The Magnetic-field Dependence of the Gaps in a Two-band Superconductor: A Point-contact Study of MgB$_2$ Single Crystals

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We present the results of directional point-contact measurements in MgB$_2$ single crystals, in magnetic fields up to 9 T parallel to the c axis. By fitting the conductance curves of our point contacts — showing clear Andreev-reflection features — with a generalized Blonder-Tinkham-Klapwijk model, we were able to extract the values of the two gaps $\Delta_\sigma$ and $\Delta_\pi$. The comparison of the resulting $\Delta_\sigma(B)$ and $\Delta_\pi(B)$ curves to the theoretical predictions of the two-band model in dirty limit, recently appeared in literature, allows the first direct test of this model and gives a clear and quantitative proof that the $\pi$ band, even in the best single crystals, is in the moderate dirty limit.

PACS numbers: 74.45.+c, 74.70.Ad, 74.25.Op

More than two years after the discovery of superconductivity in MgB$_2$ \[1\], the great experimental and theoretical efforts of the entire scientific community have led to clarification of most features of this compound, mainly related to the existence of two band systems ($\sigma$ and $\pi$) and of the relevant gaps \[2\,3\]. Point-contact spectroscopy (PCS) has proved particularly useful in investigating MgB$_2$, since it allows measuring both the $\sigma$- and $\pi$-band gaps at the same time \[4\,5\] and determining the temperature dependency of these gaps with very high accuracy \[6\]. However, some controversial points are still present. In particular, the effects of a magnetic field on the gap values and on the $\pi$-band contribution to the total density of states (DOS) are still under debate, as well as the clean or dirty limit conditions of the two bands in the best samples and their influence on the measured physical properties. Both these topics can be addressed very well by performing accurate and directional PCS experiments in high-quality MgB$_2$ single crystals in the presence of magnetic field.

This paper presents some new results we obtained by PCS with magnetic fields up to 9 T applied parallel to the c axis of MgB$_2$ single crystals. These measurements gave us the magnetic-field dependence of the two gaps ($\Delta_\pi$ and $\Delta_\sigma$) which results in good agreement with the theoretical predictions for the mixed state in a dirty two-band superconductor where the $\pi$-band diffusivity $D_\pi$ is a few times greater than the $\sigma$-band one, $D_\sigma$ \[6\]. The consistency of this result is tested by comparing the zero-bias DOS calculated from our PCS data to the averaged zero-bias DOS predicted by the same model \[6\].

The high-quality single crystals we used for our measurements were produced at ETH (Zurich) by using the growth technique described elsewhere \[7\]. To control the direction of current injection, we chose only samples with regular shape, i.e. flat upper surface and sharp edges, even if these characteristics were fulfilled only by smaller samples (up to about 0.5×0.5×0.07 mm$^3$). The point contacts were made by using either a small spot of silver conductive paint or a small piece of indium. The advantages of this technique with respect to the standard one (that employs a metallic tip pressed against the sample) have been widely explained elsewhere \[8\,9\]. The normal-state resistance of our contacts ranges from 10 to 50 $\Omega$.

Due to the rather large mean free path of our single crystals ($\ell \approx 100$ nm) \[8\], they result to be in the ballistic regime \[5\].

In the experiments presented in this paper, the contacts were always placed on the narrow side of the crystals, so that, as already pointed out in previous papers \[8\,9\], the probability of electron injection was maximum along a direction parallel to the $ab$ planes. Thus, in the following we will refer to our contacts as “$ab$-plane contacts”. The intensity of the magnetic field applied to the samples could range from 0 up to 9 T and was affected by an uncertainty of about 1%, while the angle between the field and the $ab$ planes was always $\phi = 90 \pm 2^\circ$.

The conductance curves ($dI/dV$ vs. $V$) of our “spot” contacts were obtained by numerical differentiation of the $I-V$ characteristics, and then normalized to the normal-state conductance. The upper curve in Fig 4 (symbols) was obtained at $T = 4.2$ K in a Ag-paint contact. It has exactly the shape expected for a $ab$-plane contact \[8\], featuring symmetric conductance maxima at energies corresponding to $\Delta_\sigma$ and $\Delta_\pi$. This curve can be easily fitted by using a Blonder-Tinkham-Klapwijk (BTK) model generalized to the two-band case, where the total normalized conductance is given by $\sigma = (1 - w_\pi)\sigma_\sigma + w_\pi\sigma_\pi$.
FIG. 1: (a) Normalized conductance curves of a Ag-paint ab-plane contact, in increasing magnetic fields parallel to the c axis. Symbols: experimental data. Solid lines: best-fitting curves given by the two-band BTK model (see text). The curves are vertically shifted for clarity. (b) The same as in (a) but for a In-spot ab-plane contact on a different crystal.

Here, both $\sigma_\pi$ and $\sigma_\sigma$ are calculated in the case of a spherical Fermi surface (FS), which is obviously not the case of MgB$_2$. This problem cannot be overcome since, at present, there is no analytical theory for the Andreev reflection that takes into account the complex shape of the FS of MgB$_2$.

The fit has 7 free parameters: the gap amplitudes $\Delta_\pi$ and $\Delta_\sigma$, the potential barrier coefficients $Z_\pi$ and $Z_\sigma$, the lifetime broadening parameters $\Gamma_\pi$ and $\Gamma_\sigma$ and, finally, the weight $w_\sigma$. $\Gamma$ is a phenomenological parameter that usually accounts for pair-breaking effects (e.g. due to non-magnetic impurities), broadening the conductance curves and reducing their height with respect to the ideal ones. The best-fitting curve is shown in Fig. 1 as a solid line superimposed to the experimental data. The corresponding values of the fitting parameters are: $\Delta_\pi = 7.3 \pm 0.1$ meV, $\Delta_\sigma = 2.8 \pm 0.1$ meV, $Z_\pi = 0.944$, $Z_\sigma = 0.484$, $\Gamma_\pi = 3.3$ meV, $\Gamma_\sigma = 1.46$ meV, and finally $w_\sigma = 0.75$. The gaps are in very good agreement with the predictions of the two-band model (Eliashberg formulation) $\Delta$. The same happens for the weight $w_\sigma$ that is compatible with an injection cone of about 26° $\Delta$. The fit has 7 free parameters: the gap amplitudes $\Delta_\pi$ and $\Delta_\sigma$, the potential barrier coefficients $Z_\pi$ and $Z_\sigma$, the lifetime broadening parameters $\Gamma_\pi$ and $\Gamma_\sigma$ and, finally, the weight $w_\sigma$. $\Gamma$ is a phenomenological parameter that usually accounts for pair-breaking effects (e.g. due to non-magnetic impurities), broadening the conductance curves and reducing their height with respect to the ideal ones. The best-fitting curve is shown in Fig. 1 as a solid line superimposed to the experimental data. The corresponding values of the fitting parameters are: $\Delta_\pi = 7.3 \pm 0.1$ meV, $\Delta_\sigma = 2.8 \pm 0.1$ meV, $Z_\pi = 0.944$, $Z_\sigma = 0.484$, $\Gamma_\pi = 3.3$ meV, $\Gamma_\sigma = 1.46$ meV, and finally $w_\sigma = 0.75$. The gaps are in very good agreement with the predictions of the two-band model (Eliashberg formulation) $\Delta$. The same happens for the weight $w_\sigma$ that is compatible with an injection cone of about 26° $\Delta$. The fit has 7 free parameters: the gap amplitudes $\Delta_\pi$ and $\Delta_\sigma$, the potential barrier coefficients $Z_\pi$ and $Z_\sigma$, the lifetime broadening parameters $\Gamma_\pi$ and $\Gamma_\sigma$ and, finally, the weight $w_\sigma$. $\Gamma$ is a phenomenological parameter that usually accounts for pair-breaking effects (e.g. due to non-magnetic impurities), broadening the conductance curves and reducing their height with respect to the ideal ones. The best-fitting curve is shown in Fig. 1 as a solid line superimposed to the experimental data. The corresponding values of the fitting parameters are: $\Delta_\pi = 7.3 \pm 0.1$ meV, $\Delta_\sigma = 2.8 \pm 0.1$ meV, $Z_\pi = 0.944$, $Z_\sigma = 0.484$, $\Gamma_\pi = 3.3$ meV, $\Gamma_\sigma = 1.46$ meV, and finally $w_\sigma = 0.75$. The gaps are in very good agreement with the predictions of the two-band model (Eliashberg formulation) $\Delta$. The same happens for the weight $w_\sigma$ that is compatible with an injection cone of about 26° $\Delta$. We can now try to fit in the same way the conductance curves measured in the presence of magnetic field. Due to the lack of an analytical theory of Andreev reflection for a two-band superconductor in magnetic field, this fit can be simply performed by using the lifetime broadening parameters $\Gamma_\sigma,\pi$ to mimic the effect of the magnetic field, as in Ref. 10. In this case, the total broadening parameter $\Gamma$ is considered as the sum of an intrinsic $\Gamma_i$, due to the lifetime of quasiparticles, and an extrinsic $\Gamma_f$ due to the effect of the magnetic field: $\Gamma = \Gamma_i + \Gamma_f$. This approach assumes that the field breaks pairs in a way that can be represented by the quasiparticle lifetime, while its effects on the DOS are negligible in a first-order approximation.

Unfortunately, at $T = 0$ K the effects on the DOS curves of both the magnetic field and the actual shape of the FS are very relevant $\Delta$ $\Delta$, so that our BTK-lifetime model fails in fitting them. We expect similar large effects to be also present in the Andreev-reflection conductance at $T = 0$ K. Nevertheless, at low but finite temperature (for example, $T \simeq 4$ K) the thermally-broadened theoretical DOS curves become much more similar to those given by the standard BTK-lifetime model. To clarify this point, we tried to fit with this model some theoretical DOS curves at $T = 4$ K in the presence of magnetic field parallel to the $c$ axis, i.e.: i) the local $\pi$-band DOS curves calculated at various points of the vortex-lattice unit cell $\Delta$, ii) the two-band DOS calculated by taking into account the actual (simplified) shape of the FS of MgB$_2$, made up of a distorted cylinder (for the $\sigma$ band) and a half torus (for the $\pi$ band) $\Delta$. In both cases the lifetime-broadened BTK model proved very effective in fitting the theoretical curves in all the energy range, apart from some deviations ($< 30\%$) at very small energies ($eV < 3$ meV). The gap values determined from the fit are close to the theoretical ones used to generate the curves, suggesting that $\Gamma_f$ can mimic rather well the pair-breaking effect of the field at finite temperature.

Thus, we can now proceed with the BTK fit of our experimental curves at $B \neq 0$. Up to about 1 T the fit is carried out by taking into account the contribution of the two bands, while above this field the fit can be obtained with no contribution of the $\pi$ band (i.e. by taking $\sigma_\pi = 1$). The best value of $w_\sigma$ determined from the zero-field curve was kept constant in all the other fits. As in most junctions, also the values of $Z_\pi$ and $Z_\sigma$ could be taken practically constant at the increase of the field, so that the actual free fitting parameters at $B \neq 0$ are $\Delta_\sigma, \Delta_\pi, \Gamma_\sigma$ and $\Gamma_\pi$. The solid lines in Fig. 1, represent the curves that best fit the experimental data (circles). It is clear that the fit is very good, even if it cannot reproduce the asymmetry of some experimental curves.

In Fig. 1, the experimental conductances (circles) and the corresponding best-fit curves (solid lines) are shown for another junction obtained by pressing a very small In spot on the side surface of a MgB$_2$ crystal. The best-fit parameters for the zero-field curve are: $\Delta_\sigma = 7.0 \pm 0.1$.
meV, $\Delta_\pi = 3.1 \pm 0.2$ meV, $Z_\sigma = 0.51$, $Z_\pi = 0.41$, $\Gamma_\sigma = 3.0$ meV, $\Gamma_\pi = 1.86$ meV, and $w_\pi = 0.7$. A comparison with the corresponding values of Fig.1 shows that the big difference in shape between the curves in (a) and (b) is mainly due to the reduction of $Z_\sigma$ by a factor of two, while all the other parameters are practically unchanged. This is probably due to the different nature of the contact in the two cases (Ag paint in (a), indium in (b)).

Figs. 2a and 2b report the field-dependence of the two gaps (solid circles) obtained by fitting the conductance curves of Fig. 1a and 1b, respectively. It is clearly seen that, for $B < 1$ T, the $\pi$-band gap decreases at the increase of the field while the $\sigma$-band gap remains practically unchanged. Above 1-1.2 T there is no longer trace of features related to $\Delta_\pi$ in the conductance curves and, therefore, nothing can be concluded about this gap. The vanishing of the $\pi$-band contribution was observed in all the point contacts on MgB$_2$ crystals we studied in magnetic field (more than 10). This result is in complete agreement with many other experimental results present in literature and with the theoretical predictions of Ref. 4, even if a very recent paper claims the possibility to determine the $\pi$-band gap up to about 5 T by PCS on MgB$_2$ films 17.

In both Figs. 2a and 2b, dashed lines represent the field dependence of the maximum pair potentials ($\Delta^\sigma_{\text{max}}$ and $\Delta^\pi_{\text{max}}$) calculated at the boundary of the vortex-lattice unit cell for $B \parallel c$. Even if our data rather represent an average of the conductance in different regions of the vortex lattice, the similarity between experimental data and theoretical curves is remarkable, provided that the overall shape of the curves is considered rather than the absolute gap values. In Fig.2a, the initial decrease of $\Delta_\pi$ is strikingly similar to that of $\Delta^\pi_{\text{max}}$, in the case where $D_\sigma = 0.2 D_\pi$. The behavior of $\Delta_\pi$ in Fig.2b is more linear, and is here compared to the theoretical curve calculated with $D_\sigma = D_\pi$. As far as $\Delta_\sigma$ is concerned, its field dependence agrees very well with the theoretical curve in both cases. In Fig.2b, the theoretical curve well reproduces the tendency of $\Delta_\sigma$ to saturate at low fields.

The internal consistency of the results reported so far can be checked by calculating the zero-bias DOS (ZBD) with the parameters we got from the fits, and comparing its field dependence with that reported in Ref. 6. To do this, i) we took the fitting parameters of each curve of Fig. 1a and 1b, and ii) we put $Z_\sigma,\pi = 20$ and assumed a negligible contribution of the intrinsic lifetime broadening, i.e. we put $\Gamma^\sigma,\pi = 0$; iii) we calculated with the lifetime-broadened BTK model the tunneling conductance curve at $T = 0$ K, by using the values of $\Delta_\sigma, \Delta_\pi$, $w_\pi$ and $\Gamma^\sigma,\pi$ from the fit. The separation between intrinsic and field-induced pair-breaking effects is possible since the former are reasonably field-independent and can thus be determined from the fit of the zero-field curves. This procedure is somehow similar to that used in Ref. 6 to evaluate the field-dependence of $\gamma$, which is in fact a thermodynamic probe of the low-energy DOS.

In Figs. 3a and 3b the values of the ZBD determined from the data of Fig. 1a and 1b (solid circles) are compared to the total theoretical averaged DOS at $\epsilon F = 0$ (solid and dashed curves) derived from the partial $\pi$- and $\sigma$-band ZBD calculated in Ref. 6. In the case of Fig. 3a, the agreement between the data derived from the experiments and the theoretical ZBD for $D_\sigma = 0.2 D_\pi$ is impressive. On the other hand, the data of Fig. 3b lie between the total ZBD for $D_\sigma/D_\pi = 5$ and $D_\pi/D_\sigma = 1$, thus suggesting that an intermediate value of this ratio would allow a proper fit of the experimental data. Both these last results are fully consistent with those shown in Fig. 2. However, this agreement is not trivial since the quantities reported in Fig. 2 and Fig. 3 are almost independent. In fact, it can be easily shown that, for a given DOS curve, the value of the ZBD is little dependent on the gap amplitude, but strongly depends on the values of $\Gamma^\sigma_\pi$ and $\Gamma^\pi_\sigma$. As a consequence, the consistency of the two different comparisons gives a strong evidence of the validity of our results.

To summarize, these results indicate that: i) the lifetime broadening can be used, as a first approximation, to mimic the effect of the magnetic field in the BTK fit.
of Andreev-reflection curves measured in MgB$_2$ at finite temperature; ii) the field dependencies of $\Delta_{\sigma,\pi}$ and of the ZBD deduced from the experiments provide a clear and quantitative evidence that, even in the best single crystals, the $\pi$ band is in moderate dirty limit ($D_\sigma \simeq 5D_\pi$), in complete agreement with recent STM [12] and de Haas-van Alphen [18] results on the same crystals, as well as with the model for electric transport in MgB$_2$ [13] and the theory of the mixed state in a dirty two-band superconductor [14]; iii) different crystals, even if apparently produced in the same way, may have different values of the diffusivity ratio $D_\sigma/D_\pi$, i.e. different degrees of cleanliness of the $\sigma$ band.

Some final comments are necessary on the zero-field values of $\Delta_\pi$ and on the upper critical field $B_{c2}^{\parallel c}$ implicitly reported in Fig. 2. First, our PCS values of $\Delta_\pi$ ($\simeq 2.7 - 2.8$ meV) [21] are systematically greater than those given by STM ($\simeq 2.1 - 2.2$ meV) [12]. Since the accuracy of both the techniques is out of discussion, this difference has probably a physical reason that is still under investigation. Let us just remind here that the values of $\Delta_\pi$ are distributed between 1 and 3 meV over the FS [20], with a maximum at about 2 meV. Moreover, strong-coupling calculations [22] give an average value over the FS $\Delta_\pi = 2.7$ meV. This might suggest that, while STM is more sensitive to the maximum of the distribution, PCS gives a weighed average of $\Delta_\pi$ over the FS. As far as the critical field $B_{c2}$ is concerned, we recently determined it by PCS for both $B \parallel c$ and $B \perp c$ [21]. We always got values greater than those of $B_{c2}$ measured by bulk techniques (torque magnetometry, specific heat) and smaller than the surface critical field $B_{c3}$ [21]. The results will be widely discussed in a forthcoming paper, but we can anticipate that the high values of $B_{c2}$ measured by PCS are probably related to some non-trivial surface effects.

In conclusion, in this paper we have presented the first detailed determination of the magnetic-field dependency of the gaps in a two-band superconductor by using the point-contact technique in high-quality MgB$_2$ single crystals. The results allow the first direct test of the recent theory for the mixed state in a dirty two-band superconductor. Moreover, they give clear and self-consistent evidence of the moderate dirty-limit conditions for the $\pi$ band and of the variability of these conditions from sample to sample.

We are indebted to T. Dahm, O.V. Dolgov, A.A. Golubov and I.I. Mazin for discussions and suggestions. V.A.S. acknowledges the support from RFBR (project N. 02-02-17133), the Ministry of Science and Technologies of the Russian Federation (contract N. 40.012.1.1.1357) and the INTAS project N.01-0617. This work was done within the project PRA ”UMBRA” of INFM and the ASI contract N. I/R/109/02.

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[22] In particular, we cannot say that $\Delta_\sigma = 0$ for $B \geq B^* = 1.2$ T. Thus, the identification of $B^*$ (at which the $\sigma$-band features disappear) with $B_{c2}$ might not be correct.

FIG. 3: (a) Symbols: magnetic field dependence of the zero-bias DOS (ZBD) calculated with $\Delta_{\sigma,\pi}$ and $\Gamma_{\pi,\pi}$ obtained by the fit of the curves of Fig. 2, and taking $Z_\sigma = Z_\pi = 20$. Solid line: field dependence of the theoretical ZBD for $w_\pi = 0.75$, when $D_\pi = 0.2D_\sigma$ [21]. (b) Symbols: ZBD calculated as in (a) from the curves of Fig. 1b. Solid line: same as in (a) but with $w_\pi = 0.70$. Dashed line: field dependence of the ZBD when $w_\pi = 0.70$ and $D_\pi = D_\sigma$ [21].