

Multiband model for penetration depth in MgB₂

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(Received 8 May 2002; published 19 August 2002)

The results of first-principles calculations of the electronic structure and the electron-phonon interaction in MgB₂ are used to study theoretically the temperature dependence and anisotropy of the magnetic-field penetration depth. The effects of impurity scattering are essential for a proper description of the experimental results. We compare our results with experimental data and we argue that the two-band model describes the data rather well.

DOI: 10.1103/PhysRevB.66.054524

PACS number(s): 74.20.-z, 74.70.Ad, 74.25.Nf

The electronic structure of the recently discovered superconductor¹ MgB₂ is now rather well understood and the superconductivity may be ascribed to the conventional electron-phonon mechanism²⁻⁵. The Fermi surface consists of two three-dimensional(3D) sheets, from the π bonding and antibonding bands, and two nearly cylindrical sheets from the two-dimensional σ bands. The qualitative difference between the 2D σ - and the 3D π -bands in connection with the large disparity of the electron-phonon interaction (EPI) for the different Fermi surface sheets suggested a multiband description of superconductivity.⁶⁻¹⁰ Recent reports on quantum oscillations¹¹ provided not only important information on the electronic structure near the Fermi level but it also probed directly the disparity of the EPI in the π - and σ -band systems. The excellent agreement of the calculated EPI with the de Haas-van Alphen mass renormalization clearly confirms the basic assumption of the two-gap model¹². Further experimental support of this model comes from scanning tunnel microscopy and point-contact spectroscopy,¹³⁻¹⁵ high-resolution photoemission spectroscopy¹⁶, Raman spectroscopy¹⁷, specific-heat measurements,^{9,18} and studies of the magnetic penetration depth.¹⁹⁻²¹

There is still some debate concerning the applicability of the multiband description to MgB₂, in particular since some tunneling measurements²² show only a single gap with a magnitude smaller than the BCS value of $\Delta = 1.76 T_c$. A recently proposed multiband scenario for tunneling⁸ in MgB₂ explains the reason for the differences in the observed tunneling spectra and thus helps to settle this debate.

A similar discussion has been going on concerning the penetration depth. The measured magnetic penetration depth shows a large variety of behavior (see Table I). In order to interpret these results, a microscopic model is required. In this paper we shall use the multiband model^{6,8,9} to calculate the temperature dependence and the anisotropy of the penetration depth using the Eliashberg formalism and the results of first-principles electronic structure calculations. Generalization of the BCS theory to the multiband model was first suggested in Refs. 34 and 35 and it has been observed experimentally in Nb-doped SrTiO₃.³⁶ More recently, Kresin and Wolf³⁷ suggested a two-band model in the strong-

coupling regime for describing the properties of high- T_c superconductors. Strong-coupling two-band-model calculations of the microwave response, and in particular the penetration depth, were performed in Refs. 38 and 39.

The penetration depth of the magnetic field $\lambda_{L,\alpha\beta}$ in the local (London) limit is related to the imaginary part of the optical conductivity by

$$1/\lambda_{L,\alpha\beta}^2 = \lim_{\omega \rightarrow 0} 4\pi\omega \operatorname{Im} \sigma^{\alpha\beta}(\omega, \mathbf{q}=0)/c^2, \quad (1)$$

where α, β denote Cartesian coordinates and c is the velocity of light. If we neglect strong-coupling effects (or, more generally, Fermi-liquid effects) then for a clean uniform superconductor at $T=0$ we have the relation $\lambda_{L,\alpha\beta} = c/\omega_p^{\alpha\beta}$, where $(\omega_p^{\alpha\beta})^2 = 8\pi e^2 \sum_{\mathbf{k}j} \delta(\epsilon^{\mathbf{k}j}) v_{F,j}^\alpha v_{F,j}^\beta$ is the squared total plasma frequency and $v_{F,j}^\alpha$ is the α component of the Fermi velocity in the j band. Impurities and interaction effects drastically enhance the penetration depth, and it is therefore suitable to introduce a so-called “superfluid plasma frequency” $\omega_{p,\alpha\beta}^{sf}$ by the relation $\omega_{p,\alpha\beta}^{sf} = c/\lambda_{L,\alpha\beta}$. It has often been mentioned that this function corresponds to the charge density of the superfluid condensate, but we would like to point out that this is only the case for noninteracting clean systems at $T=0$.

In the two-band model we have the standard expression (neglecting vertex corrections),^{38,39}

$$\begin{aligned} 1/\lambda_{L,\alpha\beta}^2(T) &\equiv [\omega_{p,\alpha\beta}^{sf}(T)/c]^2 \\ &= \sum_{i=\sigma,\pi} \left(\frac{\omega_{p,i}^{\alpha\beta}}{c} \right)^2 \pi T \sum_{n=-\infty}^{\infty} \frac{\tilde{\Delta}_i^2(n)}{[\tilde{\omega}_i^2(n) + \tilde{\Delta}_i^2(n)]^{3/2}}, \end{aligned} \quad (2)$$

where $\tilde{\omega}(n) = \omega_n Z(\omega_n)$ and $\tilde{\Delta}(\omega_n) = \Delta(\omega_n) Z(\omega_n)$ are the solutions of the Eliashberg equations^{8,9} and the calculated plasma frequencies for the σ and π bands are given in Ref. 8. Equation (2) corresponds to the standard parallel-conductor formula and does not contain cross terms $\tilde{\Delta}_i(\omega_n) \tilde{\Delta}_j(\omega_n)$. It is a consequence of the fact that in the

TABLE I. Penetration depth measurements by different methods and groups (MW=microwave, μ SR = muon spin relaxation, RF=radio frequency, FIR=far-infrared optical spectroscopy). Values for the estimated London penetration depth $\lambda_L(0)$, superfluid plasma frequency ω_p^{sf} , temperature dependence $\Delta\lambda(T)$, superconducting gap values Δ_0 , and ratios $2\Delta_0/k_B T_c$ are shown.

Method	$\lambda_L(0)$ (nm)	ω_p^{sf} (eV)	$\Delta\lambda(T)$	Δ_0 (meV)	$2\Delta_0/k_B T_c$	Ref.
ac + $M(H)$	200	0.99	$\sim T^{2.7}$			17
μ SR	100	1.98	two gaps	$\Delta_1=6.0, \Delta_2=2.6$	3.6, 1.6	19
H_{c1}			T			23
MW			T^2			24
μ SR+ac	85	2.33	T^2			25
RF	160 ± 20	1.24	BCS	2.8 ± 0.4	1.7 ± 0.2	26
FIR	300	0.66	BCS	2.5	1.9	27
MW	60	3.3	$T, T < T_c/2$			28
MW	110 ± 10	1.8	BCS	7.4 ± 0.25	≈ 4.5	29
RF			BCS	2.61	1.54	30
FIR	218	0.91		$2.5 < \Delta < 7.5$		31
MW ($T_c=37.9$ K)	100	1.98				32
MW ($T_c=26$ K)	1200	0.165				32
MW ($T_c=39$ K)	110	1.8	BCS, $T > 5$ K	3.8	2.26	33
MW ($T_c=36$ K)	115	1.72	BCS, $T > 5$ K	3.2	2.06	33

local limit ($\mathbf{q}=0$) the bare current vertex equals $\mathbf{v}_{F,i} \delta_{ij}$. The Eliashberg equations were solved numerically as described in Refs. 8 and 9.

The influence of impurities is incorporated into the model by including shifts of the gap function $\Delta_i^0(\omega_n)$ and the renormalization factor $Z_i^0(\omega_n)$,

$$\Delta_i \rightarrow \Delta_i^0 + \sum_j \gamma_{ij} \Delta_j^0 / 2 \sqrt{\omega_n^2 + (\Delta_j^0)^2},$$

$$Z_i(\omega_n) \rightarrow Z_i^0(\omega_n) + \sum_j \gamma_{ij} / 2 \sqrt{\omega_n^2 + (\Delta_j^0)^2},$$

in the Eliashberg equations. Intraband scattering does not change T_c and the gap values (Anderson's theorem), but influences strongly the penetration depth.

Before we start discussing the exact solutions to the Eliashberg equations we present a simplified model consisting of two independent BCS superconducting bands with different plasma frequencies and different gaps (and consequently different T_c 's). In spite of the fact that this model is clearly an oversimplification, it captures qualitatively most of the observed behavior. In this model the band with the larger T_c has the smaller plasma frequency (see Fig. 1).

For a clean system the resulting inverse squared penetration depth is the sum of the "superfluid plasma frequencies" (solid line). The kink in Fig. 1 is an artifact of the simplified model which will be smoothed out by interband coupling, but an inflection point in the temperature dependence of the penetration depth remains which has been observed experimentally, as will be discussed below (see Fig. 2). The low-temperature dependence is determined by the band with the smallest gap, whereas the high-temperature behavior results from the band with the larger gap. This is in accordance with the temperature dependence for low temperatures observed

in some experiments. If the superconducting band with the smaller gap will be "overdamped" due to impurities, then the penetration depth is only determined by the other band and it will show a BCS temperature dependence, which has also been observed in some experiments (see Table I).

For a proper understanding of the observed physical behavior of MgB₂ it is important that impurities are taken into account properly. Recently, the influence of impurities on the two-gap superconductivity has been discussed.⁴⁰ Using the same arguments we shall discuss two cases: (i) The clean case with scattering rates $\gamma_\sigma = \gamma_\pi = 2$ meV as realized in low-resistivity dense wires⁴¹ and (ii) the dirty case with $\gamma_\sigma = 54$ meV and $\gamma_\pi = 1.2$ eV. The values for the scattering

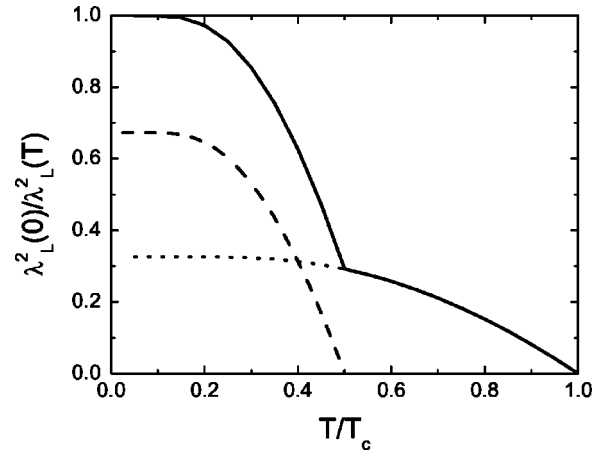


FIG. 1. Temperature dependence of the penetration depth in the model of two independent BCS superconducting bands (dashed and dotted line) with different superconducting gaps. The resulting penetration depth (solid line) clearly shows a non-BCS temperature behavior. The low-temperature behavior will be dominated by the band with the smaller superconducting gap.

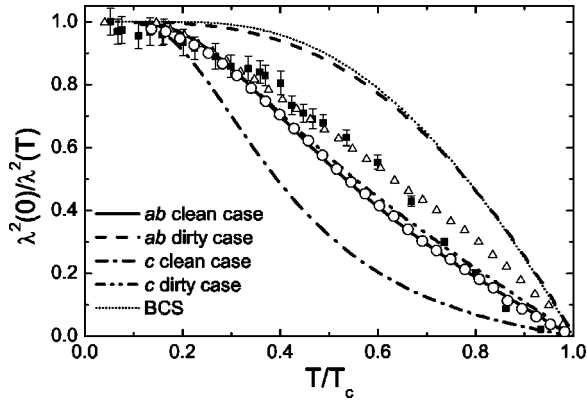


FIG. 2. The calculated temperature dependence of the penetration depth for the clean and dirty case (as defined in the text) in the ab plane and along the c axis, as well as a BCS curve corresponding to a single band case. For comparison experimental data from microwave experiments on single crystals (Δ) (Ref. 26), oriented films (\circ) (Ref. 33) and μ SR data on polycrystals (\blacksquare) (Ref. 19) are shown too.

rates in the dirty case, as well as negligibly small interband scattering rates,⁴⁰ are in accordance with the results on high resistivity films.³¹ The reason for weak interband scattering lies in the specific electronic structure of MgB₂, namely the electronic states in the 2D σ band only have a small overlap with the states in the Mg plane, where defects are most likely to occur.

Exact calculations, i.e., solving the Eliashberg equations for the effective two-band model with parameters derived from first-principle electronic structure calculations, have been carried out for the clean and dirty cases for a magnetic field along the c direction or in the ab plane. The results obtained can be presented in the form of the effective superfluid plasma frequency, ω_p^{sf} . Figure 2 displays the calculated $[\omega_p^{sf}(T)/\omega_p^{sf}(T \rightarrow 0)]^2 = [\lambda_L(T \rightarrow 0)/\lambda_L(T)]^2$ as a function of reduced temperature.

First we shall discuss the temperature dependence of λ_L^{ab} , when the magnetic field is oriented exactly along the c axis (this means that screening currents run in the ab plane). In the clean case the situation is similar to the model discussed above (Fig. 1). $\lambda_L^{ab}(T)^{-2}$ has an inflection point and the low-temperature behavior is determined by the band with the small gap Δ_π . In the dirty case the conductivity in the π band is strongly suppressed. This means that the screening currents in the ab plane are determined by the σ band with a BCS-like temperature dependence with a large gap Δ_σ . For the intermediate case the temperature dependence of $\lambda_L^{ab}(T)$ is between these limiting cases. One can even have situations with a nearly linear dependence in some temperature interval, as may be seen in Fig. 2. Experimental data from microwave experiments on single crystals²⁶ and oriented films³³ as well as μ SR data on polycrystals¹⁹ are shown for comparison in Fig. 2.

As may be seen from Eq. (2), the penetration depth in the c direction in the clean case is only determined by the π bands because of the very small plasma frequency of the σ band in this direction. It is interesting to notice that the tem-

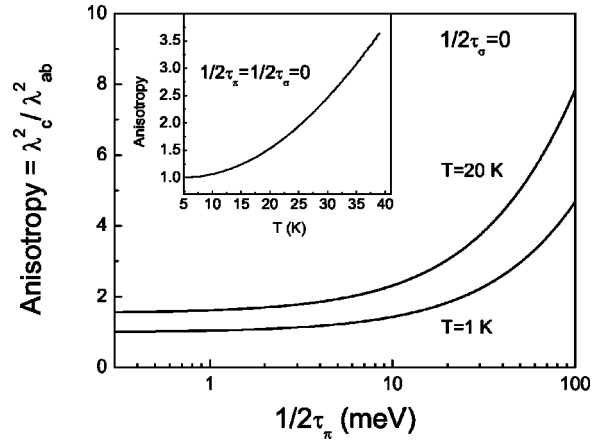


FIG. 3. The anisotropy of zero-temperature penetration depth vs impurity scattering rate in the π band. The inset shows the temperature dependence of the anisotropy for the clean limit.

perature dependence of the penetration depth in the dirty c -axis case follows the clean ab -direction case. This is caused by the fact that the σ channel is blocked by the small plasma frequency and the π channel is blocked by impurity scattering. However, the absolute values of the penetration depths differ by a factor of about 8 in these two cases. One may see that an inflection point is present in the temperature dependence even for this single-band contribution, because of the induced superconductivity at higher temperatures in the π band.

The corresponding London penetration depths at $T = 4$ K have the values $\lambda_{L,ab}^{clean} = 39.2$ nm, $\lambda_{L,c}^{clean} = 39.7$ nm, $\lambda_{L,ab}^{dirty} = 105.7$ nm, and $\lambda_{L,c}^{dirty} = 316.5$ nm. One may observe that even in the clean case the value of $\omega_{p,\alpha\beta}^{sf}(T \rightarrow 0) \approx 5$ eV from Eq. (2) differs from the total plasma frequency ≈ 7 eV as a consequence of strong-coupling effects due to electron-phonon interaction.

Table I summarizes the experimental information on the penetration depth $\lambda_L(T \rightarrow 0)$, the temperature dependence of the penetration depth $\Delta\lambda_L(T)$, and the estimated superconducting gap obtained by different experimental methods and groups. Our theoretical values of the penetration depths for the clean case are smaller than the smallest experimental value. On the other hand the values for the dirty case are in reasonable agreement with experiment. Nearly all measured penetration depths fall within our limiting cases (clean and dirty), and especially the observed BCS-like behavior at lower temperatures, reflecting the π -band contribution, is in agreement with our theoretical calculations.

It is well known that in a clean superconductor the low-temperature penetration depth is independent of the superconducting gap. In this case, the anisotropy is only determined by the ratio of the plasma frequencies in the ab plane and c directions. Hence, if the π band is very clean the penetration depth is nearly isotropic due to the small difference in the effective plasma frequencies. This is shown in Fig. 3, where one may also see that impurities in the π band drastically enhance the anisotropy. In the inset of Fig. 3 the temperature dependence of the anisotropy is shown for the clean case. The reason for the strong variation with tempera-

ture is that for high temperatures the difference of gaps also contributes. A similar observation has recently been made in a weak-coupling model.⁴²

A final remark concerns the orientation of the magnetic field. According to estimates in Ref. 8 the σ band does not contribute to the electronic transport for angles with the c axis larger than of the order of 1° . This implies that for larger angles the effective penetration depth is determined by the π band only. Only for angles approaching zero, the σ band contributes and the penetration depth decreases towards the minimal value corresponding to the screening current flowing in the ab plane, namely 39 and 106 nm for the clean and dirty case, respectively.

The above-mentioned considerations must be taken into account when interpreting the experimental data. In polycrystalline samples the penetration depth is mostly determined by the π band and therefore practically isotropic and it is similar to the c -axis penetration depth in Fig. 2. Our calculations for the dirty case describe qualitatively well the data in Ref. 19. On the other hand, the data for single crystals and oriented films correspond to our calculations of the ab -plane penetration depth, provided the magnetic field is oriented with an accuracy better than 1° along the c axis.

Therefore the data from Refs. 26 and 33 are described by our calculation for the clean case. Quantitative deviations can be attributed to a different impurity content and a possible admixture of c -axis contribution. The temperature dependence of the specific electrical resistivity is not provided in these papers however, which would be needed in order to estimate the impurity scattering rates.

In conclusion, we have used the results of first-principles calculations of the electronic structure and electron-phonon interaction in MgB_2 to calculate the magnetic-field penetration depth. The measured temperature dependence of the penetration depth is qualitatively well reproduced in a two-band model with the same set of parameters which was used to fit dc resistivity.^{31,41} We predict strong dependence of the anisotropy of the penetration depth on impurity scattering in the π band, while interband impurity scattering is negligibly small.⁴⁰ This anisotropy increases with increasing temperature.

We acknowledge many useful discussions with I. I. Mazin and A. D. Caplin. J.K. would like to thank the Schloebmann Foundation for financial support. This work was supported by the Dutch Foundation for Research on Matter (FOM).

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