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TITLE: LO PHONONS IN $La_{1.85}Sr_{.15}CuO_4$

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AUTHOR(S): T. Egami, Dept of Materials Science and Engineering, Univ of Pennsylvania
R.J. McQueeney, LANSCE-12
Y. Petrov, Dept of Physics and Astronomy, Univ. of Pennsylvania
M. Yethiraj, Oak Ridge Natl. Lab
G. Shirane, Dept. of Physics, Tohoku Univ. Sendai Japan
Y. Endoh, Dept. of Physics, Tohoku Univ. Sendai Japan

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LO Phonons in $La_{1.85}Sr_{.15}CuO_4$

T. Egami[a], R. J. McQueeney[b], Y. Petrov[c], M. Yethiraj[d], G. Shirane[e] and Y. Endoh[f]

[a]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA 19104, USA, [b]Los Alamos National Laboratory, Los Alamos, NM 87545, USA, [c]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA, [d]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, [e]Brookhaven National Laboratory, Upton, NY 11973, USA, [f]Department of Physics, Tohoku University, Sendai 980, Japan.

Abstract

Dispersion of the highest energy LO phonons in $La_{1.85}Sr_{.15}CuO_4$ was studied by neutron inelastic scattering. At $T = 10$ K the dispersion along (h, 0, 0) is anomalous, forming two dispersionless branches with a discontinuity at $h = 1/4$. A possible relation of this anomaly to the spin-charge stripes will be discussed.

When a mother compound of a superconducting cuprate is doped with carriers, the high energy LO phonons around the half-breathing mode at the ($h = 0.5$, $k = 0$, $l = 0$) point show significant softening [1]. In order to study the dispersion around this mode, inelastic neutron scattering measurements were carried out with the HB3 triple-axis spectrometer of the HFIR, Oak Ridge National Laboratory, on a pair of single crystals $La_{1.85}Sr_{.15}CuO_4$ that were used in the earlier measurements [2,3]. A Be monochromator, a graphite analyzer, the collimation of 48'-40'-80'-120', a graphite filter and the final energy of 14.87 meV were used. We focused on the LO branch (3.0 - 3.5, 0, 0) in the tetragonal indices [4] (x (h) is parallel to the Cu-O bonds in the plane). This branch is relatively free of spurious peaks, while the LO branch ($h = 4.5 - 5.0$) that was studied earlier [2] is hampered by a strong spurious peak near (4.65, 0) and 75 meV due to the Bragg scattering from the sample being incoherently scattered by the analyzer.

The intensity map made of the energy scans at $h = 3.2$, 3.25, 3.3, 3.35, 3.4, and 3.5 at T = 10 K is shown in Fig. 1. The split of the low energy branch at 70 meV and the high energy branch at 84 meV with the discontinuity around $h = 3.25$ is clearly seen. In the earlier measurement the spurious peak mentioned above was located in the middle of the gap and misled us to think that the phonon width became very wide around this point [5]. Such a discontinuity has actually been observed for $YBa_2Cu_3O_7$ [1], and for $Ba_{0.6}K_{0.4}BiO_3$ [6], but not in $La_{1.85}Sr_{.15}CuO_4$ for which the earlier measurement was made at $l = 1$ to avoid the spurious peak [1]. The most important finding here, however, is that this anomalous split is observed only in a small Q space, near $k = 0$. Outside this zone a normal continuous dispersion is observed. Figure 2 shows a set of scans along k, at $\hbar\omega = 70$ meV and T = 10 K.

The rapid decrease in the intensity away from $k = 0$ indicates that the width of the 70 meV branch is only about $\Delta k \sim 0.2$, which is twice the resolution in Q_y, and corresponds to the coherence length of 20 Å. It is of great interest to see if the same applies for $YBa_2Cu_3O_7$ and $Ba_{0.6}K_{0.4}BiO_3$.

The dispersionless branch at 70 meV that covers a small Q space, with $\Delta h \sim 0.5$ and $\Delta k \sim 0.2$, represents nearly localized phonons. If a wave packet is formed with all the phonons in this region (a la Wannier function) it will cover the real space of $2a \times 5a$, or 8×20 Å^2. Since the energy of the high energy branch corresponds to that of the undoped LO phonon (84 meV at the (0, 0) point [1]), it is reasonable to assume that the low energy branch is associated with the presence of the doped holes. A possible explanation is that the doped holes are not uniformly distributed, but are segregated in an area of $2a \times 5a$, and the 70 meV branch is the localized phonon in such areas. The 84 meV phonon should cover outside these regions. Thus the hole rich regions could be the pieces of the dynamic spin-charge stripes hypothesized earlier [7]. However, at this moment no information exists for the connectivity of these regions, so that it is premature to call them stripes. If we use the linear charge density of 0.5 per unit cell deduced from the static stripes in $La_{1.475}Nd_{0.4}Sr_{0.125}CuO_4$ [7], the hole rich region ($5a$ long) would have 2.5 holes inside it, appearing very much like a bipolaron. The width of $2a$ suggests that two Cu-O chains are involved, and the half-breathing (0.5, 0) phonon would make the two Cu-O chains alternately favored for charges to occupy to form a vibronic state. Thus it is possible that the anomalous dispersion observed here is related to the charge stripes in the cuprates and even to their superconductivity.

Acknowledgments

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References:

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Figure captions:

Fig. 1. The intensity map as a function of h and phonon energy $\hbar\omega$. The scale is linear, with 12 counts per step. The sharp line at 85 meV, $h = 3.3 - 3.5$, is due to a spurious peak. The discontinuity at $h = 3.25$ between the 70 meV branch and the 84 meV branch is clearly seen.

Fig. 2. Scans along k at $\hbar\omega = 70$ meV at various values of h. The width (FWHM ~ 0.2) corresponds to the coherence length of 20 Å.

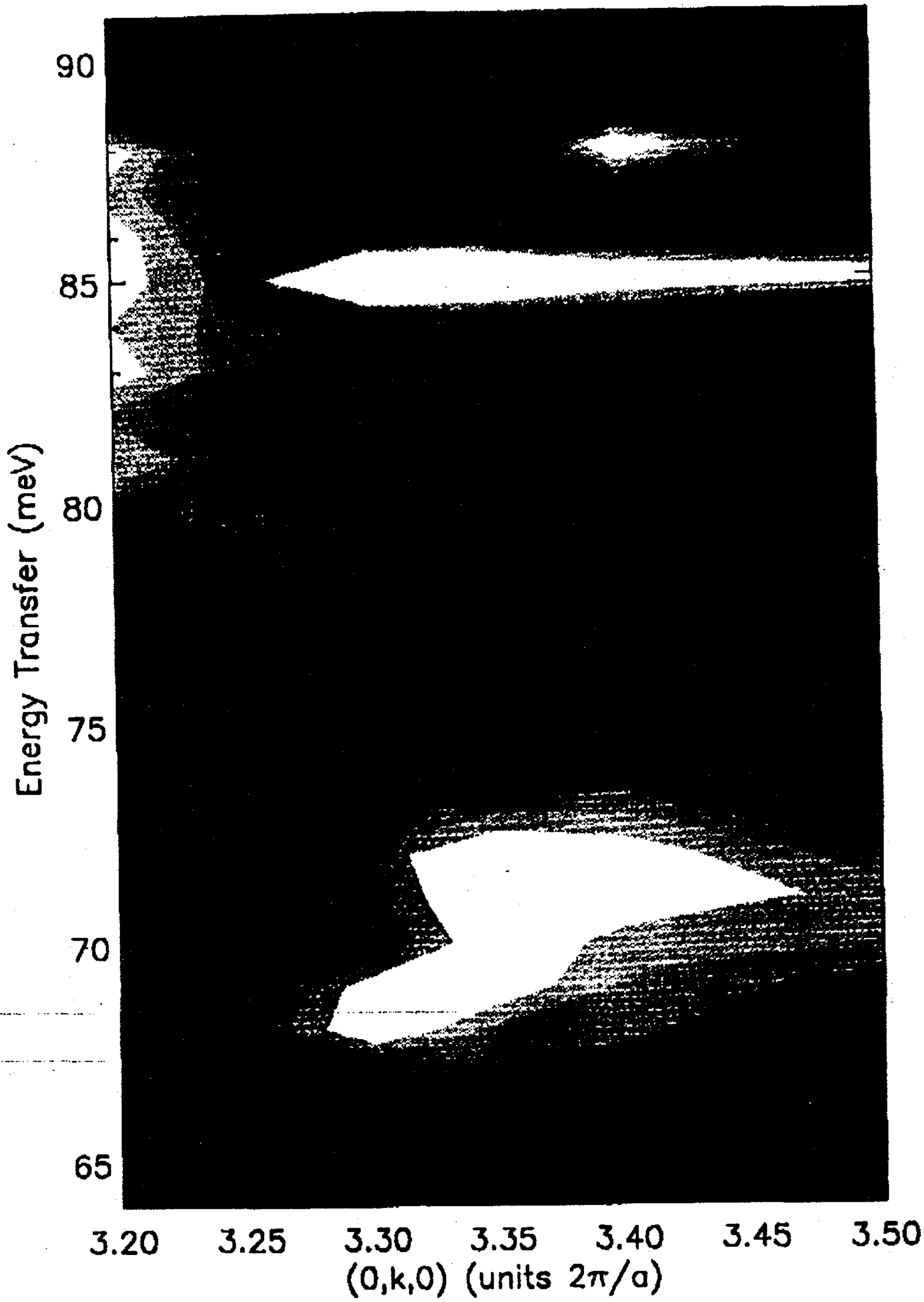
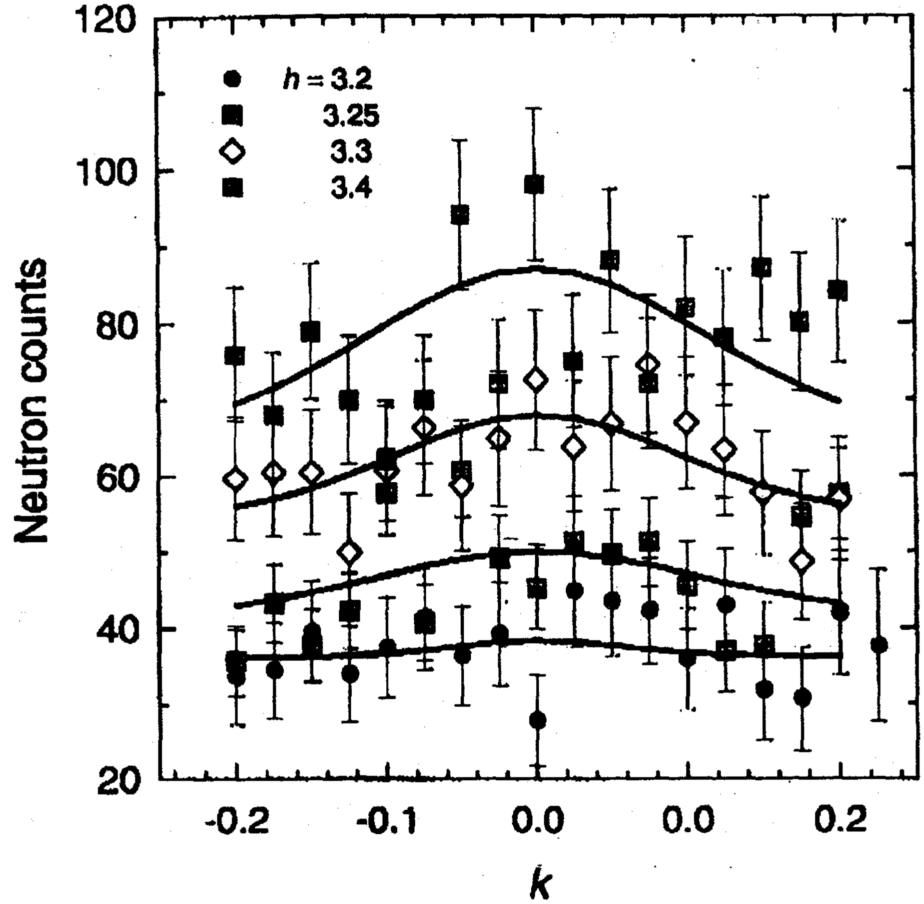

90
85
80
75
70
65
Energy Transfer (meV)
3.20
3.25
3.30
3.35
3.40
3.45
3.50
(0,k,0) (units 2π/a)

Fig. 1



Neutron counts
120
100
80
60
40
20
h = 3.2
3.25
3.3
3.4
-0.2
-0.1
0.0
0.0
0.2
k