Optical studies of charge dynamics in optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$

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Systematic temperature-dependent optical studies of optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (OP Bi2212) single crystals have been carried out. An electron-boson spectral function peaked at 43 meV is derived in the normal state at 100 K, indicating that the most significant spectral feature in OP Bi2212 is a resonance at 43 meV. The optical data below T_c show that this boson is directly involved in the pair formation in OP Bi2212. Origins of the 43 meV mode are discussed.

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For Bardeen-Cooper-Schrieffer (BCS) superconductors, the spectral function $\alpha^2F(\omega)$ contains all the relevant information concerning superconductivity.[1] Experimentally, $\alpha^2F(\omega)$ is commonly obtained from tunneling *I-V* curves using the well-developed Eliashberg theory.[2] In principle the optical conductivity can also be used to determine $\alpha^2F(\omega)$ for BCS superconductors.[3–5] Recently, it has been recognized that the same kind of analysis of the optical data can give rise to a spectral function $W(\omega)$ for *d*-wave high-T_c superconductors.[6] This has led to the conclusion that electron coupling to the spin fluctuations[7] may be the analog to the common electron-phonon interaction in BCS superconductors. The issue of electron-boson coupling in high-T_c cuprates has attracted much attention recently particularly due to the suggestion of strong electron-phonon interactions in these systems.[8] We will take a more empirical approach to discuss the experimental evidence of electron-boson coupling using optical data for different high-T_c superconductors.[9]

In this paper, we report a detailed analysis of the electron-boson interaction in optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (OP Bi2212) using new optical data. A bosonic spectral function peaked at 43 meV is identified in the normal state at 100 K. The optical data below T_c suggest that this 43 meV boson is directly involved in pair formation in OP Bi2212. The possibility of a resonant interaction of the spin resonance at 43 meV with a 44 meV phonon below T_c is discussed.

The *ab*-plane optical reflectance of OP Bi2212 has been measured previously.[10] However our systematic optical studies, with $E\|a$, b, and c axes, have revealed many new features. Large OP Bi2212 single crystals are grown using the floating-zone method for this work and the crystals are mounted on an optically black cone. The polarized reflectance from 6 K to 295 K is measured in a near-normal incidence arrangement from ≈ 30 to over 20 000 cm^{-1} on a Bruker IFS 66v/S. The absolute reflectance is determined by evaporating a gold film *in situ* in vacuum ($\approx 1 \times 10^{-8}$ Torr) over the sample.[11] The optical properties are determined from a Kramers-Kronig analysis.

In Fig. 1, raw optical data are shown for an OP Bi2212 single crystal. With $E\|a$ axis, two in-plane optic phonons at 473 and 613 cm^{-1} have been observed in reflectivity measurements. The temperature-dependent reflectance is given in Fig. 1(a) from about 100 to 2000 cm^{-1}, and the optical conductivity $\sigma_1(\omega)$ is presented in Fig. 1(b). The optical conductivity is quite isotropic in the *ab* plane for OP Bi2212; however, large phonon anisotropy is observed as shown in the inset of Fig. 1 at 295 K. Particularly, the 473 cm^{-1} phonon is absent for $E\|b$ axis while a new mode appears at 350 cm^{-1} or 44 meV. In addition, ten *c*-axis infrared-active phonons are observed instead of the $6A_{2u}$ phonons that are predicted by the D_{4h} space group for OP Bi2212.[12] A more detailed theoretical analysis is needed to account for these new experimental findings.

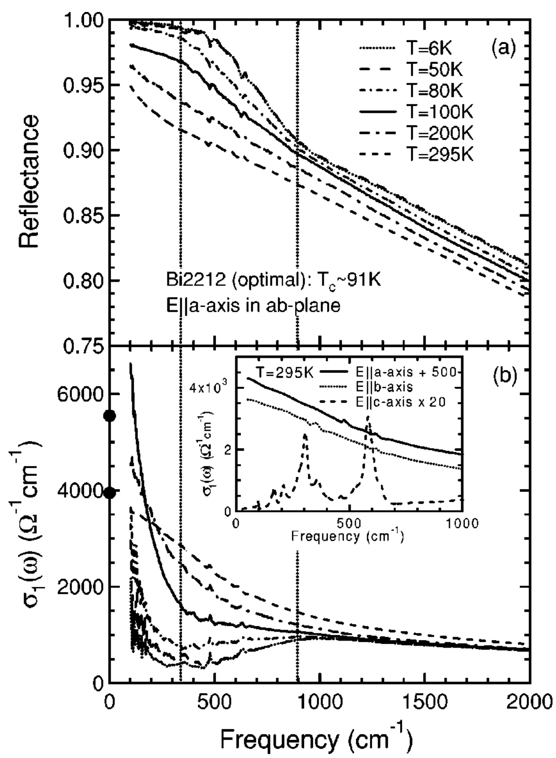

FIG. 1. The temperature-dependent *ab*-plane optical data of an OP Bi2212 single crystal with the $E\|a$ from 100 to 2000 cm^{-1}. (a) The temperature-dependent reflectance and (b) the temperature-dependent $\sigma_1(\omega)$. [The dots at zero frequency correspond to dc resistivity measurements at 200 K and 295 K, respectively. The two vertical lines at 339 cm^{-1} (42 meV) and at 893 cm^{-1} (111 meV) serve as guides to the eye.] Inset: $\sigma_1(\omega)$ at 295 K for different polarizations ($E\|a$ curve is offset for clarity).

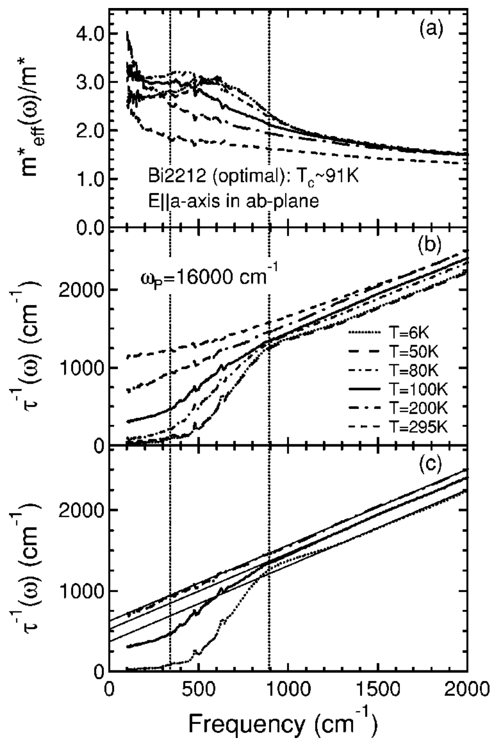

FIG. 2. The analysis of the ab-plane optical data of an OP Bi2212 single crystal with the $E\|a$ from 100 to 2000 cm^{-1}. (a) The temperature-dependent mass ratio, (b) the temperature-dependent $\tau^{-1}(\omega)$, and (c) $\tau^{-1}(\omega)$ is analyzed at 6, 100, and 200 K.

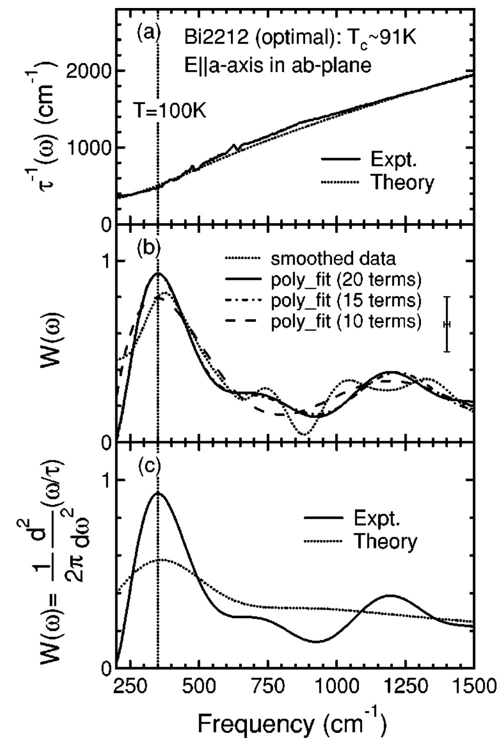

FIG. 3. An unambiguous method of extracting the spectral function $W(\omega)$. (a) The experimentally $\tau^{-1}(\omega)$ at 100 K for OP Bi2212, together with the theoretical calculation, (b) experimentally determined $W(\omega)$ using different methods (error bar for the derivative analysis is included), and (c) a comparison of experimentally and theoretically determined $W(\omega)$.

The conductivity data is analyzed in the extended-Drude formalism[13] with a frequency-dependent scattering rate $\tau^{-1}(\omega)$ and a mass ratio that are defined as

$$\tau^{-1}(\omega)=\frac{\omega_p^2}{4\pi}\mathrm{Re}\left[\frac{1}{\tilde{\sigma}}\right], \quad \frac{m^*_{eff}}{m^*}=\frac{\omega_p^2}{4\pi\omega}\mathrm{Im}\left[\frac{1}{\tilde{\sigma}}\right], \qquad (1)$$

where ω_p is the classical plasma frequency. The value of $\omega_p=16\,000$ cm^{-1} is derived from the optical conductivity sum rule at 295 K. The results of such an analysis are given in Fig. 2. The temperature-dependent mass ratio is shown in Fig. 2(a) and the scattering rate $\tau^{-1}(\omega)$ in Fig. 2(b). The frequency-dependent scattering $\tau^{-1}(\omega)$ contains all the relevant information concerning the electron-boson interaction.[3–5] Because of the unprecedented signal-to-noise ratio (≈ 1000) of these optical data, important new features in $\tau^{-1}(\omega)$ are observed for OP Bi2212 as highlighted in Fig. 2(c). The high-frequency part of $\tau^{-1}(\omega)$ is fitted with a straight line and the slopes of these linear fits are almost identical for different temperatures. At 200 K, $\tau^{-1}(\omega)$ increases linearly with frequency. However, deviations from this linear behavior are observed as a suppression of $\tau^{-1}(\omega)$ at low frequencies above T_c at 100 K and an "overshoot" of $\tau^{-1}(\omega)$ at around 900 cm^{-1} below T_c at 6 K. The overshoot of $\tau^{-1}(\omega)$ in OP Bi2212 is very similar to what has been observed in OP YBCO (Ref. 14) and this overshoot has been argued to be the key evidence for boson-mediated superconductivity.[15] Even though the suppression of $\tau^{-1}(\omega)$ in the normal state has often been interpreted in terms of a pseudogap,[13] it is more natural to explain the observed suppression of $\tau^{-1}(\omega)$ at 100 K here as due to electron-boson coupling. In fact, given that the pseudogap in high-T_c cuprates may have a spin origin, these two interpretations are consistent with each other.

The electron-boson interactions can be studied using $\tau^{-1}(\omega)$ in more detail. Carbotte *et al.*[6] and Abanov *et al.*[7] analyzed $\tau^{-1}(\omega)$ in high-T_c cuprates by defining a spectral function $W(\omega)$ using the Allen formula

$$W(\omega)=\frac{1}{2\pi}\frac{d^2}{d\omega^2}\left[\frac{\omega}{\tau(\omega)}\right]. \qquad (2)$$

It was first pointed out by Allen[3] that $W(\omega)$ is closely related to the electron-phonon spectral function $\alpha^2F(\omega)$ or any other electron-boson spectral function in the normal state for $T=0$ and in the weak-coupling limit. Shulga[15] rederived the Allen formula in the strong-coupling case and in general for $T>0$ the electron-boson spectral function is broadened.[5] On these theoretical bases, analyzing $\tau^{-1}(\omega)$ at 100 K in OP Bi2212 using Eq. (2) in terms of a bosonic spectral function is both mathematically and physically valid.

In Fig. 3 a unique way of extracting the spectral function $W(\omega)$ from the experimental data is presented. The measured $\tau^{-1}(\omega)$ at 100 K is plotted for OP Bi2212 in Fig. 3(a), together with the theoretical curve for $\tau^{-1}(\omega)$ calculated using a model developed by Schachinger and Carbotte.[16] In Fig. 3(b), the spectral function $W(\omega)$ derived from different methods using Eq. (2) is plotted. The $W(\omega)$ determined from the smoothed ω/τ gives a similar spectrum with a maximum at 350 cm^{-1} or 43 meV determined from the polynomial fits. However, in this study fitting the measured quantity ω/τ with a high-order polynomial is adopted as the unambiguous method of extracting $W(\omega)$ from the optical data. In Fig. 3(c), the experimentally and theoretically derived $W(\omega)$ functions are compared and both spectral functions contain a peak at 43 meV. It should be emphasized that this $W(\omega)$ function determined experimentally using Eq. (2) is an approximate one but it qualitatively captures the key features of the true electron-boson spectral function. The main experimental finding is that the suppression of $\tau^{-1}(\omega)$ at low frequencies at 100 K is the result of an electron-boson spectral function peaked around 43 meV.

To demonstrate that this 43 meV boson in OP Bi2212 is relevant to superconductivity, one has to invert the optical data below T_c. However, this is a complicated procedure for d-wave high-T_c cuprates. A formal inversion of the optical data below T_c is beyond the scope of this experimental work. Fortunately, a simplified visual accessibility procedure is devised by Shulga[15] for "by eye" analysis of the raw optical data below T_c in terms of electron-boson coupling. In particular, he showed that the ratio of the $\tau_s^{-1}(\omega)/\tau_n^{-1}(\omega)$ will exhibit a maximum and the ratio of $R_s(\omega)/R_n(\omega)$ will have a minimum near the frequency of $2\Delta+\Omega_{max}$, where Δ is the superconducting gap maximum and Ω_{max} is the maximum of the electron-boson spectral function.[15] This is because the coherent scattering rate below T_c grows faster than in the normal state, thereby producing an "overshoot" in $\tau_s^{-1}(\omega)$ which peaks at around $2\Delta+\Omega_{max}$. In Fig. 4(a), such ratios of the reflectance and the scattering rate are given for OP Bi2212. Interestingly, the phonon at 44 meV which is absent above T_c with $E\|a$ axis becomes infrared active below T_c as shown clearly in the scattering rate ratio in Fig. 4(a) and it has much larger linewidth compared to the other two phonons at 6 K. It is evident that a maximum in the ratio of $\tau_{6K}^{-1}(\omega)/\tau_{100K}^{-1}(\omega)$ and a minimum in the ratio of $R_{6K}(\omega)/R_{100K}(\omega)$ at around 900 cm^{-1} or 110 meV can be identified. Taking this value as $2\Delta+\Omega_{max}$ and using the measured value of $\Delta=34$ meV (Ref. 17) for OP Bi2212, a value of 42 meV is determined for Ω_{max}. This is in excellent agreement with the maximum of the bosonic spectral function at 43 meV derived at 100 K, indicating that this bosonic spectral function is directly involved in the pair formation in OP Bi2212.

Obviously, the origin of the 43 meV boson is an important question. Carbotte *et al.*[6] and Abanov *et al.*[7] argued that the 43 meV peak in $W(\omega)$ corresponds to the spin resonance peak. Furthermore, the spectral function $W(\omega)$ below T_c does contain useful information. Carbotte *et al.*[6] showed that for high-T_c cuprates, the strong peak in $W(\omega)$ below T_c is correlated with the electron-spin excitation spectral density, $I^2\chi''(\omega)$, but shifted to $\Delta+\Delta_s$, where Δ_s is the maximum of the spin resonance peak. Also, Abanov *et al.*[7] showed that features in $W(\omega)$ below T_c are related to the singularities in optical conductivity and they argued that the negative minimum in $W(\omega)$ at $2\Delta+\Delta_s$ is the signature of spin-mediated superconductivity. They also identified two weaker features at 4Δ and $2\Delta+2\Delta_s$.

The temperature-dependent $W(\omega)$ is shown in Fig. 4(b) for an OP Bi2212 single crystal. There is a large maximum in $W(\omega)$ at around 70 meV, a deep negative minimum around 110 meV, and a weak maximum around 150 meV at 6 K. According to Carbotte *et al.*[6] and Abanov *et al.*,[7] the large maximum corresponds to $\Delta+\Delta_s$, the deep minimum should be at $2\Delta+\Delta_s$, and the weak maximum at around 150 meV is related to $2\Delta+2\Delta_s$. From these observations, one can uniquely determine the values of $\Delta=35\pm3$ meV and $\Delta_s=40\pm3$ meV. These optically obtained values agree very well with the directly measured values of $\Delta=34$ meV (Ref. 17) and $\Delta_s=43$ meV (Ref. 18) for OP Bi2212. Just above T_c at $T=100$ K, $W(\omega)$ has a peak at 43 meV. However, $W(\omega)$ becomes featureless at $T=295$ K. The $W(\omega)$ functions for a detwinned OP YBCO single crystal are shown in Fig. 4(c) for comparison. One can again determine the values of $\Delta=30\pm4$ meV and $\Delta_s=40\pm4$ meV from the optical data at 6 K.[19] These optically obtained values also agree very well with the directly measured values of $\Delta=27$ meV (Ref. 20) and $\Delta_s=41$ meV (Ref. 21) for OP YBCO. The existence of a

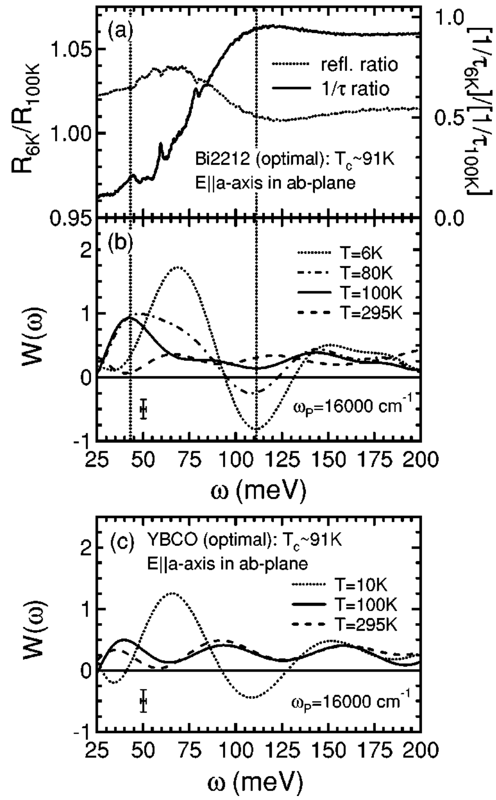

FIG. 4. The temperature dependence of the spectral function $W(\omega)$ of an OP Bi2212 single crystal and a detwinned OP YBCO single crystal with $E\|a$ in the ab plane (20-term polynomial fits are used). (a) The reflectance ratio and the scattering rate ratio below and above T_c, (b) $W(\omega)$ of an OP Bi2212 single crystal at four different temperatures (error bar for the derivative analysis is included), and (c) $W(\omega)$ of an OP YBCO single crystal at three different temperatures (error bar for the derivative analysis is included).

maximum at $\Delta+\Delta_s$ and a minimum at $2\Delta+\Delta_s$ in $W(\omega)$ below T_c is unique for spin-mediated superconductivity and these characteristic features are absent for a nonsuperconducting $(Bi_{0.5}Pb_{0.5})_2Ba_3Co_2O_\delta$ metallic sample. In all, the experimental data are consistent with the picture of spin-mediated superconductivity and the features in $W(\omega)$ below T_c can lead to the determination of Δ and Δ_s optically.[22]

The origin of the 43 meV boson in OP Bi2212 deserves some further discussion. The obvious candidate is the spin resonance peak at 43 meV since it has a similar temperature dependence as well as having the same energy. This is also the conclusion of recent photoemission[23] and tunneling[24] work on Bi2212. The observation of the 43 meV peak at 100 K would imply the existence of a pseudogap above T_c in OP Bi2212. It should be pointed out that the whole spin excitation spectrum is likely to be involved in the pairing. The spin resonance peak serves as a distinct spectroscopic signature for many types of experiments. Because the spectral function $W(\omega)$ is featureless at 295 K, this is inconsistent with the suggestion of electron coupling to a zone boundary phonon at 60–80 meV.[8] However, the spectral function analysis alone does not exclude other coupling mechanisms. In particular, the possibility that the electron-boson spectral function is in part the result of electron-phonon coupling cannot be ruled out and our suggestion that the 44 meV phonon is in fact a magnetic polaron below T_c due to the resonant interaction with the spin resonance peak should be considered. The appearance of the 44 meV phonon in the $E\|a$ axis spectra below T_c (presumably becoming infrared active due to interaction with the spin resonance peak) and its large width at 6 K add support to the resonant interaction picture. In the final analysis both spins and phonons can be important for superconductivity in high-T_c cuprates, but the most relevant spectroscopic feature, deduced from these optical measurements for OP Bi2212, is around 40 meV.

In conclusion, we have carried out a detailed analysis of the optical data for OP Bi2212 and OP YBCO single crystals. Our data are consistent with the picture of electron-boson-mediated superconductivity in high-T_c cuprates instead of theories that are based on kinetic energy mechanisms. A detailed theoretical analysis of our high-quality optical data, particularly for OP Bi2212, will lead to a better understanding of the charge dynamics in these systems that is most essential to the superconducting mechanism.

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