Resonant Raman Study of Superconducting Gap and Electron-Phonon Coupling in YbBa$_2$Cu$_3$O$_{7-\delta}$

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We investigate the electronic background as well as the O2-O3 mode at 330 cm$^{-1}$ of highly doped YbBa$_2$Cu$_3$O$_{7-\delta}$ in $B_{1g}$ symmetry. Above the critical temperature $T_c$ the spectra consist of an almost constant electronic background and superimposed phononic excitations. Below $T_c$ the superconducting gap opens and the electronic background redistributes exhibiting a $2\Delta$ peak at 320 cm$^{-1}$. We use a model that allows us to separate the background from the phonon. In this model the phonon intensity is assigned to the coupling of the phonon to inter- and intraband electronic excitations. For excitation energies between 1.96 eV and 2.71 eV the electronic background exhibits hardly any resonance. Accordingly, the intraband contribution to the phonon intensity is not affected. In contrast, the interband contribution vanishes below $T_c$ at 1.96 eV while it remains almost unaffected at 2.71 eV.

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The Fano-type line shape of the $B_{1g}$ mode in Raman experiments in the $R$Ba$_2$Cu$_3$O$_7$ ($R$-123) system with $R$=rare earth or yttrium has been subject of several investigations. Using extended Fano models like those presented by Chen et al. and Devereaux et al. the self-energy contributions to the phonon parameters as a consequence of the interaction of the phonon with low-energy electronic excitations can in principle be obtained. Moreover, a measure of the electron-phonon coupling and the “bare” phonon intensity, i.e., the one resulting from a coupling to interband excitations, can be estimated from a detailed analysis of the Raman spectra. Therefore, a simultaneous description of the real and the imaginary part of the electronic response function $\chi^e(\omega) = R^e(\omega) + i\delta^e(\omega)$ of the intraband excitations
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is needed. Such a description has recently been presented by us and applied to Ca- and Pr-doped Y-123-films. Here, we will use our description in order to investigate the different contributions to the $B_{1g}$ phonon intensity in overdoped YbBa$_2$Cu$_3$O$_7$ (Yb-123) and their resonance properties as well as the resonance of the pair-breaking peak ($2\Delta$ peak) in $B_{1g}$ symmetry.

We study a fully oxygenated high-quality Yb-123 single crystal grown with a self flux method. Due to the high oxygen content and the small rare earth ion radius, the crystal is overdoped ($T_c=76$ K). $B_{1g}$ Raman spectra $[z(x',y')\bar{z}$ in Porto notation $]$ have been taken using laser lines at 458, 514, and 633 nm (2.71, 2.41, and 1.96 eV) in a setup described elsewhere. They have been corrected for the spectral response of spectrometer and detector. For a comparison of the spectra obtained with different excitation energies the cross-section is calculated from the efficiencies using ellipsometric data of Y-123. All given temperatures are actual spot temperatures with typical heatings between 5 K and 15 K. In order to describe the line shape of the $B_{1g}$ phonon we subdivide the Raman cross-section $I_c(\omega)$ into a sum of the electronic response $\rho(\omega)$ and an electron-phonon interference term $I_p(\omega)$:

$$I_p(\omega) = \frac{C}{\gamma(\omega)(1+\epsilon^2(\omega))} \times \frac{R^2_{tot}(\omega) - 2\epsilon(\omega)R_{tot}(\omega)\rho(\omega) - \rho^2(\omega)}{C^2}. \quad (1)$$

The constant $C = A\gamma^2/g^2$ is a parameter for the intensity where $\gamma$ represents the symmetry element of the electron-phonon vertex projected out by the measurement geometry and $g$ is the lowest order expansion coefficient of the electron-phonon vertex describing the coupling to non-resonant intraband electronic excitations. $R(\omega) + i\rho(\omega) = Cg^2\chi^{\varepsilon}(\omega)$ is the electronic response in the measured units. While $\rho(\omega)$ can be obtained directly from the spectra, $R(\omega)$ has to be calculated via a Hilbert transformation. $R_{tot}(\omega) = R(\omega) + R_0$ with $R_0 = Cg(gpp/\gamma)$ where $g_{pp}$ is an abbreviated “photon-phonon” vertex that describes the coupling to resonant interband electronic excitations. The renormalized phonon frequency $\omega_p(\omega)$ and linewidth $\gamma(\omega)$ are given by $\omega^2_p(\omega) = \omega^2_p - 2\omega_pR(\omega)/C$ and $\gamma(\omega) = \Gamma + \rho(\omega)/C$, respectively, and $\epsilon(\omega) = [\omega^2 - \omega^2_p(\omega)]/[2\omega_p\gamma(\omega)]$. The bare phonon intensity $I_{pp}$ resulting from the coupling to interband excitations is given by $I_{pp} = \frac{\pi}{2}R_0^2$ (Ref. 4). The imaginary part of the measured electronic response (background) is modeled by two contributions $I_\infty \tanh(\omega/\omega_T)$ and $I_{\text{red}}(\omega,\omega_\Delta,\Gamma_\Delta,\omega_\Delta,\omega_\Delta,\omega_\Delta)$. The first term describes the incoherent background with a crossover frequency $\omega_T$ and the second the redistribution below $T_c$ using two Lorentzians, one is centered at the $2\Delta$ peak with the intensity $I_{2\Delta}$ and the other, proportional to $I_{supp}$, describes the suppression between $\omega = 0$ and $\omega = 2\Delta$. Figure (a) displays the $B_{1g}$ cross-section of Yb-123 at 20 K obtained
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with $\hbar \omega_i = 2.71$ eV as well as its description. For the description we use Eq. (1) for the $B_{1g}$ phonon and the Ba mode, Lorentzians for all other modes, and the background contributions stated above. The description yields a 2\Delta peak at $\approx 320 \text{ cm}^{-1}$. Assuming that the background is not resonant, a calculated spectrum with vanishing bare phonon intensity ($R_0 = 0$) for the $B_{1g}$ phonon is drawn in Fig. 1 (b), where other phonons are dropped for clarity. We compare this calculation to the cross-section obtained with $\hbar \omega_i = 1.96$ eV and 20 K and find a good agreement.

Results of the analysis of the $B_{1g}$ phonon line shape for measurements with $\hbar \omega_i = 2.71$ eV are shown in Fig. 2. It turns out that the strong broadening as well as the slight softening of the renormalized phonon can entirely be assigned to the redistributing background leaving anharmonic decays for the bare phonon parameters. As we obtained similar result with $\hbar \omega_i = 2.41$ eV we used a fixed parameter set $\Gamma(T)$, $\omega_p(T)$ for all excitation energies. This is especially important for the spectra recorded with $\hbar \omega_i = 1.96$ eV, where the decreasing or even vanishing bare phonon intensity hinders a reliable determination of the phonon parameters.

The upper panels of Fig. 3 display the peak height of the 2\Delta peak obtained with our description of the electronic background. Obviously, the 2\Delta peaks vanish above $T_c$. The remaining peak intensity above $T_c$ for $\hbar \omega_i = 2.71$ eV is just a compensation of a slightly underestimated electron-phonon coupling. Below $T_c$ the intensities increase in a monotonic fashion saturating, more or less pronounced, at low temperatures. With respect to the resonance properties of the 2\Delta peak we find a decreasing intensity with decreasing excitation energy. This partly explains the discrepancy between the calculated and the measured cross-sections shown in Fig. 1 (b). The energy of the 2\Delta peak decreases only slightly with increasing temperature from $\approx 310 \text{ cm}^{-1}$ at 30 K down to $\approx 260 \text{ cm}^{-1}$ at 70 K.

Regarding the temperature dependencies of the bare phonon intensity $I_{pp}$ in Fig. 3 we find similar behavior for the data sets obtained with $\hbar \omega_i = 2.71$ eV and 2.41 eV. They exhibit a slight decrease with decreasing temperature being not affected by $T_c$. In contrast, we find a dramatically decreasing intensity with $\hbar \omega_i = 1.96$ eV below $T_c$. The overall decrease of $I_{pp}$ for $T > T_c$ with decreasing excitation energy is similar to the behavior of $I_{2\Delta}$ for $T \rightarrow 0$, however, more pronounced.

The sudden drop of $I_{pp}$ below $T_c$ for $\hbar \omega_i = 1.96$ eV suggests a superconductivity-induced closing of the resonant excitation channel of the phonon. For even lower excitation energies $I_{pp}$ vanishes almost completely for $T \rightarrow 0$ as we have observed with $\hbar \omega_i = 1.71$ eV and 1.58 eV. Above $T_c$, however, the decreasing intensity with decreasing excitation energy appears to continue monotonically. This suggests that more fundamental changes
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of the band structure take place below $T_c$. They will most likely appear around the van Hove singularity at $(\frac{\pi}{a},0)$ where the electron-phonon coupling is enhanced.³ It remains open at present how far the band structure changes inferred from our data are related to the anomalies around 2 eV observed in thermal-difference reflectance spectroscopy,¹¹ or to the missing spectral weight deduced from a sum-rule type analysis of c-axis optical conductivity data.¹²

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Fig. 1.
(a) $B_{1g}$ Raman cross-section $I_c(\omega)$ at $T=20$ K obtained with $\hbar\omega_i = 2.71$ eV (dots) and description (thin solid line). The background (dashed line) and phononic contributions ($B_{1g}$ mode: thick solid line, other phonons: dotted line) are also given. (b) Calculation of the cross-section with vanishing bare phonon intensity for the $B_{1g}$ phonon (solid line) and comparison with the cross-section obtained with $\hbar\omega_i = 1.96$ eV (dots) at 20 K. Inset: Efficiencies of the Raman spectra at 700 cm$^{-1}$ (dots) in comparison with a calculation (solid line) according to ellipsometric data.

Fig. 2.
Bare (solid circles) and renormalized (open circles) frequency and linewidth of the $B_{1g}$ phonon for spectra recorded with $\hbar\omega_i = 2.71$ eV. Solid lines are fits to anharmonic decays for the data above $T_c$ (dashed line).

Fig. 3.
Temperature dependence of the peak height $I_{2\Delta}$ and of the bare phonon intensity $I_{pp}$ for $\hbar\omega_i = 2.71$, 2.41 and 1.96 eV. The dashed lines indicate $T_c$. 