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High Resolution Inelastic Neutron Scattering Study of Phonon Self-Energy Effects in YBCO.

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We report preliminary results of the high resolution inelastic neutron scattering measurements of the 42.5 meV optical phonon branch in YBCO, whose behavior at momentum transfer q=0 has been extensively studied by Raman scattering. The experiment was done on a large (75g) single crystal of $YBa_2Cu_3O_{7-x}$ (T_c~90K) with the resolution of 2 meV (full width at half maximum). In cooling from 100K to 50K we observe a small softening of the phonon energy at q=0.25,0.25,0, but no significant linewidth change.

It is well known that phonon self-energy effects in superconductors provide information about electron-phonon coupling and the magnitude and the phase of the superconducting energy gap.[1-3] Electronic contribution to the phonon self-energy is proportional to the electron-phonon coupling strength and $P(\mathbf{q},\omega)$ (the electronic polarizability at the phonon momentum $\mathbf{q}$ and energy ω). $Im(P(\mathbf{q},\omega))$ is proportional to the probability of electronic transitions with $\mathbf{q},\omega$. It contributes to the phonon linewidth, whereas $Re(P(\mathbf{q},\omega))$, (related to $Im(P(\mathbf{q},\omega))$ by a Kramers-Kronig transformation) renormalizes the peak position. In superconductors, a gap 2Δ in the density of electronic states opens below T_c, with a pileup above 2Δ, which results in changes in the phonon linewidth and the peak position, if $\omega \approx 2\Delta$. These effects depend on the topology of the Fermi surface and the phase and the magnitude of 2Δ as a function of the Fermi momentum. In $YBa_2Cu_3O_{7-x}$, broadening of the phonon linewidth (compared to the normal state) is expected in the (xx0) q-space direction if the phonon energy is just above the superconducting gap for an s-wave pairing state, and narrowing is expected for a d-wave state.[2] The most extensive study of the phonon self-energy effects has been done by Raman scattering, which is limited to the zone center.[4] The 42.5 meV phonon shows the strongest effects, presumably because its energy is close to 2Δ.[5] K. Pyka et. al. measured the temperature dependence of its peak position away from the zone center in $YBa_2Cu_3O_{7-x}$ in the (x00)/(0x0) directions by inelastic neutron scattering.[6]

We report preliminary results of the first high resolution inelastic neutron scattering measurements sensitive to linewidth of the 42.5 meV optical phonon branch.

The experiment was done on a large (75g) single crystal of $YBa_2Cu_3O_{7-x}$ (T_c~90K) with the resolution of 2meV full width at half maximum (FWHM). This resolution enabed us to probe the intrinsic linewidth, which according to the Raman results is 2-3meV. The mosaic of the largest domain (~70% of the crystal) was 2° with some smaller domains as far as 5° from the

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main domain. Our measurements were performed on the BT4 triple-axis spectrometer at the neutron Beam Split-core Reactor (NBSR) at NIST.

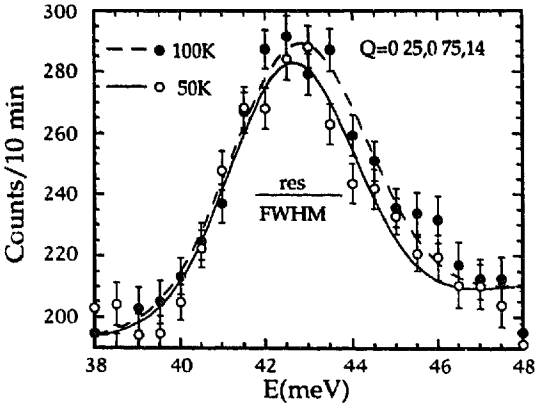

Figure 1. The 42.5meV phonon in $YBa_2Cu_3O_{7-x}$ at q=(0.25,0.25,0)

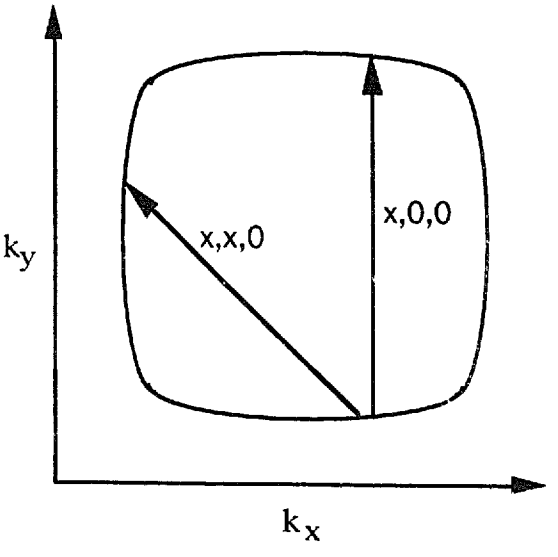

Figure 2. Schematic of the copper oxygen plane Fermi surface in $YBa_2Cu_3O_{7-x}$. Arrows represent electronic transitions in the (0x0) and (xx0) directions.

The 42.5 meV phonon was measured at q=(0.25,0.25,0) at 100K and 50 K (see Fig. 1). In cooling from 100K to 50K we observe a small softening of the phonon energy (by ~0.18±0.13 meV) but no significant linewidth change within the experimental sensitivity. Work currently in progress should clarify the exact temperature evolution of the linewidth and peak position of the 42.5 meV phonon branch in YBCO along the (x00)/(0x0) and (xx0) directions.

According to Ref. 6 softening of the same phonon in the (x00)/(0x0) direction around x=0.25 is 0.5 meV.[6] Our data show that the effect in the (xx0) direction is much weaker.

Fig. 2 shows the diagram of the Fermi surface in $YBa_2Cu_3O_{7-x}$[7] and the electronic transitions which, along with their Umclapp counterparts, contribute to the phonon self-energy. It is clear that there are more electronic states available for the decay of the (x00) phonon than of the (xx0) phonon, which might explain why the softening of the latter is smaller.

The preliminary results show that the 42.5 meV phonon in $YBa_2Cu_3O_{7-x}$ softens by ~0.18 meV at q=(0.25,0.25,0) from 100 to 50K. Smallness of the effect might be due to the lack of nesting in the (xx0) direction.

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