

Field Dependence of π -Band Superconducting Gap in MgB_2 Thin Films from Point-Contact Spectroscopy *

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We present the results of point-contact spectroscopy measurements on high-quality epitaxial MgB_2 thin films with injected current along the c -axis. The temperature and field dependences of π -band properties with the field parallel to ($H_{\parallel}$) or perpendicular to ($H_{\perp}$) the c -axis are investigated in detail. When a magnetic field is applied, either parallel or perpendicular to the c -axis, the density of the quasiparticle state (DOS) of the π -band proliferates quickly with increasing field, while the gap amplitude of the π -band decreases slowly, which is different from the recent theoretical calculations, showing a field dependent competition between the interband scattering and the pair-breaking effects.

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The binary alloy superconductor MgB_2 has stimulated plenty of efforts since its discovery because of its relatively high critical temperature ($T_c \approx 40\text{K}$).^[1] Up to now, it has been widely accepted that MgB_2 is a two-band superconductor (two-dimensional σ -band and three-dimensional π -band) with conventional electron-phonon pairing mechanism.^[2,3] Most prediction of the two-band model has been experimentally demonstrated in this system, such as high T_c value, momentum-dependent superconducting gaps and their temperature dependences, novel vortex phase diagram,^[4,5] etc. The roles of the intraband and interband scattering have been taken into account to explain the interesting evolution of the superconductivity both by applying magnetic field and by introducing various impurities.^[6–16] Recently, Koshelev *et al.*^[17] proposed a quantitative model for a dirty two-band superconductor which successfully explains the novel vortex structure in MgB_2 observed by STM.^[18] Furthermore, this model predicts the field dependences of the superconducting gaps and quasiparticle's density of states (DOS),^[17] which is in good agreement with the in-plane point-contact experiments.^[8] It was then concluded that even in the best MgB_2 crystals, the π -band is moderately dirty. As a consequence, the

averaged DOS of π -band at zero energy will proliferate quickly with increasing field and almost be saturated around H^* (below $0.2H_{c2}$), correspondingly, the maximum π -band pairing potentials will be seriously depressed below H^* . Up to date, more and more experiments are revealing diverse evolution of the two-band superconductivity by introducing both intrinsic and extrinsic disturbances, however the underlying mechanism is still not understood completely.

In this study, we concentrate on the spectra of Au-tip/ MgB_2 -film point-contact junctions measured at various temperatures and magnetic fields. The well-defined c -axis orientation of the injected current is achieved by careful preparation of junctions on the high quality thin films, and the π -band (with a weight of about 96%) dominated spectroscopy is then investigated in detail. It is surprising to find that although the temperature dependence of π -band gap (Δ_{π}) is in good agreement with the BCS prediction, the field dependence of Δ_{π} behaves very differently from that of π -band DOS. The origin of this novel field dependence of π -band gap is then discussed.

The MgB_2 films studied in this work were grown by the hybrid physical-chemical-vapour deposition technique^[19] on (0001) 4H-SiC substrates, and have

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a critical temperature of 41 K with a very sharp resistive transition. The thickness of the films is about 2000 Å. The good epitaxy with *c*-axis normal to the film surface was demonstrated by the measured x-ray diffraction pattern showing only the (001) peaks. The point-contact junctions were prepared by driving a mechanically sharpened Au tip (made of a $\phi 0.25$ mm gold wire) towards the surface of the epitaxial MgB₂ thin films.

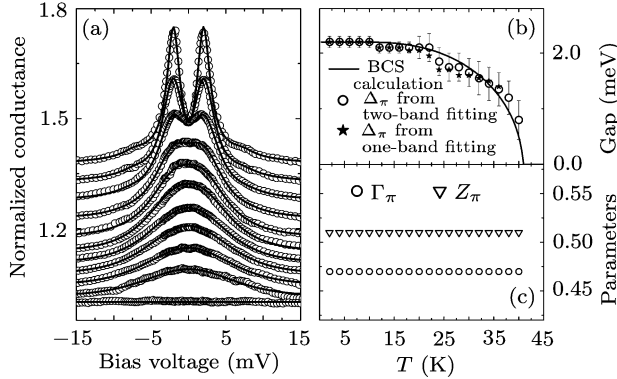


Fig. 1. (a) Normalized spectra of MgB₂ at various temperatures from 2 K to 42 K with steps of 4 K at $H = 0$ T, as shown by open circles. The solid lines are the fitting curves (all the curves except the lowest one are offset vertically for clarity). (b) The open circles and the solid stars show the temperature-dependent superconducting gap of π -band obtained by fitting the data to the two-band model and single-band model, respectively. The solid line indicates the BCS theoretical calculations. (c) Other parameters used in the BTK fitting include the broadening parameters Γ_π and the barrier height Z_π .

Figure 1(a) shows the temperature-dependent spectra from 2 K to 42 K. The sharp low-energy Andreev reflection peaks and the slight high-energy shoulders can be seen clearly on the highest curve measured at $T = 2$ K, corresponding to the contribution from the π -band gap and the σ -band gap, respectively. The well-known BTK model^[20] was used to analyse the data, in which the total normalized conductance ($G = dI/dV$) is given by $G = \omega_\sigma G_\sigma + (1 - \omega_\sigma)G_\pi$,^[21] where ω_σ is the weight of the σ -band, which is only associated with the relative orientation of the crystallographic axis with respect to the tunnelling barrier.^[12,22,23] Thus in the fitting process, the parameter ω_σ is kept to be constant for all the spectra obtained on a particular orientation at various temperatures and fields.

The fitting curves are denoted by the solid lines superposed on the experimental data. In the fits, we take seven parameters, i.e., gap amplitudes Δ_σ , Δ_π , broadening parameters Γ_σ , Γ_π , potential barriers Z_σ , Z_π , and the weight of the σ -band ω_σ . At $T = 2$ K, the fitting parameters are $\Delta_\sigma = 7.6$ meV, $\Delta_\pi = 2.2$ meV, $\Gamma_\sigma = 1$, $\Gamma_\pi = 0.47$, $Z_\sigma = 0.6$, $Z_\pi = 0.51$, $\omega_\sigma = 0.035$. Considering that the current is most possibly injected

within a finite solid angle, the very small value of $\omega_\sigma \approx 3.5\%$ is in good agreement with the theoretical prediction.^[24] Compared with the previous reports on the similar samples,^[2,8,9,12] the contribution of the σ -band is much smaller than that of π -band in this work, which makes it more easily to determine the π -band gap accurately.

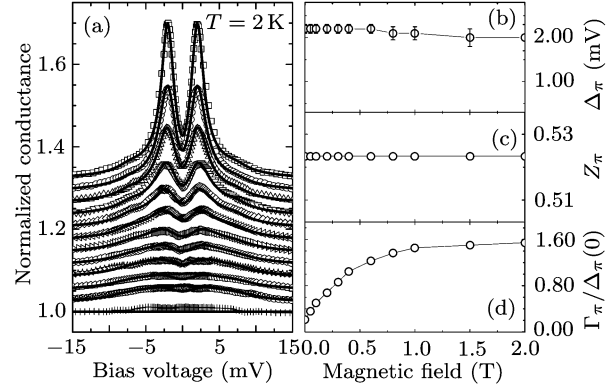


Fig. 2. (a) Normalized point-contact spectra of MgB₂ measured at $T = 2$ K in various magnetic fields $\mu_0 H = 0, 0.05, 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0, 7.0$ T with H parallel to the *c*-axis. The spectra for the fields between 2.0 T and 7.0 T are not shown because of their very weak signal (all the curves except the lowest one have been offset vertically for clarity). Here we take the fitting parameters: (b) field-dependent superconducting gaps of π -band; (c) barrier height Z_π ; (d) broadening parameters $\Gamma_\pi/\Delta_\pi(0)$.

For various temperatures, the fitting parameters of π -band are presented in Figs. 1(b) and 1(c). Due to the very small contribution of σ -band, the parameters of σ -band can not be determined accurately especially when the shoulders of the spectra are smeared out because of the thermal effect. However, this uncertainty of σ -band parameters has little influence on the parameters of π -band (which is also because of the small contribution of σ -band in this work). In Fig. 1(b), the π -band gaps determined by both the two-band model and a single-band one are compared. It can be seen clearly that both the models give the almost identical results in good agreement with the BCS prediction.

In Fig. 2(a), we present the Andreev reflection spectra measured at various magnetic fields from 0 T to 7 T at $T = 2$ K when the field is parallel to the *c*-axis. Since the signal becomes very weak at high field, we only focus on the data for the field lower than 2 T to reduce the possible artificial error. The fitting parameters of π -band are shown in Figs. 2(b)–2(d). The normalized broadening parameter of $\Gamma_\pi/\Delta_\pi(0)$ increases quickly at low field and becomes weakly field-dependent above 1 T, which is consistent with the previous reports suggesting relatively strong intraband scattering (and/or pair-breaking effect) in π -band.^[8,9,12,21] In other words, the π -band quasiparticles can be generated much more easily at low fields.

This can also be checked by directly evaluating the π -band DOS (S_{qp}), namely, $S_{qp}(H) = 1 - I(H)/I(0)$, where $I(H)$ is the area under the spectrum between ± 15 mV, which is roughly proportional to the superfluid density.^[2] In this work, $I(0) = 2.39$.

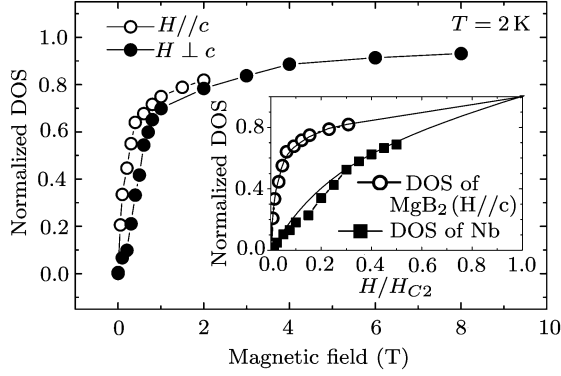


Fig. 3. Field dependence of the density of states (DOS). Inset: Comparison of the DOS with that of a conventional single band superconductor of Nb.^[25]

As shown in the inset of Fig. 3, the calculated DOS indicated by open circles increases rapidly until $H = 1$ T, above which it almost saturates and increases much slower. This is consistent with that of the STM experiment.^[18] This novel field dependence of DOS of π -band is very different from that of the conventional single band superconductors such as Nb (as presented in the inset of Fig. 3) and has drawn a great deal of attention. Moreover, the remarkable proliferation of π -band quasiparticles is a common feature for both $H_{\parallel}$ and $H_{\perp}$ although Δ_{π} extends to very different upper critical fields for these two configurations. As shown in the main panel of Fig. 3, both $DOS_{\parallel}$ and $DOS_{\perp}$ have an inflection at the same field (about 0.8 T) at which DOS becomes almost saturated while $H_{c2}^{\perp}$ is almost 4 times of $H_{c2}^{\parallel}$. This undoubtedly presents an explicit explanation of the field dependent anisotropy of MgB₂ (namely, almost isotropic at very low field while anisotropic above 0.8 T), which is in good agreement with the previous reports.^[12]

Recently, Koshelev and Golubov proposed a quantitative model to account for the vortex structure in a two-band superconductor with weak interband impurity scattering and rather strong intraband scattering rates exceeding the corresponding energy gaps (dirty limit).^[17] This model successfully explains the novel vortex structure observed in MgB₂^[18] and was demonstrated later by the in-plane Andreev reflection data^[8] in which both the field dependence of superconducting gaps and that of zero bias DOS (ZBD) are in good agreement with the theoretical prediction. However, in the present work a surprising finding is that, although the field dependence of DOS obtained in our experiments is consistent with the theoretical

calculations,^[17] the field dependence of Δ_{π} is remarkably different from the theoretical prediction. For comparison, the theoretical calculations^[17] of Δ_{π} and π -band ZBD for $D_{\sigma} = 0.2D_{\pi}$ (thin dashed lines) and $D_{\sigma} = D_{\pi}$ (thin solid lines) are presented in Figs. 4(a) and 4(b), where D_{σ} and D_{π} are σ -band and π -band diffusivity, respectively. It is obvious that the experimentally determined ZBD vs H/H_{c2} lies between the situations of $D_{\sigma} = 0.2D_{\pi}$ and $D_{\sigma} = D_{\pi}$ and much closer to the former one. On the contrary, Δ_{π} has a rather weak field dependence at low field which is inconsistent with the theoretical prediction. Furthermore, this is a common behaviour for various temperatures as shown in Fig. 4(a).

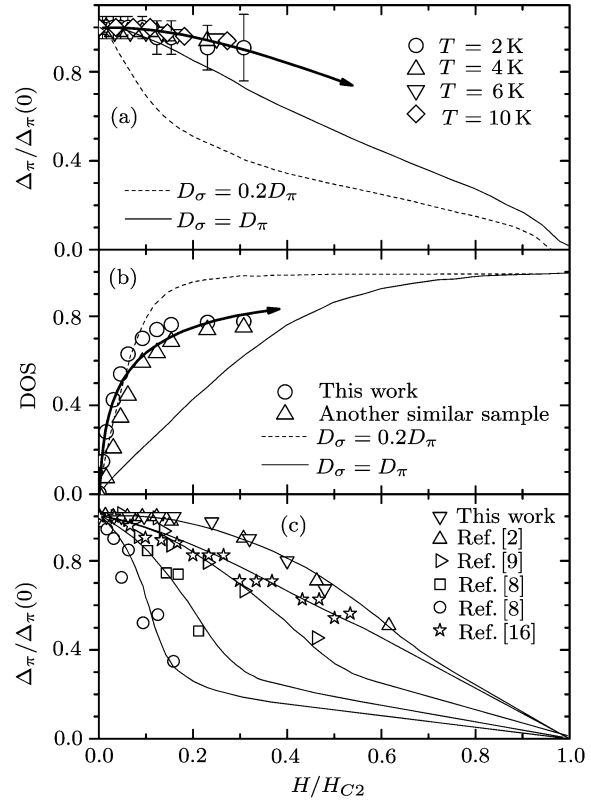


Fig. 4. Comparison of experimental results for H parallel to the c -axis and theoretical calculations for (a) superconducting gaps and (b) density of states of quasiparticles. The thick solid lines with arrows are the guides for eyes. The thin dashed lines and solid lines indicate the theoretical calculations for $D_{\sigma} = 0.2D_{\pi}$ and $D_{\sigma} = D_{\pi}$,^[17] respectively. (c) Field dependence of Δ_{π} reported by different groups. The thin solid lines in (c) are the guides for eyes.

This novel field dependence of Δ_{π} in contrast to that of ZBD can not be understood by the model proposed by Koshelev and Golubov.^[17] It has been mentioned that this model considers a two-band superconductor with weak interband scattering and rather strong intraband scattering without considering the field induced competition between interband scatter-

ing and pair-breaking. However, the π -band pairing is known to be partially induced by σ -band^[18] and hence may be sensitive to the imbalance between interband scattering and pair-breaking. This is indeed reflected by the diverse $\Delta_\pi(H)$ relations observed in various experiments as shown in Fig. 4(c). More recently, the role of interband scattering has been revealed by doping induced impurities^[10,11,13,16] and irradiation induced defects.^[14,15] Applying a magnetic field will lead to a pair-breaking effect and also change the strength of both interband and intraband scattering. Since π -band pairing strength is much weaker than that of σ -band, the field induced change of pair-breaking at low field should have stronger effect on π -band than on σ -band, meanwhile the re-balance of the pair-breaking effect and the field induced interband scattering is closely related to the practical condition of a given sample. This can reasonably explain the variable $\Delta_\pi \sim H$ relations for different measurements as shown in Fig. 4(c). In this picture, although the pair-breaking or intraband scattering excites plenty of quasiparticles in π -band, its pairing potential Δ_π can still be sustained^[5] due to the enhancement of interband scattering. Therefore, this is an interesting field-induced competition between interband scattering and pair-breaking effect which is worth further studying.

In summary, we have successfully prepared good point-contact junctions on high-quality MgB_2 thin films and investigated their spectroscopy in detail. The contribution from σ -band is demonstrated to be less than 5%, indicating the well-defined c -axis orientation of injected current. Then the physical quantities of π -band are accurately detected in a wide range of temperature and low field. When an external magnetic field is applied, either parallel or perpendicular to the c -axis, the π -band quasiparticles are rapidly excited at very low field, presenting an explicit explanation of the field dependent anisotropy of MgB_2 . On the contrary, the pairing potential of π -band decreases much slower and tends to persist up to H_{c2} , which can not be well described by the simplified two-band model recently proposed. The field induced re-balance of interband scattering and pair-breaking was then proposed to explain this novel phenomenon.

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