Effect of impurity scattering on the magnetic field penetration depth in YBa$_2$Cu$_3$O$_{7-\delta}$: comparison with experiments

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The temperature dependence of the anisotropic magnetic field penetration depth of a two-band superconductor is calculated in the model of strong $s$-wave pairing interaction in one of the bands ($S$ band) and induced superconductivity in the second band ($N$ band). The results of the calculations are compared with experimental data on the $ab$-plane and $c$-axis penetration depth in YBa$_2$Cu$_3$O$_{7-\delta}$. It is shown that all recent measurements are consistent with the two-band model over the entire temperature range. © 1995 American Institute of Physics.

1. It is well known that the electromagnetic properties of YBaCuO are not described by the standard weak-coupling BCS model. In particular, the measurements of the temperature dependence of the magnetic field penetration depth $\lambda(T)$ have revealed an increased slope of $\lambda^{-2}(T)$ near the critical temperature $T_c$ and nonexponential behavior of $\lambda(T)$ at $T<T_c/2$. These deviations could, in principle, be explained in terms of the model of strong electron–phonon interaction, with an isotropic superconducting order parameter. However, the results of microwave measurements$^{1-3}$ of $\lambda(T)$ on higher quality YBaCuO samples cannot be described by this model. According to Refs. 1–3, the temperature dependence of $\Delta\lambda_{ab}(T)$ in the $ab$ plane at $T<T_c/4$ changes from exponential$^3$ to linear$^1$ and then to a quadratic dependence$^2$ mainly with increasing oxygen deficit in a sample. Subsequent microwave measurements$^4,5$ have confirmed the unusual linear low-temperature behavior of $\Delta\lambda_{ab}(T)$. The inset to Fig. 1 shows the low-temperature part of the experimental $\Delta\lambda_{ab}(T)$ curve from Ref. 6. Strong deviations from the isotropic BCS and strong-coupling models are seen in the figure.

The existence of crossover from the linear to a quadratic temperature dependence of $\Delta\lambda(T)$ has been demonstrated by calculations done in the framework of the $d$-wave pairing model with impurity scattering taken into account.$^7$ Such a crossover has actually been observed in Ref. 4 upon doping of YBaCuO samples with Zn or Ni. However, it is impossible to reconcile the $d$-wave model with the activational exponential behavior of
\( \Delta \lambda_{ab}(T) \). Moreover, the experimentally measured slope of the \( \lambda_{ab}^2(T) \) curves near \( T_c \) is much larger than that predicted by this model. The qualitative difference between the behaviors of the \( c \)-axis penetration depth \( \lambda_c(T) \) predicted by the \( d \)- and \( s \)-pairing models was also pointed out in Ref. 8. Very recently the low-temperature behavior of \( \Delta \lambda_{ab}(T) \) was calculated in the framework of the \( s \)-wave two-band model first proposed in Ref. 10. It was shown in Ref. 9 that with increasing the concentration of magnetic impurities a crossover from the exponential to a power-law temperature dependence occurs.

Following this approach, in this paper we present a quantitative comparison between the calculations of \( \lambda_{ab}(T) \) within the two-band model in the temperature range \( 0<T<T_c \) and recent measurements in \( \text{YBaCuO} \). We assume strong electron–phonon interaction in the \( S \) band (\( \text{CuO}_2 \) planes), while superconductivity is induced in the \( N \) band (\( \text{CuO} \) chains) due to the interband proximity effect. We show that for temperatures not too close to \( T_c \) the value of \( \Delta \lambda_{ab}(T) \) is largely determined by both the intraband scattering on magnetic impurities in the \( N \) band and the ordinary scattering in the \( N \) and \( S \) bands. Furthermore, good quantitative agreement is found between the calculations in the framework of two-band model and low-frequency measurements of the penetration depth \( \lambda_c(T) \) on aligned ultrafine \( \text{YBaCuO} \) powders in Ref. 11. The results of microwave measurements of the \( \lambda(T) \) anisotropy in \( \text{YBaCuO} \) single crystals should be treated with care because (i) high precision adjustment of the sample position is necessary and (ii) the distribution of fields and currents in the sample is very complicated. Therefore, we will not be considering the microwave measurements of \( \lambda_c \).

2. In the case of a strong pairing interaction in the \( S \) band the Eliashberg strong-coupling theory is a starting point for discussing anisotropy effects, as it properly takes into account the effects of retardation and decay of quasiparticle excitations. The straight-
forward generalization of the Eliashberg equations for the many-band case leads to the system of coupled equations:

\[
\Delta'_{i,n}(i\omega_n) = \Delta_{i,n} Z_{i,n} = \pi T \sum_j \sum_{n'} \left\{ (\lambda_{ij} D_{n,n'} - \mu^*) \Delta'_{j,m} \right\} \frac{\Delta'_{i,m}}{[(\Delta'_{j,m})^2 + (\omega'_{j,m})^2]^2},
\]

(1)

\[
\omega'_{i,n}(i\omega_n) = \omega_n Z_{i,n} = \omega_n + \pi T \sum_j \sum_{n'} \left\{ \lambda_{ij} D_{n,n'} + (\gamma_{ij} + \gamma_{ij}^*) \right\} \frac{\omega'_{j,m}}{[(\Delta'_{j,m})^2 + (\omega'_{j,m})^2]^2}.
\]

(2)

Here \( D_{n,n'} = \sum_m \Omega_m^2 (\omega_n - \omega_{n'})^2 + \Omega_m^2 \)^{-1} is the phonon Green function and \( \Omega_m \) are phonon frequencies, which we choose in model form as \( \Omega_1 = 200 \text{ K}, \Omega_2 = 5 \Omega_1 = 10^3 \text{ K} \). We note that the function \( D_{n,n'} \) in Eqs. (1), (2) could stand for any other nonphonon (except for spin) interaction. Further, a particular choice of \( \Omega_i \) does not change our conclusions, because the coupling constants \( \lambda_{ij} \) are the most important parameters. The intraband coupling constants \( \lambda_{ii} \) describe the strength of the electron–phonon interaction within the \( i \)-th band. The physical meaning of the interband coupling constants \( \lambda_{ij} \) (\( i \neq j \)) is that they describe phonon-mediated transitions between different bands. In the two-band case considered below this process leads effectively to Cooper pair formation in the \( N \) band, provided that the coupling constant \( \lambda_{21} \neq 0 \). The terms \( \gamma_{ij} \) denote the scattering rates from band \( i \) into band \( j \) due to nonmagnetic impurities, \( \gamma_{ij}^* \) are the magnetic scattering rates, \( Z_{i,n} \) is a renormalization function, and \( \omega_n = \pi T (2n + 1) \) are the Matsubara frequencies. It is important to note that the interband scattering rates \( \gamma_{ij} \) (\( i \neq j \)) lead to Cooper-pair tunneling between the corresponding bands and therefore play the same role as \( \lambda_{ij} \) (\( i \neq j \)) in the case of two bands \( N \) and \( S \). For a weak coupling \( \lambda_{ij} \ll 1 \), Eqs. (1), (2) reduce to the equations of the BCS model.

The choice of parameters of the model is motivated by the situation in YBaCuO. We assume that the planes are characterized by a large coupling constant and form an \( S \) band (\( \lambda_{11} = 3 \)), whereas the chains form an \( N \) band (\( \lambda_{22} = 0 \)). A nonzero order parameter in the chains is induced through interband interactions \( \lambda_{12} = \lambda_{21} = 0.2 \). The above parameter set is consistent with \( T_c \approx 90 \text{ K} \) in YBaCuO.

We assume that the interband scattering rates \( \gamma_{ij} \) in Eqs. (1), (2) are small, \( \gamma_{12}, \gamma_{21} \ll T_c \), and we set \( \gamma_{12} = \gamma_{21} = \gamma_{11} = 0 \). We take into account the impurity scattering due to ordinary and magnetic impurities in the \( N \) band (\( \gamma_{22} \) and \( \gamma_{22}^* \), respectively) and the nonmagnetic scattering in the \( S \) band (\( \gamma_{11} \)).

The origin of magnetic scattering is that as the oxygen content decreases, the oxygen atoms move preferentially out of the chains. As a result, the chain Cu atoms develop magnetic moments which act as pair breakers. Thus, the magnetic scattering \( \gamma_{22}^* \) in the \( N \) band is the only free parameter of the model related to the oxygen deficit in \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \).
The choice of elastic scattering rates in the \(N\) and \(S\) bands should be made consistent with the absolute values and anisotropy of resistivities above \(T_c\). The resistivity of the corresponding band \((S,N)\) at \(T_c\) is estimated as

\[
\rho_s(T_c) = 8 \pi^2 \hbar^{-1} \omega_{p,1}^{-2} k_B T_c \sum_i \left[ \lambda_{1i}^{tr} + \frac{(\gamma_{1i} + \gamma_{2i}^*)}{\pi k_B T_c} \right],
\]

\[
\rho_n(T_c) = 8 \pi^2 \hbar^{-1} \omega_{p,2}^{-2} k_B T_c \sum_i \left[ \lambda_{2i}^{tr} + \frac{(\gamma_{2i} + \gamma_{2i}^*)}{\pi k_B T_c} \right],
\]

where \(\lambda_{ij}^{tr}\) are transport coupling constants, and \(\omega_{p,1}\) and \(\omega_{p,2}\) are the plasma frequencies of the \(S\) and \(N\) bands, respectively. With plasma frequencies 3.6 eV for planes and 3.2 eV for chains\(^{12}\) and with elastic scattering rates in the \(N\) and \(S\) bands \(\gamma_{1i} = \gamma_{22} = (2 - 4) T_c\) (16–32 meV), the model (1)–(3) is consistent with absolute values of the resistivity 50–100 \(\mu\Omega\cdot\text{cm}\) at 100 K.

The electromagnetic response of a two-band superconductor can be calculated by generalization of the standard approach developed for strongly coupled superconductors\(^{9,13}\). The penetration depth in the \(ab\) plane is given by:

\[
\lambda_{ab}^{-2}(T) = \frac{Q_1(T) + Q_2(T)}{Q_1(0) + Q_2(0)},
\]

where the corresponding kernels for two bands are

\[
Q_{1,2}(T) = \omega_{p,1,2}^2 \pi T \sum_{\omega_n = 0}^{\infty} \frac{\Delta_{1,2}^2(i \omega_n)}{[\omega_n^2 + \Delta_{1,2}^2(i \omega_n)]^{3/2} Z_{1,2}(i \omega_n)},
\]

We assume that the conductivity in the \(c\) direction is nonmetallic\(^{14}\), i.e., transport along the \(c\) direction occurs via incoherent hopping. In this limit the penetration depth \(\lambda_c\) is given by the Josephson interaction between neighboring pairs of planes and chains and is determined by

\[
\frac{\lambda_c^{-2}(T)}{\lambda_c^{-2}(0)} = 8 \gamma^* \frac{T}{T_c} \sum_{\omega_n = 0}^{\infty} \frac{\Delta_1(i \omega_n) \Delta_2(i \omega_n)}{\sqrt{\omega_n^2 + \Delta_1^2(i \omega_n) \omega_n^2 + \Delta_2^2(i \omega_n)}},
\]

where \(\gamma^* = 1.78\) is Euler’s constant.

3. With the parameters specified above, the Eliashberg equations are solved numerically for two bands. A set of \(\lambda_{ab}^{-2}(t)\) curves for \(\gamma_{22} = 1.6\) meV with different values of \(\gamma_{11} = \gamma_{22}\) is shown in Fig. 2. The single-crystal data from Refs. 4 and 5 \((\rho_{ab} \approx 50 \mu\Omega\cdot\text{cm})\) are in good agreement with the calculations except at temperatures close to \(T_c\). The linear term at \(T < 0.5 T_c\) is well described by the model.

It was demonstrated explicitly in Ref. 15 that a small gap exists in the \(N\) band for \(\gamma_{22} = 0\) and decreases rapidly with an increase of \(\gamma_{22}^*\). As a result, at sufficiently large \(\gamma_{22}^*\) a gapless state develops in the system. The inset to Fig. 2 displays the results of calculations of \(\Delta \lambda_{ab}(T)\) for different \(\gamma_{22}^*\) values. As a consequence of the development of the gapless state, a crossover takes place at low \(T\) from an exponential temperature dependence for \(\gamma_{22} = 0\) to a linear temperature dependence at larger \(\gamma_{22}^*\). The data of
Ref. 3 are compared with our results for $\gamma_{22}^*=0$. The good agreement between the theory and experiment indicates that the exponential temperature dependence at low $T$ can be attributed to the absence of magnetic impurities in fully oxygenated YBaCuO films.\textsuperscript{3}

With increase of $\gamma_{22}^*$ and $\gamma_{22}$ the contribution of the $N$ band to the penetration depth vanishes, and the behavior of $\lambda_{ab}(T)$ becomes closer to that predicted by the isotropic strong-coupling model. Such a crossover, illustrated in Figs. 1 and 3, correlates well with the increase of the resistivity above $T_c$.

Figure 1 presents a quantitative comparison of the calculations of $\lambda_{ab}^{-2}(T)$ with the data on an electron-beam evaporated YBaCuO film.\textsuperscript{6} The parameters $\gamma_{11}=\gamma_{22}=32$ meV correspond to the experimental value of the resistivity of the film, $\rho_{ab} \approx 80$ $\mu\Omega\cdot$cm at 100 K.

The computed $\lambda(T)$ curves are shown in Fig. 3 alongside the data on YBaCuO powders.\textsuperscript{11} At low $T$ the experimental dependence $\Delta\lambda_{ab}^{-2}(T) \sim T^2$ is in agreement with theory. A fit of the calculated $\lambda_c(T)$ curve to the experimental data\textsuperscript{11} is presented in Fig. 3. Our results for different sets of parameters $\gamma_{22}^*$ and $\gamma_{22}$ point to the absence of linear behavior of $\lambda_c(T)$, which is in contradiction to the predictions of the $d$-wave model.\textsuperscript{7,8}

Thus, the influence of impurity scattering on the magnetic field penetration depth in YBaCuO manifests itself in the following way. As discussed in Refs. 9, 10, the magnetic
scattering rate $\gamma_{22}$ in the $N$ band may serve as a quantitative measure of the oxygen deficit in YBa$_2$Cu$_3$O$_{7-\delta}$. In fully oxygenated YBa$_2$Cu$_3$O$_7$ films magnetic pair-breaking in the chains ($N$ band) is absent, i.e., $\gamma_{22} \approx 0$. In this case the two-band model and the measurements exhibit an exponential temperature dependence at low $T$, with an exponent given by a small proximity-induced energy gap in the chains. Even for relatively low concentrations of magnetic impurities $\gamma_{22}$, the superconducting state in the chains becomes gapless. The gaplessness results in a linear term in the contribution of the chains to $\Delta \lambda_{ab}(T)$ at low $T$. The data of Refs. 4 and 5 obtained in YBa$_2$Cu$_3$O$_{6.95}$ single crystals, indeed show a linear dependence of $\Delta \lambda_{ab}(T)$ in accordance with the model. When going from oxygen-deficit single crystals to oxygen-deficient YBa$_2$Cu$_3$O$_{7-\delta}$ thin films and powders the ordinary and magnetic scattering in the chains ($\gamma_{22}$ and $\gamma_{22}^*$) increase. This leads to suppression of the superconductivity in the chains and to a decrease of the chain contribution to the total penetration depth. As a result, a crossover at low $T$ from the linear to a quadratic temperature dependence of $\Delta \lambda_{ab}$ takes place. This behavior correlates well with the experimental data corresponding to different values of resistivity above $T_c$.

In conclusion, we have demonstrated for the first time that all the recent measurements of $\lambda_{ab}(T)$ in YBaCuO are consistent with the two-band model. The approach of Refs. 9, 10 for calculation of $\lambda_{ab}(T)$ has been extended to the entire temperature range 0<$T$<$T_c$ at arbitrary concentration of nonmagnetic impurities. The model correctly de-
scribes the disappearance of linear term in $\lambda_{ab}(T)$ with increasing sample resistivity. The
temperature dependence of $\lambda_c$ has been calculated within the two-band model in the
approximation of Josephson interaction between the layers. In this approach the linear
term never appears in $\lambda_c(T)$ at low $T$. The key experiments to check the two-band
description for YBaCuO would be measurements of $\lambda_c(T)$ on YBaCuO single crystals
and of $\lambda_{ab}(T)$ in oxygen-depleted and Fe- or Ga-doped YBaCuO, when the supercon-
ductivity of the CuO chains is destroyed.

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