Energy gap substructures in conductance measurements of MgB₂-based Josephson junctions: beyond the two-gap model

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Abstract
Several theoretical analyses of the two superconducting energy gaps of magnesium diboride, Δₓ and Δᵧ, predict substructures within each energy gap. We report additional experimental evidence for these features, in tunneling conductance data using multiple samples measured at very low temperatures. The absence of these features in c-axis tunneling, and a sharp peak in the subgap (associated with the counter electrode material), support the conclusion that these features are intrinsic to MgB₂. By demonstrating the inadequacy of a simple two-gap model in fitting the data, we illustrate that distinctions between theoretical models of energy gap substructures are experimentally accessible.

Keywords: magnesium diboride, Josephson junctions, superconducting energy gap, tunneling spectroscopy, multi-gap superconductivity, two-gap superconductivity, energy gap substructure

Introduction
Magnesium diboride (MgB₂) has two well-separated energy gaps, which makes it a particularly interesting object of study. Although there had long been both experimental [1, 2] and theoretical [3–5] suggestions of two-gap superconductivity, MgB₂ was the first material to put the matter beyond dispute [6]. Multi-gap superconductivity has recently attracted increased interest, with its demonstration in a variety of materials, including pnictides [7].

As theories were developed for understanding superconductivity in MgB₂, it was recognized that its superconducting energy gap must be both anisotropic and multi-valued: the higher energy gap is associated with the strong σ bonds in the Boron planes, and the lower energy gap is associated with the weaker three-dimensional π bonds. Three theoretical analyses predict sub-features within each energy gap of MgB₂, due to its electron-phonon interactions. Figure 1 shows portions of these theoretical results, which we compare with our data. The model of Choi et al [8]. (hereafter referred to as theory I) was among the earliest to show a distribution in gap energies explicitly. The model of Floris et al [10] (theory III) revealed that, near the Fermi energy (ϕ – EF = 0), each energy gap is a distribution, rather than a single energy. A more recent model from Margine and Giustino [9] (theory II) also exhibits a distribution in the superconducting gaps of MgB₂. Although each model determines the gap distribution from first principles, differing assumptions and parameter values are applied. These lead to differences in the features of the gap distributions, and the energies at which they appear. While a large number of measurements have provided evidence for two superconducting energy gaps in MgB₂...
create a complete physical model of the dynamics of the junctions. Instead, we chose the simplest possible models, with the fewest free parameters—models which were sufficient for much of the published data revealing two gaps (see, e.g. [13]). Our data clearly resolve the difference between these simple models and the true nature of the energy gap distribution of MgB$_2$. As a result, our findings are one of only a few published data sets [17–21] able to help distinguish between competing more complete theoretical models.

We begin our analysis with the current–voltage characteristics of a generalized junction between two materials,

$$I(V) = G_n \int_{-\infty}^{\infty} N(E)N_2(E + eV) \times [f(E) - f(E + eV)] \, dE,$$

where $G_n$ is the normal-state conductance of the junction (assumed constant), $N(E)$ is the density of states for each electrode, and $f(E)$ is the Fermi distribution. Using the BCS density of states for each superconducting electrode

$$N(E) = \Re \left\{ \frac{E^2}{\sqrt{E^2 - \Delta^2}} \right\},$$

one is able to reproduce the current–voltage characteristics of a basic tunnel junction (neglecting the Josephson supercurrent). Because each junction used in our study has two different electrode materials, each density of states will use a different energy gap $\Delta_1$ and $\Delta_2$, where $\Delta_1$ ($\Delta_2$) represents the lower (higher) of the two gaps.

In the simplified model we have used (matching that described in [13]), two additional effects are considered: Broadening Factor $\Gamma$: Dynes et al [23] found a broadening in conductance peaks that could not be attributed to temperature. Instead, the quasiparticle lifetime provides a broadening that can be accounted for by replacing all instances of $E$ with $E + i\Gamma$ in the BCS density of states.

$\Gamma$ has also been used to simulate the effect of a convolution of the theoretical conductance with a distribution of gap values [13]. In this paper, we model the gap distribution as distinct gap energies, with a broadening that phenomenologically matches the experimental gap distribution from our experiments.

Including a constant $\Gamma$ reveals a feature in the subgap region of the $I$–$V$ curve, which we have observed and used in our analysis. When $\Gamma$ is included, the modified BCS density of states is nonzero, even at $E = 0$, whether or not the transparency of the junction is zero. This allows the formation of peaks at $\Delta_1$ and $\Delta_2$ in the subgap region, down to $T = 0$, in the absence of Andreev reflections (which require a finite transparency). Because of their strong sensitivity to thermal broadening, the peaks virtually disappear above 3 K in theoretical calculations using values similar to those of our junctions. But, the peak at $\Delta_1$ becomes quite sharp as $T \to 0$.

Weighting for multiple gaps: an additional refinement must be made when considering a multi-gap superconductor. For a model including both the $\pi$ and $\sigma$ gaps of MgB$_2$, the

Simple two-gap and four-gap theory

In our analysis, we compare and contrast our data with two-gap and four-gap theoretical fits. The fits are not an attempt to

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**Figure 1.** Normalized conductance data of MgB$_2$, obtained using MgB$_2$/I/Pb and MgB$_2$/I/Sn junctions, compared with theory. Curves are offset for clarity. For the data, the counter electrode gap energy has been subtracted, leaving only the contribution from MgB$_2$. Theory I [8] and theory II [9] show the local density of states versus superconducting energy gap, for energies within 0.01 eV of the Fermi energy at $T = 0$. A histogram of its points, at the Fermi energy, would produce distributions analogous to theories I and II. The data resolve features that may be useful in refining theoretical models. (Theory I reprinted with permission from Macmillan Publishers Ltd: [8], copyright 2002. Theory II reprinted with permission from [9]. Copyright 2013 by the American Physical Society. Theory III reprinted with permission from [10]. Copyright 2005 by the American Physical Society.)

[6, 11–16], the predicted substructures within each energy gap have been found in relatively few experiments [17–21]. These fine features have been thought to be unobservable in physically-realistic samples [22]. Their observation opens a new avenue for exploring superconductivity in MgB$_2$.

We have conducted differential conductance measurements on MgB$_2$/I/Pb and MgB$_2$/I/Sn junctions with a variety of film geometries. The samples were cooled to temperatures ranging from several Kelvin down to 20 mK, to reduce thermal broadening in order to access higher resolution in the energy gap. Above $T_c$, of the Pb or Sn counterelectrode, our results are consistent with a simple two-gap model. However, below $T_c$ and down to 20 mK, our results distinguish between predictions from simplified two-gap and four-gap models. Therefore, we demonstrate the need to go beyond the two-gap model, and provide data useful in refining more advanced models.
density of states becomes:

\[ N(E) = w_\pi N_\pi(E) + w_\sigma N_\sigma(E). \]  

(3)

Because the sum of the weights must equal 1, a single weighting factor may be used (substituting \( w_\pi = 1 - w_\sigma \)). If additional peaks are observed, they can be modeled as additional gaps, each with its own gap energy \( \Delta \), its own broadening factor \( \Gamma \), and its own weight \( w \), as long as the sum of the weights equals 1.

The weighting factors for MgB2 depend on junction geometry, with \( w_\pi = 1 - w_\sigma \) ranging from less than 1% for pure \( c \)-axis tunneling, to \( \sim 33\% \) for pure \( a-b \) plane tunneling [13].

However, as indicated by the theories shown in figure 1, two smoothly-broadened gaps (one each for \( \pi \) and \( \sigma \)) are not sufficient to represent the density of states of MgB2. As a result, within the \( \pi \) (or \( \sigma \)) gap, substructures are necessary, each with its own weighting factor. For simplicity, we have chosen to model each structure as its own gap, with its own broadening.

From the Fermi surface of MgB2, it is evident that the observable contributions to each gap will be dependent on the tunneling direction. Therefore, the weights for each substructure should differ for different samples.

We have chosen to compare and contrast our data with a simple two-gap model (one gap for \( \pi \) and one for \( \sigma \)) versus a model consisting of four-gaps (two each for \( \pi \) and \( \sigma \)). We have observed that, below \( T_c \) of the Pb or Sn counter-electrode, a four-gap model is superior. Above that temperature, the features are sufficiently broadened that only two peaks may be distinguished, whether a two-gap or four-gap model is used (see figure 2).

Hereafter, we will refer to these gaps as \( \pi_1, \pi_2, \sigma_1 \), and \( \sigma_2 \), with subscripts 1 (2) referring to the lower- (higher-) energy sub-peaks of the \( \pi \) and \( \sigma \) gaps. We assume a single sample-dependent gap value \( \Delta \), broadening parameter \( \Gamma \), and weight \( w \) for each gap. We emphasize that we are not suggesting a physical source for these gap values. Instead, they serve as a convenient model for the true gap distribution.

**Experimental design**

Tunneling conductance curves are well-suited for determining the energy gaps and densities of states of superconducting materials. The differential conductance of an NS junction at \( T = 0 \) is proportional to the density of states of the superconductor; at finite temperature, it is smeared by \( \sim \pm 2kT \) [24].

In SIS' junctions, the 'very sharply peaked densities of states at the gap edges of both materials helps to counteract the effects of thermal smearing [24]' (see figure 2). By using SIS' junctions at mK temperatures, incorporating extremely high-quality MgB2 films, we maximize our ability to resolve features within the energy gaps.

For this study, we used MgB2/Pb and MgB2/I/Sn tunnel junctions incorporating high purity MgB2 thin films grown by hybrid physical-chemical vapor deposition (HPCVD) on single-crystal SiC substrates [19]. As found by Dai et al [18], on smooth 0° SiC, a largely-planar MgB2 film forms, exposing primarily the \( c \)-axis for tunneling. On SiC whose polished surface is tilted 8° from the \( c \)-axis, the MgB2 film takes on a ‘terraced’ shape, exposing the \( a-b \) plane. On rough 0° SiC, the growth of the MgB2 film forms columnar structures, exposing even more of the \( a-b \) plane, while still maintaining clean high-quality films. (See figure 3).

The insulating barrier is formed by a native oxide, which forms upon exposure of the film to air, and creates a good tunnel barrier under proper conditions. A Pb or Sn counter-electrode \( \sim 0.3 \) mm wide is then thermally evaporated on a \( \sim 0.3 \) mm exposed strip of the film.

These junctions are cooled in a helium dilution refrigerator with a base temperature \( \sim 20 \) mK. This system is designed for measurements at very low temperatures. Therefore, it is difficult to maintain steady temperatures above 4 K, and the thermometer closest to the sample is calibrated for 6 K and below. As a result, no data are presented above 6 K. Complementary data on similar junctions may be found in [18], at temperatures from 1.8 to 40 K. As those results use a completely different experimental platform, on a number of other samples, our results are proven to be robust and reproducible.

The current bias for our junction was provided by sweeping the voltage from an Agilent 3220A function generator, through a bias resistor. By ensuring \( R_{bias} \gg R_{junction} \), this combination behaves effectively as a current source. The resulting voltage across the junction was amplified, then recorded.

The current bias was swept at between 10 mHz and 1 Hz, while measurements were acquired from 10 to 48 kHz. Such oversampling allows numerical differentiation to produce high-resolution results, by averaging adjacent data points. The number of points in each average was proportional to the time spent near any given voltage. All results were robust under a variety of averaging methods, and a number of results were verified using an SR830 lock-in amplifier, demonstrating that the features are not an artifact of the averaging process. Averaging oversampled data proved an efficient and effective
method in these high-resolution measurements, and provided several advantages.6

Electrical isolation of the cryostat was provided by Stanford Research 560 amplifiers operating in differential mode. Additionally, the conductive path through the vacuum pumping lines was broken using plastic clamps and centering rings. High-frequency signals were filtered via thermally-grounded Thermocox cables, followed by LC and copper powder filters mounted to the cold finger. Magnetic fields were excluded via cryoqerm shielding, and below ∼1 K, the Aluminum sample box expels magnetic fields. Vibration damping pillars supported the cryostat. For most measurements, a National Instruments (NI) 9239 DAQ was used to acquire data and store it to the computer. Its inputs are well-isolated, with minimal crosstalk.

Voltage amplification for the ‘columnar’ junction was provided by an SR 560 amplifier operating in differential mode. For the ‘terraced’ and c-axis junctions, a home-built battery-powered amplifer using four JFETs in parallel was used.7 The high input impedance of the JFETs ensures that very little current flows along the voltage measurement lines, and severely limits the ability of noise signals to return to the junction.

Key results

We seek to identify sub-features within each of the energy gap peaks of conductance data of MgB2-based junctions, by contrasting fits using only two peaks (i.e. in the absence of these structures) with fits using four peaks (a gross simplification of the theoretical gap distributions shown in figure 1). The distinguishing features will be far more prominent at the energy gap peaks (ΔPb/Sn + ΔMgB2)/e than at any other part of the conductance curves (as indicated in figures 8, 9, 11, and 12, below). However, by making use of other portions of these curves, we gain confidence that these features within each energy gap are indeed properties of MgB2 and (not the counterelectrode material), and significantly reduce the parameter space for fitting the data.

A two-gap fit for these SIS’ junctions has seven independent parameters. Two are associated with the counterelectrode material: its energy gap Δ and broadening factor Γ. Then, each of the two energy gaps of MgB2 has a gap energy (ΔMgB2,π and ΔMgB2,σ) and a broadening factor (ΓMgB2,π and ΓMgB2,σ). Finally, there is one independent weighting factor wπ = 1−wσ. Similarly, a four-gap fit has 13 parameters: gap energies and broadening factors for the counterelectrode and each of the four energy gaps of MgB2, together with three independent weighting factors (where wπ1 + wπ2 + wσ1 + wσ2 = 1).

We can derive three of these parameters from data, before using any feature of the energy gap peaks (ΔPb/Sn + ΔMgB2)/e:

1. From the region between the π and σ peaks, we determine (to moderate precision) the relative weights of the MgB2 π and σ gaps.
2. From peaks within the subgap region, we determine the energy gap Δ and the broadening factor Γ of the counterelectrode material (Pb or Sn).

Calculating gap weights

When properly normalized, both theoretical and experimental conductance curves must approach 1 as V approaches infinity. As indicated in figure 4, the conductance is quite close to 1 for V ∼ 14 mV for the MgB2/I/Pb junction shown in this model. We use the conductance at the maximum acquired voltage, well above the σ peak at (ΔMgB2,π + ΔPb/Sn)/e, as our normalization factor Gπ.

When two-or four-gap models are used, the conductance in between the gap voltages is lower than it otherwise would have been, if there had been only a single gap at the lower gap energy. (See the shaded region near 6–7 mV in figure 4.) The greater the weight that is assigned to the higher gap, the greater this suppression in the conductance will be, in this

Figure 3. AFM images of representative MgB2 films on SiC (reprinted with permission from J. Appl. Phys. 113 083902. Copyright 2013, AIP Publishing LLC [18]). Each image represents a 2 x 2 μm area. (a) A ‘terraced’ film on 8° SiC, similar to that used for the MgB2/I/Sn junction discussed below. (b) A ‘columnar’ film on rough c-axis SiC, similar to that used for the MgB2/I/Pb junction discussed below.
Figure 4. Four-gap models of normalized conductance, for an MgB$_2$/I/Pb junction with varying weights associated with the $\pi$ and $\sigma$ gaps. At high $V$, the normalized conductance approaches 1, regardless of the relative gap weights. (See the shaded region $\sim$14 mV). The conductance of data in this region is used to normalize the conductance data of all three junctions. Between the gap voltages, the conductance decreases as $w_\pi$ increases. (See the shaded region $\sim$6–7 mV.) This provides a measure of $w_\pi$ and $w_\sigma$, independent of features of the gap peaks themselves.

Obtaining $\Delta_{\text{Pb}}$ and $\Delta_{\text{Sn}}$ from subgap features

As discussed above, when a nonzero $\Gamma$ is used, conductance peaks are expected to appear at the gap voltages $\Delta/e$ of each superconductor (Pb or Sn in our case). It is unusual to observe this peak in a low-transparency/high-barrier junction. It is especially unusual for it to be sharp enough to use for establishing an energy gap value. Our data in the subgap region of the conductance curves, shown in figures 6 and 7 attest to the high purity of the samples, the low transparency of the contacts, and the low noise inherent in our measurement system.

These peaks are extremely useful, for three reasons. First, they allow us to determine the gap energy of the Pb and Sn counterelectrode to high precision, particularly as $T \to 0$. Second, because these subgap peaks are sharp and narrow, we are confident that the features we observe in the $(\Delta_{\text{MgB}_2} + \Delta_{\text{Pb/Sn}})/e$ peaks (below) are due to MgB$_2$ rather than the counterelectrode material. Finally, they establish that $\Gamma$ for the counterelectrode material is small.

We also note that the peak at $\Delta_{\text{MgB}_2}/e$ is quite broad, which is appropriate given the distribution in gap values expected in MgB$_2$.

At higher $T$, the peak at $(\Delta_{\text{MgB}_2} - \Delta_{\text{Pb/Sn}})/e$ appears (above 1.69 K in figure 6 and above 4.5 K in figure 7). This peak is due to quasiparticles thermally excited across the energy gap [24]. The well-defined peaks at both $(\Delta_2 + \Delta_1)/e$ and $(\Delta_2 - \Delta_1)/e$ are widely used to find unique numerical values for both gaps. In this case, however, the $(\Delta_2 - \Delta_1)/e$ peak takes on a rounded appearance due to the distribution in the $\pi$ gap energies of MgB$_2$, in addition to thermal broadening. Therefore, the sharp subgap peaks at $\Delta_{\text{Pb/Sn}}/e$ combined with the peaks at $(\Delta_{\text{Pb/Sn}} + \Delta_{\text{MgB}_2})/e$ provide far better measures of the values for each gap.

Many of the observed features are reasonably consistent with the simple two-gap (one for $\pi$ and one for $\sigma$) and four-gap (two each for $\pi$ and $\sigma$) models described above, as can be seen in the subgap portions of figures 8–10. However, a more sophisticated model is required to completely reproduce all of the features in the subgap region. (For example, an Andreev reflection peak at $(\Delta_{\text{Pb}} + \Delta_{\text{MgB}_2})/3e$ appears at low temperature in figure 7.) A full discussion is beyond the scope of this paper, and will be addressed in a future article.

Having determined the gap energies and broadening factors of the counterelectrodes, we now discuss the gap structures themselves.

$\pi$ gap substructure

A majority of Cooper pairs tunneling into an MgB$_2$ surface are expected to tunnel to the $\pi$ gap. However, the precise
details will be sample-dependent. Here, we consider the three significantly different film geometries described above.

‘Columnar’: on a rough 0° SiC substrate, an MgB$_2$ film, w$_0$ $\sim$ 20%, indicating significant tunneling along the a-b plane. MgB$_2$/PbSn results, with w$_0$ $\sim$ 6%. MgB$_2$/Pb results with a 12° planar ‘c-axis’ MgB$_2$ film, with negligible contribution from the $\sigma$ gap. Peaks in these three curves are shifted in voltage due to the difference between the energy gaps of lead ($\Delta_{Pb} \approx 1.4$ meV) and tin ($\Delta_{Sn} \approx 0.57$ meV).

Figure 5. Conductance data for two different counterelectrode materials and three film geometries. These data were used to determine the gap weights. (a) MgB$_2$/Pb results with a ‘columnar’ MgB$_2$ film, w$_0$ $\sim$ 20%, indicating significant tunneling along the a-b plane. (b) MgB$_2$/PbSn results, with w$_0$ $\sim$ 6%. (c) MgB$_2$/Pb results with a planar ‘c-axis’ MgB$_2$ film, with negligible contribution from the $\sigma$ gap. Peaks in these three curves are shifted in voltage due to the difference between the energy gaps of lead ($\Delta_{Pb} \approx 1.4$ meV) and tin ($\Delta_{Sn} \approx 0.57$ meV).

The peak in the subgap region establishes $\pi$ gap is quite far from the real behavior of MgB$_2$, although $\pi$ gap cannot be sample-dependent, due to differences in the accessibility to the various portions of the Fermi surface, and in the effects of electron scattering on smearing out fine structures. Additionally, shown in figure 8, display a double peak at the gap voltage ($\Delta_{MgB_2,\pi} + \Delta_{Pb}/e$).

Complementary data on junctions with similar film geometry and quality may be found in [17] and [18]. Qualitatively, the features are quite similar. The precise details will be sample-dependent, due to differences in the accessibility to the various portions of the Fermi surface, and in the effects of electron scattering on smearing out fine structures. Additionally, the data presented in this paper is at a somewhat higher resolution, through a combination of measurement technique and lower temperatures.

Clearly, a model possessing a single $\pi$ gap cannot reproduce this structure. However, a simple model reflecting features for both $\pi_1$ and $\pi_2$ (in addition to multiple $\sigma$ gaps, described below) produces remarkable agreement.

Because different portions of the Fermi surface are associated with different portions of the gap distributions of the theories in figure 1, this suggests that all portions of the Fermi surface are accessible for tunneling, in similar proportions; a conclusion supported by the remarkably high w$_0$ for this tunnel junction. It further suggests that a two-peaked character is the correct one for the $\pi$ peak.

The peak in the subgap region establishes $\Delta_{Pb}$, while the level of the normalized conductance between $\sim 5$ and $\sim 8$ mV establishes w$_{\pi}$ in a two-gap model, or ($w_{\pi 1} + w_{\pi 2}$) in a four-gap model. Using the taller peak at ($\Delta_{MgB_2,\pi} + \Delta_{Pb}/e$, $\Delta_{MgB_2,\pi}$ was determined to a high precision: 1.78 meV with an uncertainty of $\pm 0.02$ meV. (All uncertainties are estimated by finding a range of parameters that produce reasonable fits, similar to the method outlined in [13].)

The remaining parameters in the four-gap model are less certain. Given the asymmetry of the $\pi_2$ shoulder, reasonably good four-gap fits yield $\Delta_{MgB_2,\pi}$ of 2.32 meV with an uncertainty of $\pm 0.10$ meV. The weights $w_{\pi}$ and the broadening parameters $I_{\pi}$ are more uncertain, because according to the model, any peak may have its height decreased by increasing $I_{\pi}$ or by decreasing $w_{\pi}$, and vice versa.

However, as seen in figure 1, none of the theoretical results produce two simple sharp peaks for the $\pi$ gap; and the broadening parameter is here being used exclusively as a means of approximating a distribution in the gap energies. So, although $w$ and $I$ are necessary parameters in the fit, they do not affect our goal in establishing the need for more than a single broadened $\pi$ gap.

Therefore, we have demonstrated that a single gap energy for the $\pi$ gap is quite far from the real behavior of MgB$_2$, which forms columnar structures.

Figure 6. Conductance data in the subgap region, for a ‘terraced’ MgB$_2$/I/Pb junction with $R_t = 15 \Omega$ and $R_{oh}$ $\gtrsim$ 600 $\Omega$, from 53 mK to 2.9 K. Curves have been offset for clarity. The sharp peak at $\Delta_{Sn}/e$ (full width $< 0.07$ meV) is used to establish $\Delta_{Sn}$ in our analysis. This is superior to using the thermally-broadened peak at ($\Delta_{MgB_2,\pi} - \Delta_{Sn})/e$.

![Figure 5](image5.png)

![Figure 6](image6.png)
while a $\pi$ gap possessing two distinct sub-bands is a reasonable approximation.

‘Terraced’: the MgB$_2$/I/Sn ‘terraced’ junction used an MgB$_2$ film formed of parallel tilted layers, each exposing a portion of the $a$–$b$ plane as well as the $c$-axis.

Once again, a single $\pi$ gap model fits the data very poorly. As shown in figure 9, our simple model including $\pi_1$ and $\pi_2$ is less successful than for the ‘columnar’ sample, though it still does capture some of the main features. Here, fitting to the tallest peak yields a $\pi_1$ gap energy of 1.77 ± 0.04 meV. However, the broad shoulder can be fit by a wide range of $\pi_2$ gap energies, with an uncertainty of $\sim 0.2$ meV.

Within our model, it was not possible to faithfully fit the data, as shown in figure 9. This is not surprising: as indicated by the lower value of $w_0$ for this junction, a higher proportion of the tunneling is along the $c$-axis. This indicates that less of the Fermi surface of MgB$_2$ is accessible for tunneling than in the ‘columnar’ junction of figure 8.

So, some portions of the gap distribution within the $\pi$ peak will be relatively unexplored, while others that may seem low in the models of figure 1 will be relatively overrepresented. Additionally, the shorter height of the crystallites will tend to increase electron scattering. Each of these effects can easily lead to a distribution that is not well-approximated by two rounded peaks. Similar results were found by Dai et al [18] from 40 to 1.8 K, with some further broadening due to temperature.

Even so, this prominent shoulder at $V \sim 2.7$ mV ($\Delta_{\text{MgB}_2,\pi_2} \sim 2.3$ mV) demonstrates that a single $\pi$ gap, no matter how it is broadened, is inconsistent with the data. Therefore, even with samples that do not fully explore the Fermi surface, we demonstrate that the $\pi$ gap must form a distribution rather than a single gap value, which may prove illuminating in refining theoretical models.

$c$-axis: in pure $c$-axis tunneling, almost all of the tunneling is to the $\pi$ gap, with minimal contribution from the $\sigma$ gap. Moreover, the distribution within the $\pi$ gap should be more limited than in cases where the $a$–$b$ plane is exposed, since less of the Fermi surface is being explored.

Low-temperature data on a $c$-axis MgB$_2$/I/Pb junction are shown in figure 10. It consists mainly of a single peak, centered at the lower-energy $\pi_1$ sub-gap. (That is, the peak appears at a voltage ($\Delta_{\text{MgB}_2,\pi_1} + \Delta_{\text{Pb}}$)/$e$.) However, using a single-gap theory with variable $\Gamma$, it was not possible to find a combination of $\Delta$ and $\Gamma$ which make the peak broad enough to match the data. A model including two $\pi$ gaps also fails to provide a good match.

From these data alone, it is not clear whether a distribution in gap energies is required, or if a different broadening (which cannot be modeled using $\Gamma$) is sufficient.

However, we gain increased confidence in the significance of features observed in the other film geometries because, as expected, this junction shows a more limited distribution. All three films were fabricated using similar methods, all were deposited on SiC, and all were measured using the same apparatus. So, if there were any spurious artifacts in the conductance curves, one would expect them to appear in these $c$-axis samples as well. Their absence supports our conclusion that the gap structures seen in the other samples are inherent properties of MgB$_2$.

$\sigma$ gap substructure

The high $T_c$ of MgB$_2$ is due to the Cooper pairs forming in the $\sigma$ band. Therefore, understanding the $\sigma$ gap is of key importance in theoretical models. As shown in figure 1, there are appreciable differences between different models, so high-resolution gap measurements may be of value.
As seen in figure 5(c), tunneling to a \( c \)-axis \( \text{MgB}_2 \) surface naturally shows no features in the \( \sigma \) gap. However, the other contact geometries do produce useful information. The ‘columnar’ \( \text{MgB}_2/\text{I}/\text{Pb} \) junction data exhibit features that are clearly incompatible with a simple two-gap model, as shown in figure 11. If there is only a single \( \sigma \) gap, then the resulting curve must take on the shape of a broadened BCS density of states: a steeper low-energy edge, and a gradual decay toward its limiting value of 1 at higher energies. Our data reveal exactly the opposite: a relatively sharp peak at high energies, together with a prominent lower-energy shoulder. These features are reasonably well-modeled by two separate \( \sigma \) gaps (which, together with the two \( \pi \) gaps form a four-gap model). However, there are some features that cannot be fit by two sub-gaps within \( \sigma \). Indeed, the theoretical models shown in figure 1 suggest that two peaks are insufficient to accurately portray the \( \sigma \) gap.

The ‘terraced’ \( \text{MgB}_2/\text{I}/\text{Sn} \) junction also exhibits a sharper peak at higher energies, and a prominent lower-energy shoulder. However, since \( \eta \) is \( \sim 6\% \) (in contrast to the ‘columnar’ junction’s \( \sim 20\% \)), the peaks are less pronounced. As shown in figure 12, a two-gap model (with a single \( \sigma \) gap) is far from adequate for representing the data, while a four-gap model (with two \( \sigma \) sub-peaks) models the data fairly well.

**Discussion**

We have summarized our results in table 1 and figure 1. These results show that our experiments can resolve features in the gap structures of \( \text{MgB}_2 \) less than 0.5 meV apart, with a precision as low as 0.02 meV.

As noted earlier, features in NS conductance data are expected to be thermally smeared by \( \sim k_T^2/\Delta \). This corresponds to 0.69 meV at 4 K, and 0.17 meV at 1 K. SIS’ conductance data should be even sharper. This suggests that physical separations of this order are observable at the temperatures of this study, using SIS’ junctions. The fact that we have observed independent features associated with the counter-electrode materials in the subgap region, to similar precision, further support the conclusion that these features are inherent in \( \text{MgB}_2 \).

Scattering will also limit the ability to resolve features within the energy gaps. The scattering rate \( \Gamma \) may be calculated from \( \gamma \gg (\Delta)^2/\Delta \) [22], where \( \langle \Delta \rangle \) is the average order parameter, and \( \Delta \) is the variation of the order parameter over the Fermi surface. If we equate these with the average energy gap value and the resolution of our energy gap data, respectively, we find a scattering rate on the order of 1 meV. This implies a mean free path beyond 300 nm. Since this distance is on the same order as irregularities in the film surface [18], it is surprising to observe this energy gap substructure, even with extremely clean samples. Nevertheless, prior tunneling
Figure 12. Normalized conductance, showing the $\sigma$ gap for the MgB$_2$/I/Sn ‘terramed’ junction. As above, a prominent shoulder appears at a voltage below that of the main peak. Therefore, the $\sigma$ gap cannot consist of a single peak. Note that, due to junction self-heating near the $\sigma$ gap voltage, the lowest stable temperature for observing the $\sigma$ peak was 53 mK.

Table 1. Comparison of energy gap values of MgB$_2$ derived from fits to experimental data versus peaks in theoretical density of states calculations. Experimental uncertainties are estimated by the range to experimental data versus peaks in theoretical density of states approximate, as it is not easily separated into two sub-peaks.

| Feature | ‘Columnar’ data | ‘Terramed’ data | Theory I [8] | Theory II [9] |
|---------|-----------------|-----------------|--------------|--------------|
| $\Delta_{\sigma_1}$ (meV) | 1.78 ± 0.02 | 1.77 ± 0.04 | 1.51 | 1.3 |
| $\Delta_{\sigma_2}$ (meV) | 3.23 ± 0.10 | 2.3 ± 0.2 | 2.06 | 2.2 |
| $\Delta_{\pi_1}$ (meV) | 7.49 ± 0.30 | 7.30 ± 0.20 | 6.61 | ~8.2 |
| $\Delta_{\pi_2}$ (meV) | 7.96 ± 0.05 | 7.88 ± 0.05 | 7.13 | ~8.7 |

spectroscopy experiments at temperatures from 7.0 to 1.8 K have exhibited such resolved features [17, 18], in addition to our experimental results presented here.

Table 1 and figure 1 also show that none of the three published theoretical models showing a distribution of gap energies [8–10] matches the data precisely. However, theory I [8] bears the strongest qualitative similarity, most notably in the shape of the sigma gap structures (with the strongest feature at the highest energy). In fact, if the features from theory I are scaled up in energy by a factor of 11%, there is very good agreement with our data (see table 1). There are several reasonable explanations for this.

Similar experiments using similar samples find that both the $\pi$ and $\sigma$ gap energies of MgB$_2$ are significantly elevated when using SiC as the substrate for the MgB$_2$ film, when compared with MgO [17, 18]. This is logical, considering the thermal contraction that occurs as the sample is cooled after growing the film—MgO has a much smaller mismatch in expansion coefficients with MgB$_2$, than SiC. Therefore, MgB$_2$ films on SiC will experience a tensile strain.

Pogrebnyakov et al [27] have found that tensile strain increases $T_c$ in MgB$_2$ films deposited by HPCVD. They attribute this increase to the softening of the $E_{2g}$ phonon mode (associated with the $\sigma$ gap). For MgB$_2$ films on SiC, they find $T_c$ is approximately 41.5 K, rather than the bulk value of 39.4 K. Because each gap energy is proportional to $T_c$, (with $2\Delta_0 = 4.18k_BT_c$ and $2\Delta_0 = 1.59k_BT_c$) [28], elevating $T_c$ from 39.4 to 41.5 K provides a roughly 5.3% increase in the energy gap values for each gap.

The remaining discrepancy may be due to assumptions used to simplify the theoretical analyses. These experimental results may prove useful in developing improved models.

Conclusion

We have performed high-resolution tunneling measurements of low-transparency MgB$_2$ tunnel junctions using ‘terramed’, ‘columnar’, and $c$-axis geometries, at low (4 K) to very low (23 mK) temperatures. With these measurements, we have probed the substructures within the $\pi$ and $\sigma$ gaps of MgB$_2$.

Within the subgap, we observed very sharp peaks that identify, to high precision, the values of the energy gaps of the junction counter-electrodes (Pb and Sn). These lead us to conclude that the substructures seen in the $\pi$ and $\sigma$ gaps are due to MgB$_2$, consistent with prior reported measurements [17–21].

Using a simplified two-band and four-band model with variable gap weights and broadening factors, we demonstrate how these sub-structures illustrate the need to go beyond a two gap model.

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