



**Experiment title:**  
Phonon anomalies induced by electron-phonon interaction investigated by inelastic X-ray scattering in  $\text{HgBa}_2\text{CuO}_{4+d}$

**Experiment number:**  
HE 1369

**Beamline:**  
ID16

**Date of experiment:**  
from: 31 August 2002 to: 08 September 2002

**Date of report:**  
25 February 2003

**Shifts:**  
21

**Local contact(s):**  
Dr. Paola GIURA

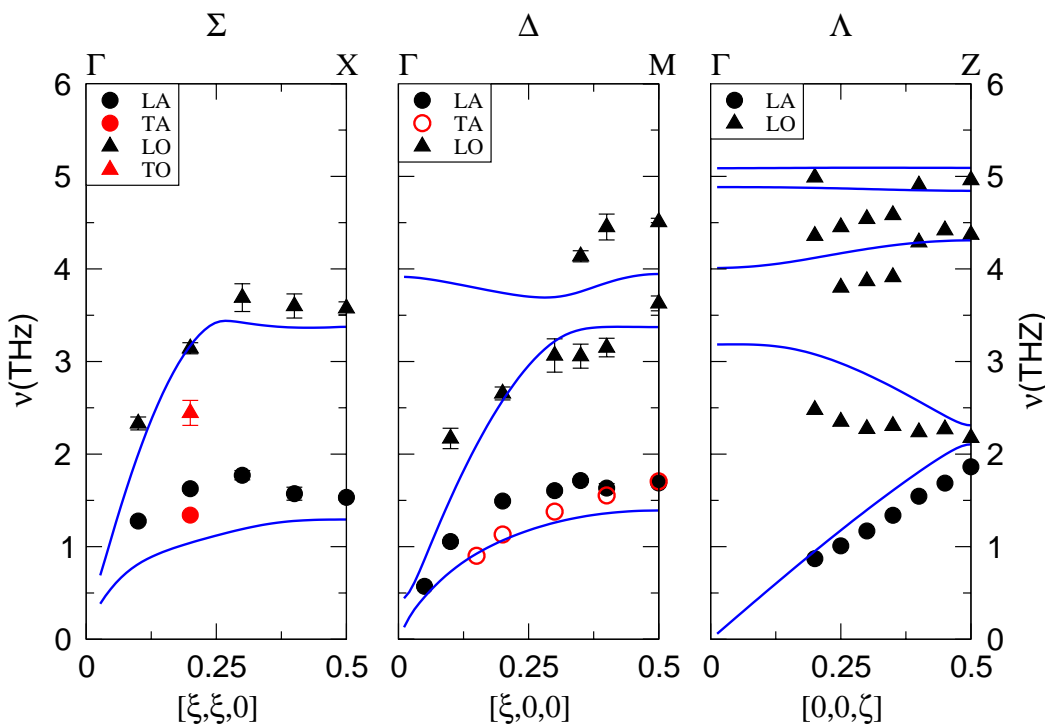
*Received at ESRF:*

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Report:

$\text{Hg}_2\text{BaCuO}_{4+\delta}$  is the 1-layer hole doped cuprate with the highest superconducting transition temperature ( $T_c=90$  K). For this system, the synthesis of superconducting crystals is possible only for volume up to  $0.1 \text{ mm}^3$ , a size which is too small for inelastic neutron scattering (INS) to observe high energy optical phonons. The measurement of phonons by inelastic x-ray scattering (IXS) represent also a difficult task [1], because



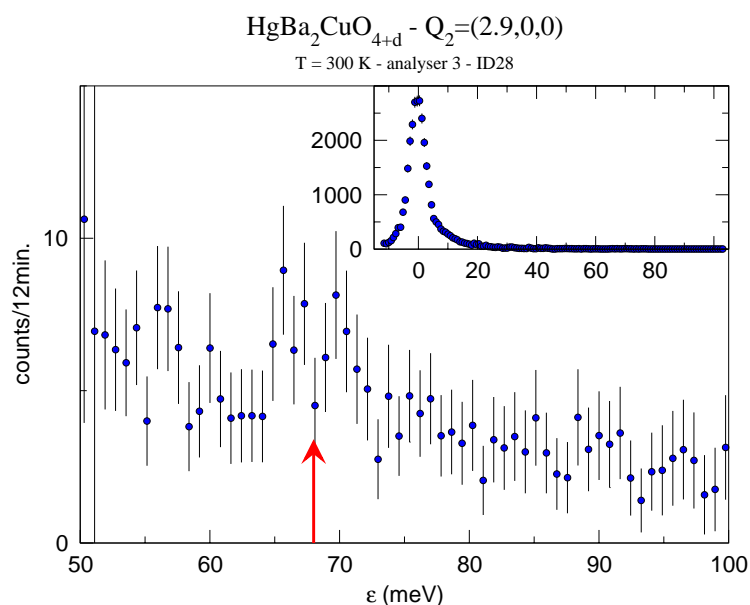
**Fig.1:**  
 $\text{Hg}_2\text{BaCuO}_{4+\delta}$  phonon dispersion along the main symmetry direction extracted from IXS spectra refinement. All the spectra were recorded on ID28 at room temperature. The line

*indicates a shell model calculation of the longitudinal modes.*

the high energy branches involve displacements of low  $Z$  oxygen and, partially, of copper ions, where the absorption is mainly due to high  $Z$  ions, as neodymium in [1] or mercury and barium in the present work. Therefore, after a first measurement with the vertical 3m spectrometer arm on ID16 at low resolutions (using Si(777) and Si(888) with about 8 and 6.6 meV resolutions), we decided to measure the phonon dispersion on ID28 using the higher  $Q$  and  $\omega$  resolution of the 6m arm, and therefore gain in the contrast between the low and the high energy excitations. However, with this set up, there is a loss in intensity due to the lower dynamical structure factor at lower  $Q$  (the ID28 6m arm is limited to  $50^\circ$ , compared to  $120^\circ$  of the vertical 3m arm on ID16), and to the reduced solid angle accepted by the analyser.

For a first investigation, we focus our attention on the low energy acoustical and optical modes, both longitudinal and transverse (See Fig. 1). Indeed, for these modes, the existing shell model [2], based of phonon density of state from INS, fails to calculate the dispersion for all the modes. In particular, the calculation gives instable transverse acoustical phonons. Therefore, using the present data, we are able to find a correct set of inter-atomic potential for the shell model.

This will give the possibility to have a reliable calculation of the phonon intensity in the different Brillouin zones, and therefore, it will be the starting point for forthcoming investigation on this compound on high energy LO phonon modes.



**Fig. 2 : IXS phonon spectrum, of Hg<sub>2</sub>BaCuO<sub>4+δ</sub>. The red arrow indicates the expected position of the high energy in plane LO mode near the zone centre.**

Moreover, a very low signal on the high energy LO phonons has been detected as shown in Fig. 2, which will permit us to plan for future experiments.

Indeed, with the support of this measurement and the calculation from the shell model, we will estimate the expected intensity, and plan the strategy for the next measurements.

The future experiments can benefit from using bigger samples (the present one was about the size of the beam spot), and from the present improving under commissioning of the beam-line ID28, aimed to increase the flux on the sample.

## References.

- [1] M. d'Astuto *et al.* *Phys. Rev. Lett.* **88** 167002 (2002).
- [2] B. Renker, *et al.* *J. Low Temp. Phys.* **105**, (1996) 843.