In-plane anisotropy and temperature dependence of oxygen phonon modes in $YBa_2Cu_3O_{6.6}$

Lothar Pintschovius [a,1], Winfriedt Reichardt [a,b], Thomas Wolf [a], Marion Klaeser [a]

[a] *Forschungszentrum Karlsruhe, IFP, P.O.B. 3640, D-76021 Karlsruhe, Germany*
[b] *Laboratoire Léon Brillouin, CE-Saclay, F-91191 Gif-sur-Yvette Cedex, France*

Abstract

The dispersion of the Cu-O bond-stretching and bond-bending vibrations in $YBa_2Cu_3O_{6.6}$ has been studied by inelastic neutron scattering. While the behavior of the bond-bending vibrations can be well accounted for by a simple potential model, the bond-stretching vibrations show a highly anomalous behavior. The displacement pattern of the most anomalous phonons is in principle consistent with dynamic charge stripe formation. However, the pattern is rotated by 90 degrees to what was expected from the magnetic fluctuations reported in the literature. Temperature dependent measurements revealed only moderate changes of phonon frequencies between 12 K and 300 K.

Key words: phonons; stripes;$YBa_2Cu_3O_{6.6}$

1. Introduction

There is a large body of evidence that doping gives rise to a strong renormalization of high-energy Cu-O bond stretching modes in cuprate superconductors [1]. Recently, this phenomenon has attracted renewed interest because it possibly supports the hypothesis that the charge distribution in the Cu-O planes is inhomogeneous and in particular may take the form of metallic stripes [2]. Charge ordering in superconducting samples is assumed to be dynamic in nature and therefore cannot be detected by diffraction methods. Phonon measurements appear to be a promising technique because dynamic charge stripe formation should reveal itself by an anomalously low energy of phonons with an elongation pattern closely related to that produced by the dynamic charge structure. As the extra-charge residing on the stripes will modulate the Cu-O bond length, the Cu-O bond-stretching vibrations are expected to couple most strongly to the charge stripes. The present paper describes results of inelastic neutron scattering measurements on $YBa_2Cu_3O_{6.6}$ (O6.6) with the aim to clarify whether this compound exhibits phonon anomalies consistent with dynamic charge stripe formation as was reported earlier [3,4].

[1] Corresponding author. Present address: Forschungszentrum Karlsruhe, IFP, P.O.B. 3640, D-76021 Karlsruhe, Germany E-mail: pini@ifp.fzk.de

2. Experimental

The experiments were carried out on the 1T triple-axis spectrometer at the ORPHEE-reactor at Saclay. A Cu220-crystal was used as monochromator to achieve high resolution. Pyrolithic graphite was used as analyzer crystal. The sample was grown using the top-seed melt texturing method. Annealing led to a composition O6.6 (T_c = 60 K). The volume was 1.3 cm^3 and the mosaic spread was 1.3 degree. Some additional measurements were performed on a somewhat larger sample with an oxygen composition O6.2. High resolution in conjunction with a steep dispersion in the [0X0]-direction allowed us to assign high-energy phonon peaks to the [X00]- or to the [0X0]-direction though the sample was twinned.

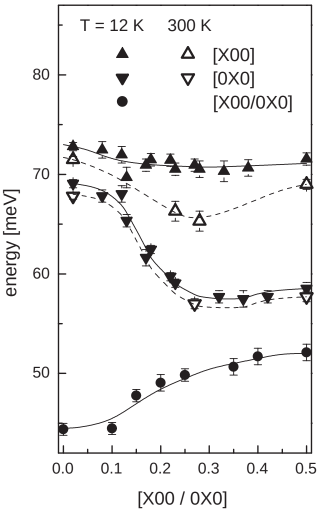

Fig. 1. Phonon dispersion of the Cu-O bond-stretching (E<55 meV) and of the Cu-O bond-bending (E>55 meV) modes in $YBa_2Cu_3O_{6.6}$ in the [X00]- and in the [0X0]-direction.The data shown refer to modes of Δ4-symmetry, i.e. to modes where the atoms in the Cu-O bi-layer vibrate in opposite phase. Lines are a guide to the eye only.

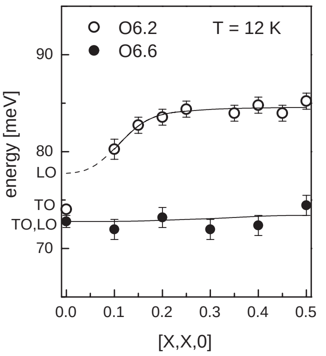

Fig. 2. Phonon dispersion of the Cu-O bond-stretching modes in the [XX0]-direction in insulating $YBa_2Cu_3O_{6.2}$ and in superconducting $YBa_2Cu_3O_{6.6}$. Note that there is an LO-TO splitting in the insulator but no such splitting in metallic $YBa_2Cu_3O_{6.6}$. Lines are a guide to the eye.

3. Results and Discussion

The Cu-O bond-bending modes were found to show an upward dispersion from the zone center to the zone boundary (Fig. 1) as is expected from shell-model calculations using an empirical potential model [5]. Moreover, no anomalous line broadening was observed for these modes in contrast to what has been reported in [3]. We note that this result does not speak against dynamic charge stripe formation in O6.6 because the bond bending modes are not expected to couple strongly to dynamic charge stripes because they do not involve a modulation of the Cu-O bond length.

On the other hand, the bond-stretching vibrations were found to show a highly anomalous behavior : a sharp drop of frequencies was observed on going from the zone center towards the zone boundary at wavevectors q about 0.2. This behavior was observed, however, only for the [0X0]-direction, whereas the corresponding branches in the [X00]- and in the [XX0]-direction are flat, at least at T = 12 K. We note that the displacement pattern of the softest modes around q = 0.25 is well suited for a strong coupling to dynamic charge stripes with a periodicity of 4 lattice constants, i.e. similar to the periodicity of the static stripes reported for $La_{1.6-x}Nd_{0.4}Sr_xO_4$ in [6]. We further note that the restriction of the phonon anomaly to just one direction matches the stripe picture as well : stripes are expected to extend along a particular crystallographic axis. However, the direction of the dynamic charge stripes inferred from our phonon results is in conflict with the direction concluded from the magnetic fluctuations in O6.6 observed by Mook et al. [4], i.e. the a-axis instead of the b-axis. Therefore, we do not think that the phonon anomaly observed in O6.6 can be considered as evidence of dynamic charge stripe formation.

In addition, the temperature dependence of the bond-stretching modes speaks against an interpretation of the phonon results in terms of the stripe picture : precursor effects of a structural phase transition depend in general strongly on temperature whereas the phonon anomaly observed in O6.6 does not. Surprisingly, the strongest temperature effect was found in the branch which shows a rather normal behavior at low temperatures but develops a sizeable dip at elevated temperatures.

Finally, we would like to point out that the steep drop of frequencies in the [0X0]-direction around X = 0.2 is a very conspicuous feature but that the flat branches in the [x00]- and in the [XX0]-direction are renormalized with respect to the insulating parent compound as well (see Fig.2).

In conclusion, the phonon anomaly observed in O6.6 is evidence of a strong electron-lattice coupling but can hardly be seen as evidence for dynamic charge stripe formation.

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