PHYSICAL REVIEW B, VOLUME 65, 180517(R)

Multiband model for tunneling in MgB_2 junctions

A. Brinkman, A. A. Golubov, and H. Rogalla
Department of Applied Physics and MESA+ Research Institute, University of Twente, 7500 AE, Enschede, The Netherlands

O. V. Dolgov, J. Kortus, Y. Kong, O. Jepsen, and O. K. Andersen
Max-Plank Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569, Stuttgart, Germany

(Received 6 November 2001; published 9 May 2002)

A theoretical model for quasiparticle and Josephson tunneling in multiband superconductors is developed and applied to MgB_2-based junctions. The gap functions in different bands in MgB_2 are obtained from an extended Eliashberg formalism, using the results of band structure calculations. The temperature and angle dependencies of MgB_2 tunneling spectra and the Josephson critical current are calculated. The conditions for observing one or two gaps are given. We argue that the model may help to settle the current debate concerning two-band superconductivity in MgB_2.

DOI: 10.1103/PhysRevB.65.180517 PACS number(s): 74.50.+r, 74.70.Ad, 74.80.Fp, 85.25.Cp

Soon after the discovery of superconductivity in MgB_2[1], first principle calculations were performed to determine the electronic structure of this material. It was found that the Fermi surface consists of two three-dimensional sheets, from the π bonding and antibonding bands, and two nearly cylindrical sheets from the two-dimensional σ bands[2–5]. The multiband picture has given rise to the concept that two superconducting energy gaps can coexist[6,7] in MgB_2.

Two-band superconductivity is a phenomenon that has been observed in Nb doped $SrTiO_3$.[8] Recent experimental STM and point-contact spectroscopy,[9–11] high-resolution photo-emission spectroscopy,[12] Raman spectroscopy,[13] specific heat measurements,[14] and muon-spin-relaxation studies of the magnetic penetration depth[15] support the concept of a double gap in MgB_2 (see Ref. 16 for a review of experiments). However, there is an ambiguity in the interpretation of point-contact data concerning the existence of two gaps.[9–11] Moreover, some tunneling measurements[17] show only one gap with a magnitude smaller than the BCS value of $\Delta = 1.76\ k_BT_c$.

In order to resolve this discrepancy, we address the question, how multiband superconductivity will manifest itself in tunneling. We present the theoretical model for quasiparticle and Josephson tunneling in MgB_2-based junctions. Using the results of band-structure calculations, we apply an extended Eliashberg formalism to obtain the gap functions in different bands, taking strong coupling effects into account. Tunneling from a normal metal (N) into MgB_2 is considered in an extended Blonder-Tinkham-Klapwijk (BTK) model.[18] The temperature dependencies and absolute values of the I_cR_N product (I_c is the critical current and R_N is the normal state resistance) are calculated in MgB_2-based SIS tunnel junctions, where S denotes a superconductor and I an insulator. Tunneling in the direction of the *a-b* plane, in the *c*-axis direction and under arbitrary angle is considered. Furthermore, the Josephson supercurrent between a single-gap superconductor and MgB_2 is calculated.

According to the labeling of Liu *et al.*,[6] the four Fermi surface sheets in MgB_2 are grouped into quasi-two-dimensional σ bands and three-dimensional π bands. Hence, normal and superconducting properties of MgB_2 can be described by an *effective two-band model*. Within this model, Liu *et al.*[6] estimated the coupling constants and energy gap ratio in the weak coupling regime. More recently, the band decomposition of the superconducting and transport Eliashberg functions $\alpha^2_{ij}F_{ij}(\omega)$ (where i and j denote σ or π bands), which describe the electron-phonon coupling in MgB_2 as function of the frequency ω, was provided in Ref. 19. This allows to perform a strong coupling calculation of the superconducting energy gap functions $\Delta_i(\omega_n)$ in different bands. The functions $\Delta_i(\omega_n)$ in turn determine the Josephson critical current in a tunnel junction between multiband superconductors, which is given by a straightforward generalization of the well-known result[20] to the case of several conducting bands[21] as well as strong coupling. The critical current component for tunneling from band i into j is given by

$$I_{ij}=\frac{\pi T}{eR_{ij}}\sum_{\omega_n}\frac{\Delta_{\mathcal{L}i}(\omega_n)\Delta_{\mathcal{R}j}(\omega_n)}{\sqrt{\omega_n^2+\Delta^2_{\mathcal{L}i}(\omega_n)}\sqrt{\omega_n^2+\Delta^2_{\mathcal{R}j}(\omega_n)}}, \qquad (1)$$

where $\mathcal{L}$ and $\mathcal{R}$ denote left and right superconductors respectively, $R_{ij}^{-1}=\min\{R^{-1}_{\mathcal{L}ij},R^{-1}_{\mathcal{R}ij}\}$ is the normal-state conductance of a junction for the bands (i,j) which is given by the integral over the Fermi surface $S_{\mathcal{L}i(\mathcal{R}j)}$

$$(R_{\mathcal{L}(\mathcal{R})ij}\mathcal{A})^{-1}=\frac{2e^2}{\hbar}\int_{v_x>0}\frac{D_{ij}v_{n,\mathcal{L}i(\mathcal{R}j)}d^2S_{\mathcal{L}i(\mathcal{R}j)}}{(2\pi)^3v_{F,\mathcal{L}i(\mathcal{R}j)}}, \qquad (2)$$

where $\mathcal{A}$ is the junction area, v_n is the projection of the Fermi velocity v_F on the direction normal to the junction plane, and D_{ij} is the probability for a quasiparticle to tunnel from band i in $\mathcal{L}$ into band j in $\mathcal{R}$. The total critical current is the sum of the components $I_c=\Sigma_{ij}I_{ij}$.

The gap functions $\Delta_i(\omega_n)$ can be calculated with an extension of the Eliashberg formalism[23] to two bands

$$\Delta_i(\omega_n)Z_i(\omega_n)=\pi T\sum_j\sum_{\omega_m}\frac{(\lambda_{ij}-\tilde{\mu}^*_{ij})\Delta_j(\omega_m)}{\sqrt{\omega_m^2+\Delta_j^2(\omega_m)}}, \qquad (3)$$

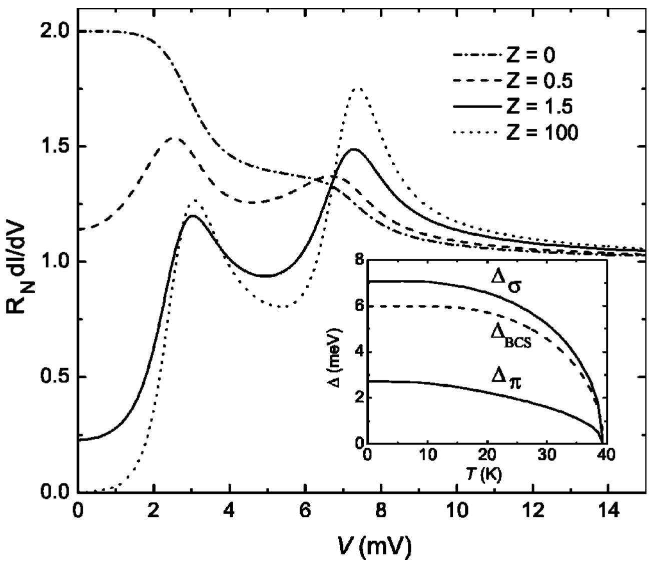

FIG. 1. The normalized conductance of MgB_2-I-N junctions as function of voltage at 4.2 K, with $Z=U_0/\hbar v_F$. The superconducting gaps for the different bands are shown in the inset.

$$Z_i(\omega_n)=1+\frac{\pi T}{\omega_n}\sum_j\sum_{\omega_m}\lambda_{ij}\frac{\omega_m}{\sqrt{\omega_m^2+\Delta_j^2(\omega_m)}}, \qquad (4)$$

where $\lambda_{ij}=2\int_0^\infty \omega\alpha_{ij}^2F_{ij}(\omega)d\omega/[\omega^2+(\omega_m-\omega_n)^2]$, $Z_i(\omega_n)$ are the Migdal renormalization functions and $\omega_n=\pi T(2n+1)$. These equations are solved numerically with the electron-phonon $\alpha_{ij}^2F_{ij}(\omega)$ functions from Ref. 19. The cutoff frequency ω_c is taken equal to 10 times the maximum phonon frequency. The functions $\tilde{\mu}_{ij}^*$ represent a matrix of the Coulomb pseudopotentials defined at ω_c, calculated up to a common prefactor that is used as an adjustable parameter to get $T_c=39.4$ K. The matrix μ^* at the frequency $\omega_{\ln}$ (relevant for the McMillan expression for T_c in the isotropic case) is given by $\mu^*=[1+\tilde{\mu}^*\ln(\omega_c/\omega_{\ln})]^{-1}\tilde{\mu}^*$, where $\omega_{\ln}$ follows from $0=\int_0^\infty \ln(\omega/\omega_{\ln})\omega^{-1}\alpha_{ij}^2F_{ij}(\omega)d\omega$. The corresponding matrix elements are $\mu_{\sigma\sigma}^*=0.13$, $\mu_{\sigma\pi}^*=0.042$, $\mu_{\pi\sigma}^*=0.03$, $\mu_{\pi\pi}^*=0.11$ and $\lambda_{ij}(\omega_m=\omega_n)$ from Ref. 19 are $\lambda_{\sigma\sigma}=1.017$, $\lambda_{\sigma\pi}=0.213$, $\lambda_{\pi\sigma}=0.155$, $\lambda_{\pi\pi}=0.448$. Due to the interband coupling terms in Eqs. (3) and (4) both gaps close at the same T_c. The resulting temperature dependencies of the energy gaps, $\Delta_i(T)$, are plotted in the inset of Fig. 1 and it is found that $\Delta_\sigma(T=0)=7.09$ meV and $\Delta_\pi(T=0)=2.70$ meV, with the $2\Delta/T_c$ ratios being equal to 4.18 and 1.59, respectively. For comparison, also the BCS curve is shown for $T_c=39.4$ K. The BCS value for the gap that corresponds to $T_c=39.4$ K is 6.0 meV at 0 K. It can be seen that the temperature dependencies are qualitatively different from the BCS temperature dependence. The ratio of the gaps Δ_σ/Δ_π increases for increasing temperatures, as was experimentally observed for example in Ref. 9.

The influence of impurities can be incorporated into the model. Intraband scattering does not change the two gaps (Anderson's theorem), while the interband scattering can be included by terms $\gamma_{ij}\Delta_j/\sqrt{\omega_n^2+\Delta_j^2}$, $\gamma_{ij}\omega_n/\sqrt{\omega_n^2+\Delta_j^2}$ in the

TABLE I. Calculated plasma frequencies, average Fermi velocities and gap values for the σ and π bands.

	ω_p^{a-b}(eV)	ω_p^c(eV)	v_F^{a-b}(m/s)	v_F^c(m/s)	Δ(meV)
σ band	4.14	0.68	$4.40\ 10^5$	$0.72\ 10^5$	7.09
π band	5.89	6.85	$5.35\ 10^5$	$6.23\ 10^5$	2.70

Eliashberg equations (3) and (4) respectively. The smallness of γ_{ij} compared to πT_c indicates that the double-gap feature should experimentally be observable, also in thin films, even for a certain amount of impurity scattering. A large amount of impurity scattering (γ_{ij} exceeding the maximum phonon frequency) will cause the gaps to converge to the same value. From Eqs. (3) and (4) and including the scattering terms an asymptotic value of $\Delta_\sigma=\Delta_\pi=4.1$ meV and $T_c=25.4$ K is found, giving a $2\Delta/k_BT_c$ ratio of 3.7.

In order to obtain the normal state resistance, we have to evaluate the effective junction transparency components D_{ij}. In the case of a specular barrier, $U(x)=U_0\delta(x-x_0)$, D_{ij} is given by

$$D_{ij}=\frac{v_{n,\mathcal{L}i}v_{n,\mathcal{R}j}}{\frac{1}{4}(v_{n,\mathcal{L}i}+v_{n,\mathcal{R}j})^2+U_0^2/\hbar^2}. \qquad (5)$$

It follows from Eqs. (2) and (5) and as first pointed out in Ref. 22, that the normal state conductance R_{ij}^{-1} in the large U_0 limit is proportional to the Fermi-surface average $\langle Nv^2\rangle_i$. The latter is proportional to the contribution of the electrons in band *i* to the squared plasma frequency $(\omega_p^i)^2$. This essentially simplifies the task of summing up the interband currents since the partial plasma frequencies are available from the band structure calculations[2–5]. The normal state junction conductance is thus proportional to $(\omega_p^i)^2_{\mathcal{L}}\langle v_n\rangle_{\mathcal{R}j}$, where $\langle v_n\rangle_{\mathcal{R}j}$ is the average Fermi velocity projection in the corresponding band (see Table I). In order to sum up the contributions of different bands, we restrict ourselves to the weighing factors $(\omega_p^i)^2$, neglecting the difference in $\langle v_n\rangle_{\mathcal{R}j}$. This is a reasonable approximation since the difference between v_F in the σ and π bands in the *a*-*b* plane is rather small, while for *c*-axis tunneling only the π band contributes, as will be shown later, so that the problem of summation does not appear in this case.

SIN tunneling. The conductance in a MgB_2-I-N tunnel junction is the sum of the contributions of two bands. Each of the conductances is given by the BTK model,[18] where the corresponding normal state conductances R_{Ni}^{-1} are proportional to the minimum of the square of the plasma frequencies at the N and MgB_2 sides. Since the plasma frequency in a typical normal metal (e.g. Au, Ag) is larger than the plasma frequencies in MgB_2, the conductances are limited by the electrons on the MgB_2 side

$$R_{N\sigma}^{-1}/R_{N\pi}^{-1}=(\omega_p^\sigma)^2/(\omega_p^\pi)^2. \qquad (6)$$

Finally, the normalized conductance of an N-I-MgB_2 contact is given by

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$$\sigma(V)\equiv\frac{\left(\frac{dI}{dV}\right)_{NIS}}{\left(\frac{dI}{dV}\right)_{NIN}}=\frac{(\omega_p^\pi)^2\sigma_\pi(V)+(\omega_p^\sigma)^2\sigma_\sigma(V)}{(\omega_p^\sigma)^2+(\omega_p^\pi)^2}. \quad (7)$$

Here, the dimensionless conductances $\sigma_{\sigma,\pi}(V)$ are provided by the BTK model, with the calculated values for the gaps and plasma frequencies, as shown in Table I.

In the conductance versus voltage plot (Fig. 1) for tunneling in the a-b direction, two peaks are clearly visible, in qualitative agreement with the experimental data.[9–11]. The ratio of peak magnitudes is not only determined by the ratio of the plasma frequencies, but also by thermal rounding and by the barrier strength $Z_{\rm BTK}=U_0/\hbar v_F$ (where v_F is taken constant for the different bands for the same reason as was given in the determination of R_{ij}). In particular, the peak at the smaller gap dominates in the small $Z_{\rm BTK}$ regime (point-contact), while the second peak dominates at large values of $Z_{\rm BTK}$ (tunneling), as may be seen in Fig. 1 at 4.2 K.

Due to the smallness of ω_p^σ in the c-direction, it can be seen from Eq. (7) that the conductance in the c-direction is only determined by the π band. In this case, no double-peak structure is expected in the conductance spectrum. This explains, together with the dependence on $Z_{\rm BTK}$, why in some experiments only one peak was observed[17] or why the second peak was weak.[9–11]

Note, that the assumption of the ratio of the normal state conductivities being equal to the ratio of the square of the plasma frequencies holds when the interface is a δ-function shaped tunnel barrier, with large $Z_{\rm BTK}$. This means that for small $Z_{\rm BTK}$, the results should be considered as a qualitative indication only. In the latter case, as well as for other types of barriers, a numerical integration of Eqs. (2) and (5) must be performed.

SIS Josephson tunneling. We consider Josephson tunneling between two MgB_2 superconductors. With the values for the plasma frequencies, $\omega_p^\sigma<\omega_p^\pi$, this gives $R_{\sigma\pi}=R_{\pi\sigma}=\max(R_{\sigma\sigma},R_{\pi\pi})=R_{\sigma\sigma}$ and $R_{\sigma\pi}/R_{\pi\pi}=R_{\sigma\sigma}/R_{\pi\pi}=(\omega_p^\pi/\omega_p^\sigma)^2>1$. The total conductance is given by $R_N^{-1}=\Sigma_{ij}R_{ij}^{-1}$.

For tunneling in the a-b plane (as can be realized for example in an edge configuration), with $R_{\sigma\pi}=R_{\pi\sigma}$ and $I_{\sigma\pi}=I_{\pi\sigma}$, the total I_cR_N product becomes

$$I_cR_N=\frac{I_{\sigma\sigma}R_{\sigma\sigma}+2I_{\sigma\pi}R_{\sigma\pi}+I_{\pi\pi}R_{\pi\pi}(\omega_p^\pi/\omega_p^\sigma)^2}{3+(\omega_p^\pi/\omega_p^\sigma)^2}. \quad (8)$$

The results of numerical calculations are presented in Fig. 2. Due to strong-coupling and interband coupling effects, the temperature dependencies of $I_{ij}R_{ij}$ differ from the well-known Ambegaokar-Baratoff result for an SIS junction between isotropic superconductors, most clearly demonstrated by the positive curvature of the $I_{\pi\pi}R_{\pi\pi}$ contribution. The I_cR_N value at $T=4.2$ K is 5.9 mV.

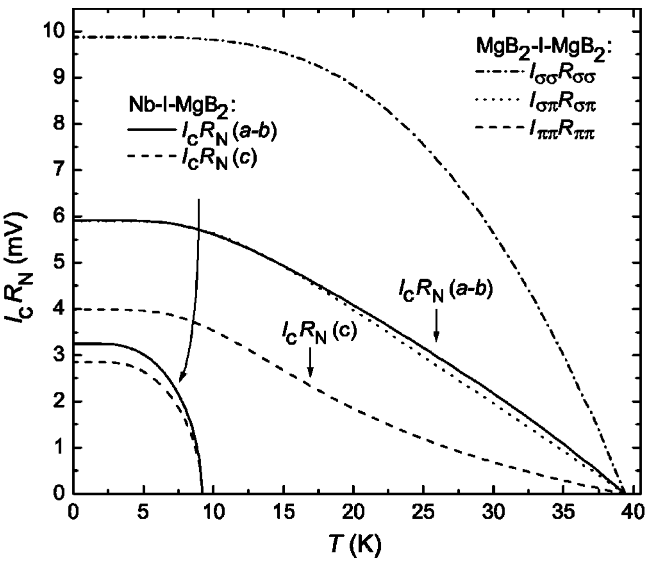

FIG. 2. I_cR_N temperature dependence for different tunneling components. The resulting I_cR_N for tunneling in the direction of the a-b plane and c-axis direction are indicated, for MgB_2-I-MgB_2 and Nb-I-MgB_2 junctions (see text).

For tunneling along the c-axis, the only contribution to the I_cR_N product comes from $I_{\pi\pi}R_{\pi\pi}$, because of the negligible value for ω_p^σ in the c-axis direction. This gives $I_cR_N=4.0$ mV at $T=4.2$ K.

The plasma frequency in a certain direction, under an angle φ with the a-b plane, can be determined from the ellipsoid equation $(\omega_p^i)^2=(\omega_{p,x}^i)^2+(\omega_{p,z}^i)^2$, and $(\omega_{p,z}^i/\omega_{p,c}^i)^2+(\omega_{p,x}^i/\omega_{p,a-b}^i)^2=1$, where $\omega_{p,x}^i$ and $\omega_{p,z}^i$ form the decomposition of ω_p^i. Because of the negligible value of $\omega_{p,c}^\sigma$, it is evident that ω_p^σ is negligible for nonzero values of $\varphi=\arctan(\omega_{p,z}^i/\omega_{p,x}^i)$. This implies that tunneling under a nonzero angle with the a-b plane gives the same result as tunneling in the c-axis direction, namely $I_cR_N=4.0$ mV at $T=4.2$ K. For angles approaching zero (of the order of 0.6°), I_cR_N rapidly increases towards the maximal value for tunneling from a-b plane to a-b plane, namely $I_cR_N=5.9$ mV at $T=4.2$ K. For a large amount of impurity scattering the $I_{ij}R_{ij}$ values converge to the same value. It follows in that case from Eq. (8), with the plasma frequencies from Table I, that I_cR_N becomes almost isotropic.

Finally, tunneling from MgB_2 into a superconductor S' with a single gap will be considered (we take Nb as an example). The resulting $I_{iS'}R_{iS'}$ temperature dependencies are calculated numerically, using 1.4 mV for the energy gap in Nb. The ratio of resistances is determined from Eq. (2). Since typical values of plasma frequencies in other superconductors are bigger than in MgB_2 (e.g., 9.47 eV for Nb, 12.29 eV for Al, and 14.93 eV for Pb, see Ref. 24), the following expression is obtained

$$I_cR_N=\frac{I_{\sigma S'}R_{\sigma S'}+I_{\pi S'}R_{\pi S'}(\omega_p^\pi/\omega_p^\sigma)^2}{1+(\omega_p^\pi/\omega_p^\sigma)^2}, \quad (9)$$

when tunneling occurs into the a-b plane of the MgB_2. In the case of c-axis tunneling, only the $I_{\pi S'}R_{\pi S'}$ contribution remains. The results for tunneling from Nb to MgB_2 are also indicated in Fig. 2. Other superconductors give qualitatively similar results. The only scaling parameter is the critical temperature of the superconducting counter-electrode.

Our results for Josephson tunneling provide an upper bound for I_cR_N products, being 5.9 mV and 4.0 mV for tunneling into the *a-b* plane and *c* direction respectively. There have already been several observations of Josephson currents in MgB_2 junctions,[25] with I_cR_N values that are much lower than our predictions. This can be due to extrinsic reasons such as a degradation of the T_c of surface layers in the vicinity of the barrier, the barrier nature and barrier quality. From our model, however, it follows that polycrystallinity does not reduce the Josephson coupling very much, as indicated by the calculated value of I_cR_N of 4.0 mV for *c*-axis transport, neither does strong impurity scattering because of the relatively large average gap of 4.1 meV in this case.

In conclusion, Josephson tunneling in MgB_2-based junctions is discussed theoretically in the framework of a two-band model. The gap functions in different electronic bands are calculated using the Eliashberg formalism together with band structure information. This provides a basis to interpret electronic transport in MgB_2. We have shown the possibility to observe either one or two gaps in point-contact spectra of MgB_2, depending on the tunneling direction, barrier type and amount of impurities. The results are also relevant for the electronic application of MgB_2 since they provide the limit for the Josephson coupling strength in MgB_2 based junctions. For MgB_2 in the clean limit we have shown that I_cR_N values as high as 5.9 mV can be expected for MgB_2 tunnel junctions if tunneling occurs in the direction of the *a-b* plane. In other cases the limiting I_cR_N values will not exceed 4.0 mV. Our predictions for the gap and I_cR_N anisotropy and for the I_c vs T dependence in MgB_2-based junctions can be verified experimentally and thus may help to settle the current debate on two-band superconductivity in MgB_2.

The authors thank D.H.A. Blank, H. Hilgenkamp, and I.I. Mazin for useful discussions. This work was supported by the Dutch Foundation for Research on Matter (FOM).

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