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Oxygen isotope effect in a high-temperature superconductor under high pressure

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Abstract

The role of phonons is addressed by combining the information obtained from the measurements of Raman scattering and magnetic susceptibility in an optimally doped high-temperature superconductor. We show that the high-pressure behavior of the oxygen isotope exponent can be predicted from the changes in both the phonon frequency and superconducting transition temperature based on a phonon-mediated d-wave BCS-like model. The isotope exponent is found to decrease with increasing pressure but remain small and positive within the pressure regime studied. These results point to the important role of the electron–phonon interaction for high-temperature superconductivity.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Understanding the high-temperature superconductivity in cuprate superconductors is at the heart of current research in solid-state physics. Isotope substitution [1] and pressure [2] have been realized to be two very effective ways in revealing the underlying pairing mechanism of superconductivity. Measurements of the isotope effect on the superconducting transition temperature T_c provided key experimental evidence for the phonon-mediated pairing and supported strongly the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity in conventional materials. A much richer and more complex situation has been established for copper-oxide superconductors [1]. Such an effect in an individual material and the difference between the different systems is still poorly understood. Meanwhile, a record high T_c of 164 K was achieved under high pressure in $HgBa_2Ca_2Cu_3O_{8+\delta}$ [3]. Observing how the pressure influences the individual parameters of the lattice in the normal and superconducting state of a single sample allows a clean quantitative test of the validity of theoretical models. In conventional metal superconductors, there is a correlation between the pressure coefficient

of the electronic stiffness and the isotope effect [4]. For high-T_c materials, a similar doping dependence for both the copper isotopic exponent and the pressure coefficient of T_c, $d \ln T_c/dP$, was found in $YBa_2Cu_3O_{7-\delta}$ [5]. These findings point directly to the equivalent importance of the pressure and isotope effects on superconductivity. Since many materials, such as 23 elements [2] and even spin-ladder cuprate [6], become superconductors only under sufficiently high pressure, measurements of the isotope effect in these materials must be performed under high pressure. Interestingly, Crespi and Cohen [7] proposed that cuprates under high pressure are a hopeful candidate for attaining negative values for α, which would provide support for an anharmonic model for high-T_c superconductivity. Until now, there is little information regarding how α changes with pressure in high-T_c cuprates. Such investigations are highly desirable for elucidating the mechanism of high-T_c superconductivity.

In this work we study the role of phonons based on the information obtained from the high-pressure measurements of the Raman scattering and superconducting transitions in the optimally doped $YBa_2Cu_3O_{7-\delta}$. We obtain the pressure dependence of the oxygen isotope exponent in terms of a phonon-mediated d-wave BCS-like model. We find that the isotope exponent indeed decreases with increasing pressure, but remains small and positive in the pressure ranges studied. This result cannot serve as evidence for supporting the anharmonic model.

2. Experimental details

Samples of $YBa_2Cu_3O_{7-\delta}$ single crystals were grown by a self-flux technique. The superconducting transition temperature T_c was determined to be 92.5 K, with a 10–90% transition width of 0.5 K in susceptibility, indicating the very good quality of the samples. Samples, together with ruby chips, were loaded into Mao–Bell cells with liquid helium as the pressure medium. The cells were made from hardened Be–Cu alloy. The gaskets were made of non-magnetic Ni–Cr alloy. The pressure was applied and measured at low temperatures by taking the $R1$ fluorescence line of ruby as a gauge [8]. Both Raman and T_c measurements were reported in [9].

High-pressure Raman measurements were taken by using an angular excitation geometry. The optical layout was detailed in [9]. To be compatible with this geometry, the diamond seat was modified to allow off-axis entry of the incident light. Specially designed tungsten carbide seats having angular conical holes were used for this purpose. Synthetic ultra-pure anvils were chosen to reduce diamond fluorescence. An argon ion laser ranging from 476.2 to 568.2 nm was used for the excitation of Raman signals, and the laser power on the sample was kept below 5 mW.

Measurements of T_c under high pressure were performed by using a highly sensitive magnetic susceptibility technique [10]. The technique is based on the quenching of the superconductivity and suppression of the Meissner effect in the superconducting sample by an external magnetic field. The magnetic susceptibility of the metallic parts of the high-pressure cells is essentially independent of the external field. Therefore, the magnetic field applied to the sample inserted in the diamond cell mainly affects the change in the signal coming from the sample. The T_c is then identified as the point where the signal goes to zero because of the disappearance of the Meissner effect.

3. Results and discussion

Representative Raman spectra of an optimally doped $YBa_2Cu_3O_{7-\delta}$ single crystal are shown in the inset of figure 1. These spectra in the $y(xx)\bar{y}$ ($A_{1g} + B_{1g}$) geometry were taken at

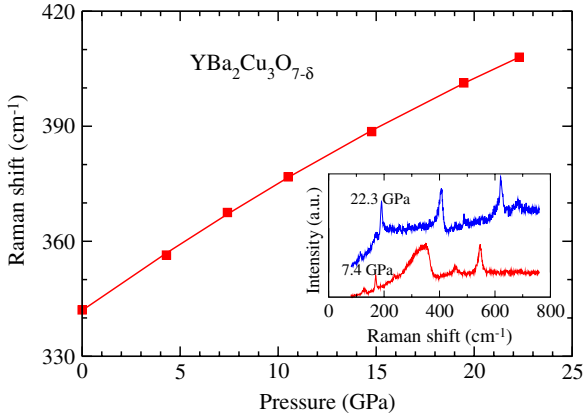

Figure 1. Pressure dependence of the Raman shift of the B_{1g} phonon mode taken at 25 K in the optimally doped $YBa_2Cu_3O_{7-\delta}$. Inset: Raman spectra in the $y(xx)\bar{y}$ ($A_{1g} + B_{1g}$) geometry taken at 25 K and at pressures of 7.4 and 22.3 GPa.

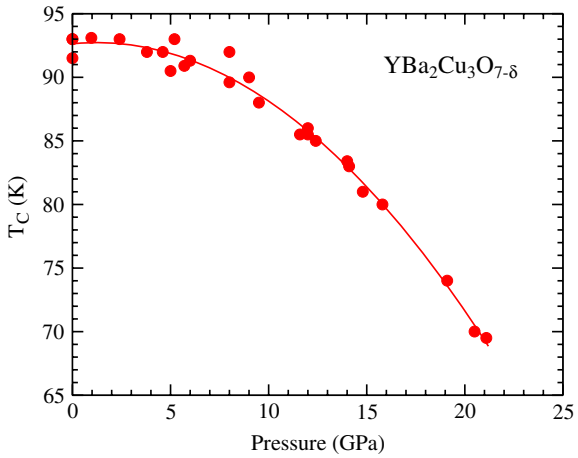

Figure 2. Pressure dependence of the superconducting transition temperature T_c in the optimally doped $YBa_2Cu_3O_{7-\delta}$.

25 K and at different pressures up to 22.3 GPa. An increase in the phonon wavenumbers is observed with increasing pressure. The most pronounced spectral change under pressure is a significant enhancement of the B_{1g} phonon mode near 300 cm^{-1}. The B_{1g} phonon acquires a peculiar lineshape, which is impossible to fit with a simple Fano formula alone. A Green's function approach is used to determine the linewidth and wavenumber shift [9]. The results of the Raman shift, ω_{B1g}, of the B_{1g} phonon mode as a function of pressure are summarized in figure 1. Within the interesting pressure regime, ω_{B1g} increases with pressure in a nearly linear way.

Figure 2 shows the pressure dependence of T_c in the optimally doped $YBa_2Cu_3O_{7-\delta}$. The superconducting transition is identified as the temperature where the signal goes to zero on the high-temperature side, which is the point at which magnetic flux completely enters the sample. The superconducting transition of 92.5 K is obtained at ambient pressure, and it shifts with the applied pressure. As can be seen, as the pressure is increased, T_c increases initially until passing

saturation at critical pressure, and at higher pressures T_c slightly decreases. The measured $T_c(P)$ behavior of this material is consistent with other independent measurements [11, 12]. A similar non-monotonic pressure dependence of $T_c(P)$ was also reported in the sister bilayer compounds $Tl_2Ba_2CaCu_2O_{8+\delta}$ [13] and $Bi_2Sr_2CaCu_2O_{8+\delta}$ [14] at the optimal doping. This behavior can be well understood within the framework of a d-wave BCS-like theory [14, 15]. This ubiquitous behavior may serve as an indicator of a hallmark of hole-doped high-T_c cuprates.

To obtain the high-pressure behavior of the isotope exponent, we use a phonon-mediated BCS-like gap equation for the d-wave superconductors:

$$1 = \frac{1}{N}\sum_k V g^2(k)\chi_k \theta\left(\omega_0 - |\varepsilon_k - \mu|\right), \tag{1}$$

where V is the in-plane pairing interaction strength, $g(k) = \cos k_x - \cos k_y$, $\chi_k = (2E_k)^{-1}\tanh(\beta E_k/2)$ with the quasiparticle spectrum $E_k = \sqrt{(\varepsilon_k - \mu)^2 + |\Delta_k|^2}$ and $\beta = (k_B T_c)^{-1}$, ω_0 is a cutoff on the spectrum, ε_k is the quasiparticle dispersion, μ is the chemical potential, and the step function $\theta(x)$ takes care of the condition $|\varepsilon_k - \mu|$ or $|\varepsilon_{k'} - \mu| < \omega_0$. The T_c equation is then obtained by solving equation (1) with $\Delta = 0$. The validity of the d-wave BCS formalism in describing the superconducting state of cuprates has been supported by recent measurements of ARPES [16] and transport properties [17]. For phonon-mediated pairing, ω_0 is assumed to vary with the isotope mass M as $M^{-1/2}$. By differentiating equation (1) with respect to both T_c and ω_0, we can express α as

$$\alpha = \frac{\frac{1}{N}\sum_k T_c g^2(k)\tanh\left(\frac{\omega_0}{2T_c}\right)\delta\left(\omega_0 - |\varepsilon_k - \mu|\right)}{\frac{1}{N}\sum_k g^2(k)\,\mathrm{sech}^2\left(\frac{|\varepsilon_k - \mu|}{2T_c}\right)\theta\left(\omega_0 - |\varepsilon_k - \mu|\right)}. \tag{2}$$

Just like the case at ambient condition, the change in α with pressure is assumed to be through the changes in both T_c and ω_0 and is then expressed by $\alpha(P) = \alpha[T_c(P), \omega_0(P)]$. For the cutoff phonon frequency $\omega_0(P)$, we take the pressure dependence of the frequency ω_{B1g} of the B_{1g} Cu–O bond-buckling phonon, which has been ascribed as a bosonic mode influencing high-T_c superconductivity [18]. The information on $\omega_{B1g}(P)$ has been obtained by high-pressure Raman scattering measurements. We thus have $\omega_0(P) = [\omega_0(0)/\omega_{B1g}(0)]\omega_{B1g}(P)$. The $\alpha(P)$ behavior can be derived from equation (2) based on the $T_c(P)$ and $\omega_{B1g}(P)$ determinations.

In the calculations, we use the dispersion $\varepsilon_k = 0.057\,26\cos k_x \cos k_y + 0.032\left(\cos 2k_x + \cos 2k_y\right)$ eV, pairing interaction strength $V = 0.037\,62$ eV, and cutoff frequency $\omega_0 = 0.060$ eV. The choice of these parameters can bear the parabolic relation between the T_c and hole content with a maximum T_c of 92.5 K at the optimal doping observed experimentally for $YBa_2Cu_3O_{7-\delta}$. The dispersion used can reproduce the band width and Fermi-surface shape of this material.

In figure 3 we present the calculated α as a function of pressure up to 25 GPa in the optimally doped $YBa_2Cu_3O_{7-\delta}$, which was reported in [19]. The zero-pressure value of α is 3.5×10^{-3}, which is in good agreement with experiments [20]. As pressure is increased, α decreases slightly in a similar manner for $\mathrm{d}\ln T_c/\mathrm{d}P$, as expected from an anharmonic model [7], but α remains small and positive within the pressure regime studied. To our knowledge this is the first prediction of the change in the isotope effect under pressure in cuprate superconductors. The similarity of the isotope effect and the pressure effect both at ambient condition and under high pressure indicates that both effects are playing an equivalent role in shedding important light on high-T_c superconductivity in cuprates. There have been no reports of isotope measurements under high pressure in cuprates so far. The prediction made here for $\alpha(P)$ awaits further experimental studies.

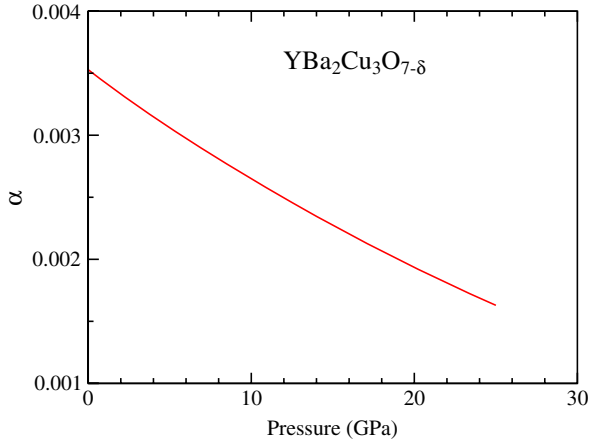

Figure 3. Calculated oxygen isotope exponent α as a function of pressure up to 25 GPa in the optimally doped $YBa_2Cu_3O_{7-\delta}$.

4. Conclusion

We have addressed the role of phonons played in high-temperature superconductivity by using the information obtained from the measurements of the Raman scattering and magnetic susceptibility in the optimally doped $YBa_2Cu_3O_{7-\delta}$. We have found that, as the pressure is increased, the Raman shift ω_{B1g} of the B_{1g} phonon mode increases in a nearly linear way, whereas T_c exhibits a non-monotonic dependence. We have shown that a phenomenological phonon-mediated d-wave BCS-like model can be used to predict the pressure dependence of the oxygen isotope exponent. The obtained small and positive oxygen isotope effect seemingly does not support the anharmonic model. Our results strongly suggest that the electron–phonon interaction should be taken into account for explaining the superconducting properties in copper-oxide superconductors.

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