ESRF	Experiment title: Lattice dynamics in the novel Co-based superconductor $Na_xCoO_2 \cdot yH_2O$	Experiment number: HS2696
Beamline: ID-28	**Date of experiment**: from: 03/03/05 to: 13/03/05	**Date of report**: 29/07/05
Shifts: 32	**Local contact(s)**: A. Bossak	*Received at ESRF:*

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Report:

Na_xCoO_2 layered compounds have been under intensive scrutiny, since the recent discovery of superconductivity in the hydrated samples. The material consists of alternating layers of Na and CoO_2 planes, stacked along the c axis, in the hexagonal lattice [1]. During the hydration process, part of the Na content is reduced, while ice-like sheets are inserted in the structure, expanding the c axis. The precise nature of superconductivity is still a matter of debate, but various results points to a non-conventional character. From the point of view of superconductivity, weak or strong electron-phonon coupling also needs to be carefully investigated. In that context, probing lattice dynamics is of prime relevance.

We report here on the determination of phonon dispersion in hydrated (NCOH, x=0.7)) and non-hydrated (NCO, x=0.35) single crystals by inelastic x-ray scattering (IXS). The experiment was performed on the ID-28 beamline at ESRF. The IXS spectrometer was operated at 3 meV energy resolution, using the Si(999) reflection of the 5 crystal analyzers. To prevent dehydration, NCOH was mounted in a closed-cycle cryostat, and kept at low temperature (100 K) during the measurements. The crystals orientation was checked prior to measurements with the on-line CCD camera installed on the spectrometer horizontal arm, and the lattice parameters were estimated. The diffraction results, are consistent with those reported in the literature for both samples, and confirm that hydration of NCOH was preserved.

The phonon dispersion was measured along the Γ-M direction (longitudinal modes) and Γ-A direction (transverse modes) in both samples. Typical IXS spectra along Γ-M are illustrated in figure 1 (left) for the non-hydrated phase. The spectra show well defined phonons excitations with energies up to 80 meV, and dispersion is clearly observed. Low energy features (below 10 meV) are likely to be related to impurities in the sample – for instance close to zone boundary (1.5,0,0), where no low-energy phonon modes are expected. The spectra were systematically fitted by Lorenzian functions weighted by the Bose factor. The resulting phonon dispersion is represented in figure 1 (bottom right) for NCO.

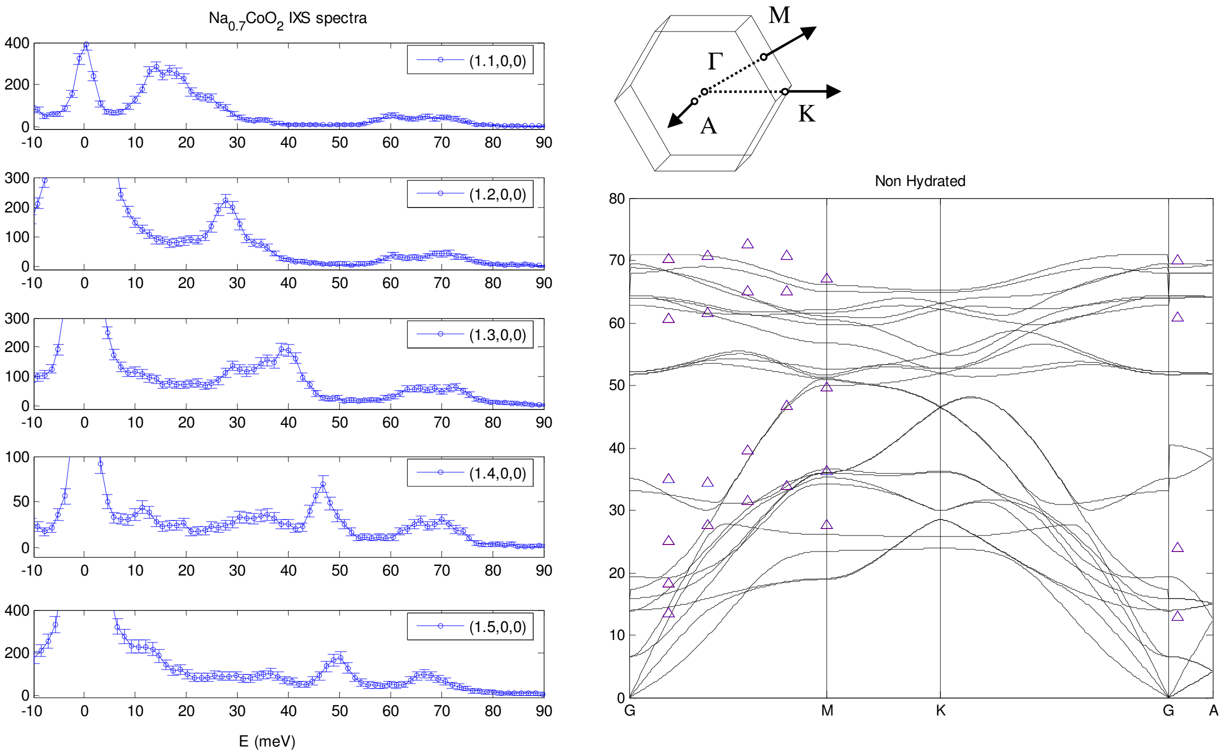

***Figure 1** : (Left) IXS spectra in NCO measured along the Γ-M direction; (top Righ): High symmetry directions in the hexagonal Brillouin zone; (bottom Right) Experimental (open symbols) and calculated (solid lines) phonon dispersion in NCO*

The experimental data are compared to first-principle calculations in the LDA approximation [2] carried out by M. Calandra at IMPMC (Paris). The number of electrons in the system was artificially reduced to account for the partial occupancy of the Na sites. The change in the negative charges is compensated by adding a positive background, which is uniformely distributed. The agreement with the experiment is excellent considering indeterminations in the measurements due to the finite q resolution and crystal mosaicity, and the complexity of the NCO electronic structure. The phonon dispersion in the hydrated sample, not shown here, differs mainly by the strong softening of the acoustic branch, visible in the 40-50 meV region along Γ-M in figure 1. This branch is mainly associated to longitudinal modes of the cobalt atoms, while the high-energy optic branches are associated to the oxygen atoms. This softening may be related to Fermi surface nesting, around ‘hole pockets’ that are supposed to form in the hydrated sample. The occurrence of hole pockets was first proposed in LDA band calculations [3]. But, their existence has not been experimentally confirmed yet, in particular not by photoemission [4], and is still a controversial issue. The confirmation of nesting vectors, responsible for electron phonon anomalies, would be a step forward in the understanding of the onset of superconductivity in NCO. Also, analysis is under way to estimate the electron-phonon coupling in both samples.

References :

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[2] P. Giannozzi et al, Phys. Rev. B, **43** , 7231 (1991)
[3] D. J. Singh, Phys. Rev. B **61**, 13397 (2000)
[4] M. Z. Hasan, Phys. Rev Lett. **92**, 246402 (2004)