Relevance of electron-lattice coupling in cuprates superconductors

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We study the oxygen isotope (¹⁸O/¹⁶O) and finite size effects in Y₁₋ₓPrₓBa₂Cu₂O₇₋δ by in-plane penetration depth (λ₁²) measurements. A significant change of the length L_c of the superconducting domains along the c-axis and λ₁² is deduced, yielding the relative isotope shift ΔL_c/L_c ≈ Δλ₁²/λ₁² ≈ −0.14 for x = 0, 0.2 and 0.3. This uncovers the existence and relevance of the coupling between the superfluid, lattice distortions and anharmonic phonons which involve the oxygen lattice degrees of freedom.

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Since the discovery of superconductivity in cuprates by Bednorz and Müller¹ a tremendous amount of work has been devoted to their characterization. The issue of inhomogeneity and its characterization is essential for several reasons, including: First, if inhomogeneity is an intrinsic property, a re-interpretation of experiments, measuring an average of the electronic properties, is unavoidable. Second, inhomogeneity may point to a microscopic property, a re-interpretation of experiments, measurements and their phase-purity was examined using powder x-ray diffraction. For each doping concentration the samples were reground in a mortar for about 60min. Powder samples with a grain size of < 10μm were obtained by using a system of 20/15/10μm sieves. Oxygen isotope exchange was performed by heating the powder in ¹⁸O₂ gas. In order to ensure the same thermal history of the substituted (¹⁸O) and not substituted (¹⁶O) samples, two experiments (in ¹⁶O₂ and ¹⁸O₂) were always performed simultaneously ². To achieve complete oxidation the exchange processes were carried out at 550°C during 30 h, followed by slow cooling (20°C/h). The ¹⁸O content, determined from a change of the sample weight after the isotope exchange, was found to be 89(2)% for all samples. Field-cooled (FC) magnetization measurements were performed with a Quantum Design SQUID magnetometer in field range 0.5 to 10mT and a temperature range 5K to 100K. The powder samples (~100mg) were put in a quartz ampule. To guarantee the same experimental conditions (sample geometry and the background signal from the sample holder), the same ampule was used. The absence of weak links between grains was confirmed by the linear scaling of the FC magnetization measured at 5K in 0.5mT, 1mT and 1.5mT. The Meissner fraction f was calculated from the mass and the x-ray density, assuming spherical grains. An example of f versus T is displayed in the insert of Fig.¹ Assuming spherical grains of radius R, the data were analyzed on the basis of the Shoenberg formula ³, allowing to calculate the temperature dependence of the effective penetration depth λ_eff(T)/λ_eff(0). For sufficiently anisotropic extreme type II superconductors, including Y₁₋ₓPrₓBa₂Cu₂O₇₋δ, λ_eff is proportional to the in-plane penetration depth, so that λ_eff = 1.31λ_ab ⁴. Since it is not possible to extract the absolute value of λ_ab from our measurements we take λ_ab(0K) from μSR measurements ⁴ to normalize the data. In the main panel of Fig.¹ we displayed the resulting temperature dependence of ¹⁶λ₂⁰₀(ab) / λ₂⁰₀(T) for the ¹⁶O and ¹⁸O samples of Y₀.7Pr₀.3Ba₂Cu₃O₇−δ. For comparison we included ¹⁶λ₂⁰₀(ab) / λ₂⁰₀(T) = ¹⁶λ₂⁰₀(ab) / λ₂⁰₀(ab) (1−T/T_c)² with the critical exponent ν = 2/3, ¹⁶T_c = 54.9K and ¹⁸T_c = 53.7K to indicate the asymptotic critical behav-
ior for an infinite superconducting domain. Apparently, the data are inconsistent with such a sharp transition. It clearly uncovers a rounded phase transition which occurs smoothly and with that a finite size effect at work. In this context it is important to emphasize that this finite size effect is not an artefact of $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ or the particular technique used to evaluate $1/\lambda^2_{ab}(T)$. Indeed, this rounding is also seen in the data for $YBa_2Cu_3O_7$ \cite{18}, La$_{2-x}$Sr$_x$CuO$_4$ with $x=0.1, 0.15$ and 0.2 \cite{19}, and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ single crystals \cite{20,21}. Moreover, independent evidence for superconducting domains of finite extent, stems from the analysis of specific heat data \cite{10}. Given the mounting evidence for these domains, their behavior upon oxygen isotope exchange is expected to offer valuable clues on the relevance of local lattice distortions in the mechanism mediating superconductivity.

To elucidate this issue we perform a finite size scaling analysis of the in-plane penetration depth data for $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ with $^{16}O$ and $^{18}O$. Supposing that cuprate superconductors are granular, consisting of spatial superconducting domains, embedded in a non-superconducting matrix with spatial extent $L_a$, $L_b$ and $L_c$ along the crystallographic $a$, $b$ and $c$-axes, the correlation length $\xi_{i}$ in direction $i$, increasing strongly when $T_c$ is approached cannot grow beyond $L_{i}$. Consequently, for finite superconducting domains, the thermodynamic quantities like the specific heat and penetration depth are smooth functions of temperature. As a remnant of the singularity at $T_c$ these quantities exhibit a so called finite size effect \cite{22}, namely a maximum or an inflection point at $T_{p_i}$, where $\xi_{i}(T_{p_i})=L_{i}$. There is mounting experimental evidence that for the accessible temperature ranges, the effective finite temperature critical behavior of the cuprates is controlled by the critical point of uncharged superfluids (3D-XY) \cite{3,21}. In this case there is the universal relationship

$$\frac{1}{\lambda^2_{i}(T)} = \frac{16\pi^3k_BT}{\Phi_0^{2}\xi^4_{i}(T)},$$

(1)

between the London penetration depth $\lambda_{i}$ and the transverse correlation length $\xi_{i}$ in direction $i$ \cite{21}. As aforementioned, when the superconductor is inhomogeneous, consisting of superconducting domains with length scales $L_{i}$, embedded in a non-superconducting matrix, the $\xi_{i}$'s do not diverge but are bounded by

$$\xi_{i}^f \leq L_c^2, \quad i \neq j \neq k.$$  

(2)

A characteristic feature of the resulting finite size effect is the occurrence of an inflection point at $T_{p_i}$ below $T_c$, the transition temperature of the homogeneous system. Here

$$\xi_{i}^f(T_{p_{x}}) \xi_{j}^f(T_{p_{x}}) = L_{c}^2, \quad i \neq j \neq k,$$

and Eq. (1) reduces to

$$\frac{1}{\lambda_{i}(T)} \frac{1}{\lambda_{j}(T)} \bigg|_{T=T_{p_{x}}} = \frac{16\pi^3k_BT_{p_{x}}}{\Phi_0^{2}L^2_{c}}.$$  

(4)

In the homogeneous case $1/\lambda_{i}(T)\lambda_{j}(T)$ decreases continuously with increasing temperature and vanishes at $T_{c}$, while for superconducting domains, embedded in a non-superconducting matrix, it does no vanish and exhibits an inflection point at $T_{p_i} < T_c$, so that

$$d\left(\frac{1}{\lambda_{i}(T)\lambda_{j}(T)}\right)/dT \bigg|_{T=T_{p_{x}}} = \text{extremum}$$  

(5)

We are now prepared to perform the finite size scaling analysis of the penetration depth data. In Fig. 2 we displayed $^{16}\lambda^2_{ab}(T=0)/^{16}\lambda^2_{ab}(T)$ and $d\left(\lambda^2_{ab}(T=0)/^{16}\lambda^2_{ab}(T)\right)/dT$ versus $T$ for $Y_{0.7}Pr_{0.3}Ba_2Cu_3O_{7-\delta}$. The solid lines are \cite{18,19}$^{16}\lambda^2_{ab}(0)/^{16}\lambda^2_{ab}(T)$, \cite{18} and the dash dot lines the corresponding derivatives, indicating the leading critical behavior of a domain, infinite in the $c$-direction. The extreme in the first derivative around $T \approx 52.1K$ and $51K$ for $^{16}O$ and $^{18}O$ respectively clearly reveal the existence of an inflection point, characterizing the occurrence of a finite size effect in $1/\lambda^2_{ab}(T)$. Using Eq. (1) and the estimates for $T_{p_i}$, \cite{18} $^{16}\lambda^2_{ab}(T_{p_i})/^{16}\lambda^2_{ab}(0)$, \cite{18} $^{18}\lambda^2_{ab}(T_{p_i})/^{16}\lambda^2_{ab}(0)$ and \cite{18} $^{16}\lambda^2_{ab}(0)$ listed in Table I, we obtain $^{16}L_{c} = 19.5(8)\text{Å}$.
and $x = 0.2$ and extracted the in-plane penetration depth, as outlined above. In Fig. 4 we show $^{16}\lambda^2_{ab}(T = 0) / \lambda^2_{ab}(T)$ and $d(\lambda^2_{ab}(T = 0) / \lambda^2_{ab}(T)) / dT$ versus $T$ for YBa$_2$Cu$_3$O$_{7-\delta}$ with $^{16}$O and $^{18}$O. The solid lines are $(^{16}\lambda_{ab}(0) / ^{16}\lambda_{ab}(T))^2 = 3.9 (1 - T / ^{16}T_c)^{2/3}$, $(^{18}\lambda_{ab}(0) / ^{18}\lambda_{ab}(T))^2 = 3.55 (1 - T / ^{18}T_c)^{2/3}$ with $^{16}T_c \approx 18T_c = 90.3K$ and the dash dot lines the corresponding derivatives, indicating the leading critical behavior of the homogeneous system. The finite size estimates for various quantities and the corresponding isotope shifts, for an $^{16}$O content $89\%$ are summarized in Table I (we define the relative oxygen isotope shift of a physical quantity $X$ as $\Delta X / X = (^{18}X - ^{16}X) / ^{16}X$). While the isotope effect on $T_c$ and the inflection points $T_{p_c}$ is very small, there is an appreciable shift of $1/\lambda^2_{ab}$. As indicated in Fig. 3 we used a quadratic fit around the inflection point to determine $T_{p_c}$. Nevertheless, the error (0.1 to 0.2K) leads to the main uncertainty in terms of $\lambda^2_{ab}(T_{p_c}) / \lambda^2_{ab}(0)$. From Table I several observations emerge. First, $L_c$ increases systematically with reduced $T_{p_c}$. Second, $L_c$ grows with increasing $x$ and upon isotope exchange ($^{16}$O, $^{18}$O). Third, the relative shift of $T_{p_c}$ is very small. This reflects the fact that the change of $L_c$ is essentially due to the superfluid, probed in terms of $\lambda^2_{ab}$. Accordingly, $\Delta L_c / L_c \approx \Delta \lambda^2_{ab} / \lambda^2_{ab}$ for $x = 0, 0.2$ and $0.3$. Indeed the relative shifts of $T_{p_c}$, $\lambda^2_{ab}(T_{p_c})$ and $L_c$ are not independent. Eq. (4) implies,

$$\frac{\Delta L_c}{L_c} = \frac{\Delta T_{p_c}}{T_{p_c}} + \frac{\Delta \lambda^2_{ab}(T_{p_c})}{\lambda^2_{ab}(T_{p_c})},$$



and $^{18}L_c = 22.6(9)\AA$ for the spatial extent of the superconducting domains along the c-axis. Note that the rather broad peak around the inflection point reflects the small value of $L_c$. Indeed, in Bi2212, where the same analysis gives $L_c \approx 68\AA$, this peak was found to be considerably sharper [24].

To explore the dependence of this change on Pr concentration we performed analogous magnetization measurements on Y$_{1-x}$Pr$_x$Ba$_2$Cu$_3$O$_{7-\delta}$ with $x = 0$ and $x = 0.2$ and extracted the in-plane penetration depth, as outlined above. In Fig. 4 we show $^{16}\lambda^2_{ab}(T = 0) / \lambda^2_{ab}(T)$ and $d(\lambda^2_{ab}(T = 0) / \lambda^2_{ab}(T)) / dT$ versus $T$ for YBa$_2$Cu$_3$O$_{7-\delta}$ with $^{16}$O and $^{18}$O. The solid lines are $(^{16}\lambda_{ab}(0) / ^{16}\lambda_{ab}(T))^2 = 3.9 (1 - T / ^{16}T_c)^{2/3}$, $(^{18}\lambda_{ab}(0) / ^{18}\lambda_{ab}(T))^2 = 3.55 (1 - T / ^{18}T_c)^{2/3}$ with $^{16}T_c \approx 18T_c = 90.3K$ and the dash dot lines the corresponding derivatives, indicating the leading critical behavior of the homogeneous system. The finite size estimates for various quantities and the corresponding isotope shifts, for an $^{16}$O content $89\%$ are summarized in Table I (we define the relative oxygen isotope shift of a physical quantity $X$ as $\Delta X / X = (^{18}X - ^{16}X) / ^{16}X$). While the isotope effect on $T_c$ and the inflection points $T_{p_c}$ is very small, there is an appreciable shift of $1/\lambda^2_{ab}$. As indicated in Fig. 3 we used a quadratic fit around the inflection point to determine $T_{p_c}$. Nevertheless, the error (0.1 to 0.2K) leads to the main uncertainty in terms of $\lambda^2_{ab}(T_{p_c}) / \lambda^2_{ab}(0)$. From Table I several observations emerge. First, $L_c$ increases systematically with reduced $T_{p_c}$. Second, $L_c$ grows with increasing $x$ and upon isotope exchange ($^{16}$O, $^{18}$O). Third, the relative shift of $T_{p_c}$ is very small. This reflects the fact that the change of $L_c$ is essentially due to the superfluid, probed in terms of $\lambda^2_{ab}$. Accordingly, $\Delta L_c / L_c \approx \Delta \lambda^2_{ab} / \lambda^2_{ab}$ for $x = 0, 0.2$ and $0.3$. Indeed the relative shifts of $T_{p_c}$, $\lambda^2_{ab}(T_{p_c})$ and $L_c$ are not independent. Eq. (4) implies,

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an electronic mechanism, without coupling to local lattice distortions and anharmonic phonons, implies $\Delta L_c = 0$. On the contrary, a significant change of $L_p$, upon oxygen exchange uncovers the coupling to local lattice distortions and anharmonic phonons involving the oxygen lattice degrees of freedom. A glance to Table I shows that the relative change of the domains along the c-axis and the in-plane penetration depth $\Delta L_c$ at fixed Pr concentration is accompanied by essentially the same relative change of $\lambda_{ab}^2$, which probes the superfluid. This uncovers unambiguously the existence and relevance of the coupling between the superfluid, lattice distortions and anharmonic phonons involving the oxygen lattice degrees of freedom. Potential candidates are the Cu-O bond-stretching-type phonons showing temperature dependence, which parallels that of the superconductive order parameter $\lambda_{ab}^2$.

Independent evidence for the shrinkage of limiting length scales upon isotope exchange stems from the behavior close to the quantum superconductor to insulator transition where $T_c$ vanishes. Here the cuprates become essentially two dimensional and correspond to a stack of independent slabs of thickness $d_s$. It was found that the relative shift $\Delta d_s/d_s$ upon isotope exchange adopts a rather unique value, namely $\Delta d_s/d_s \approx -0.03$. In conclusion, we reported the first observation of the combined finite size and oxygen isotope exchange effects on the spatial extent $L_c$ of the superconducting domains along the c-axis and the in-plane penetration depth $\lambda_{ab}$. Although the majority opinion on the mechanism of superconductivity in the cuprates is that it occurs via a purely electronic mechanism involving spin excitations, and lattice degrees of freedom are supposed to be irrelevant, we have shown the relative isotope shift $\Delta L_c/16 L_c \approx \Delta \lambda_{ab}^2/16 \lambda_{ab}^2 \approx -0.15$ uncovers clearly the existence and relevance of the coupling between the superfluid, lattice distortions and anharmonic phonons which involve the oxygen lattice degrees of freedom.

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