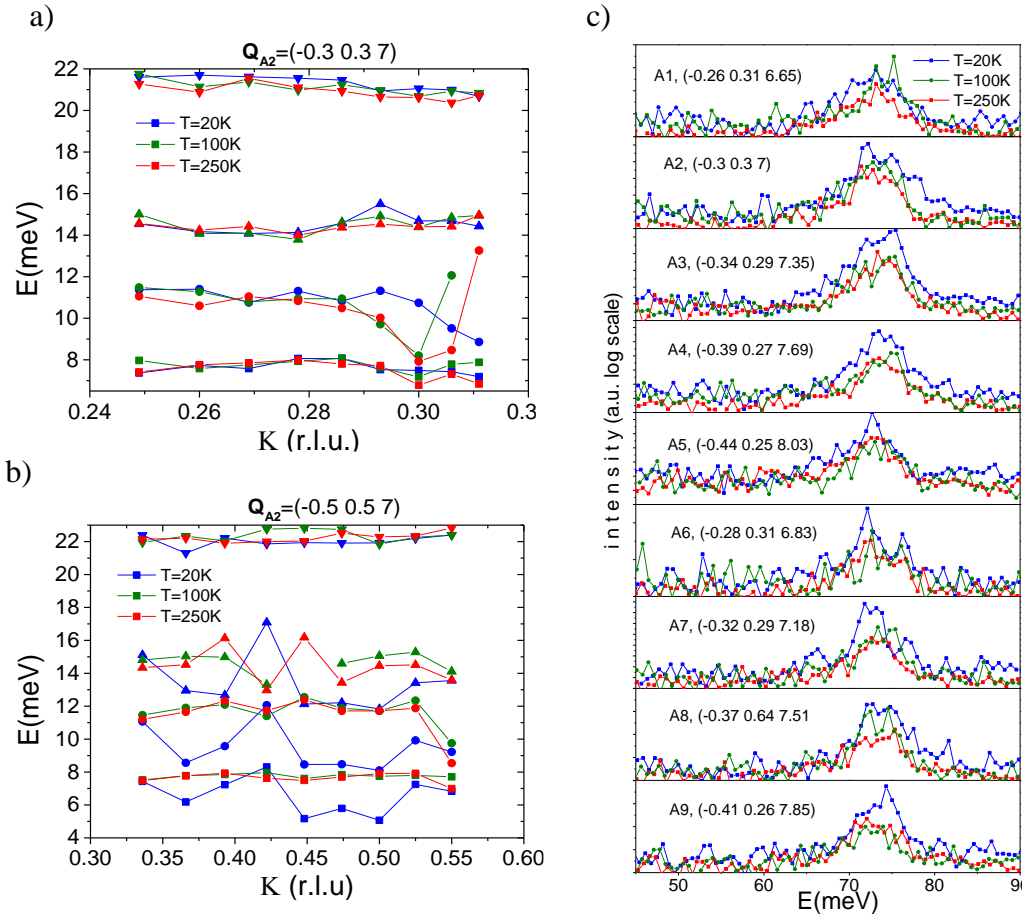


Fig. 2. a,b: Dispersion relation of the phonons fitted to four peaks in $E < 25\text{meV}$ energy range. The dispersion relation is plotted along *K* direction and the analyser positions are presented by red and green points in Fig. 1a. Note the difference between the spectra at $T=20\text{K}$ and other temperatures at $K \approx 0.3\text{ r.l.u.}$ Fig. 2a, and a possible anomaly at $K \approx 0.42\text{ r.l.u.}$, Fig. 2b. **c** the background subtracted spectra reveals a bunch of mixed high energy phonons with likely intensity increase at $T=20\text{K}$.

In conclusion, we have carefully tracked *c*-polarised phonons around momentum transfer $\mathbf{Q}=(-0.5\ 0.5\ 7)$ and $\mathbf{Q}=(-0.3\ 0.3\ 7)$. We have found:

- a clear anomalous behaviour for $T=20\text{K}$ and close to $\mathbf{q}=(1/2, 1/2, 0)$ (possibly due to spin fluctuations)
 - some difference between $T=20\text{K}$ and $T=100, 250\text{K}$ for low energy ($E=11\text{meV}$) phonons (with momentum transfer $\mathbf{Q}=(-0.3\ 0.3\ 7)$)
 - some increased intensity in 75meV region, again observed mainly for the momentum transfer $\mathbf{Q}=(-0.3\ 0.3\ 7)$.
- The further analysis is in progress.

References:

- [Li] Y. Li et al., Nature 468, 283 (2010); Y. Li, et al., Nature Phys. 8, 404 (2012)