Pressure dependence of $T_c$ and $H_{c2}$ of a dirty two-gap superconductor, carbon-doped MgB$_2$

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Abstract

We have measured $T_c$ and $H_{c2}(T)$ of carbon-doped MgB$_2$ under hydrostatic pressures up to 15.6 kbar. $dT_c/dP$ is determined to be $-0.20$ K/kbar and $H_{c2}(T = 0)$ decreases with pressure at a rate that is consistent with the theoretical value for pure MgB$_2$, $dH_{c2}/dP = -0.036$ T/kbar. By analyzing our results within the theoretical framework of a dirty two-gap superconductor, we determine values for the interband coupling and the ratio between the diffusivities associated with the two bands at three different pressures. We also extract the diffusivities and coherence lengths associated with each band. Finally, we estimate the pressure dependence of the charge carrier concentration in the $\sigma$ band to be $d \ln n/dP = -0.013$/kbar.

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1. Introduction

MgB$_2$ [1] has two superconducting gaps [2–9], and this has been shown to play a crucial role in understanding the temperature dependence of its upper critical field, $H_{c2}$ [10, 11]. In particular, doping MgB$_2$ can dramatically alter the temperature dependence of $H_{c2}$ and, in some instances, lead to significant enhancement of $H_{c2}(0)$ due to its two-gap nature [12–17]. Previously we reported on $H_{c2}(T)$ of carbon-doped MgB$_2$ at ambient pressure [17]. In the study of superconductivity, pressure has been shown to be an indispensable tool. For example, Si, normally a semiconductor, was predicted to become metallic and then superconducting under pressure. This was soon confirmed by experiments [18, 19]. Also, the highest transition temperature ever recorded is that of HgBa$_2$Ca$_2$O$_{8+\delta}$ under pressure [20].

In this paper, we report the pressure effects on $T_c$ and $H_{c2}(T)$ of a dirty two-gap superconductor, carbon-doped MgB$_2$, up to 15.6 kbar. We use two quantities relevant in the context of two-gap superconductivity as fitting parameters for $H_{c2}(T)$. We then extract $\xi_\sigma$ and $\xi_\pi$ the coherence lengths associated with the $\sigma$ band. Finally, under the assumption that the $\sigma$ band is still the dominant band, and that it still has a cylindrical Fermi surface after carbon doping, we deduce the pressure dependence of the carrier density in the $\sigma$ band.

2. Experiment

The synthesis of carbon-doped MgB$_2$ is described in Ref. [21]. It has been determined to have two phases. The majority phase, having the MgB$_2$ structure with 10% of the B-sites replaced by carbon atoms, is the superconducting phase. The minority phase, MgB$_2$C$_2$, which is nonsuperconducting, is about 20% by weight. Resistance vs. temperature measurements are carried out by the four-probe technique using a linear AC resistance bridge operating at 16 Hz. Measurements are performed in magnetic fields up to 15 T in a superconducting magnet. We use a BeCu piston-cylinder self-clamping pressure cell that can generate pressures up to 20 kbar. The pressure medium used is Fluorinert. Pressure
is converted from the 4-probe resistance measurement of a calibrated manganin coil inside the pressure cell next to the sample. Due to the ‘freezing out’ of Fluorinert, the pressure is non-constant upon cooling; this effect has been calibrated and is taken into account in the analysis.

3. Results and discussion

$T_c(P)$ at four pressures, $P = 0, 2, 6, 15.6$ kbar are plotted in Fig. 1. $dT_c/dP = -0.20$ K/kbar. The inset shows $R$ vs. $T$ at $P = 0, 2, 6$ and 15.6 kbar.

We have fitted the 2-gap theoretical curves to our data. We plot $H_{c2}(T)$ at $P = 6$ and 15.6 kbar in Fig. 2. As in the case of ambient pressure [17], there are roughly two linear regimes, one near $T_c$, which has a lower absolute slope, and the other at low temperatures with a higher absolute slope. Fig. 2 also shows the Werthamer-Helfand-Hohenberg (WHH) prediction, fit to the experimental data (resistive midpoint or resistive onset midpoint) near $T_c$. Clearly, WHH underestimates $H_{c2}$ at low temperatures. Linear extrapolations of the low temperature data (between 5 and 10 K) yield $H_{c2}(0)$ values between 25 and 35 T. As we show below, the true $H_{c2}(0)$, obtained by fitting experimental data to the relevant theoretical model, is very close to the linear extrapolations of the low temperature data between 5 and 10 K. The naive $H_{c2}(T)$ prediction from WHH, $H_{c2}(T = 0) = 0.69$ $T_c$, $dH_{c2}(T = T_c)/dT$, underestimates $H_{c2}(T)$ by a factor of four to six.

In Fig. 3, we have plotted the pressure dependence of $H_{c2}(T = 0)$. We treat the difference between the $H_{c2}(0)$ obtained from the midpoint data and the onset data as the uncertainty. $H_{c2}(T = 0, P)$ for pure MgB$_2$ has not been measured. However, X. Chen et al. calculated $dH_{c2}(T = 0)/dP$ for pure MgB$_2$, and it is $-0.036$ T/kbar [23]. Our result, with admittedly large uncertainty, is consistent with this value.

We have fitted the 2-gap theoretical curves to our data. We first introduce relevant parameters from Ref. [10]. The $\lambda$ matrix is defined by $\lambda_{mm'} = \lambda_{m'm}^{(ep)} - \mu_{mm'}$, $m, m' = 1, 2$, where $\lambda_{m'm}^{(ep)}$
The equation for \( H_{c2}(T) \) for a 2-gap superconductor (Eq. (34), Ref. [10]) has four parameters, \( a_0, a_1, a_2 \) and \( \eta \). Good fits to our data are achieved by employing the values of \( a_0 \) obtained from the \( \lambda \) matrix calculated for pure MgB\(_2\). However \( a_2 \) must be altered, as discussed in Ref. [17]. Since \( a_1 + a_2 = 2 \), the theoretical fits have two independent parameters, \( a_2 \) and \( \eta \), that can be adjusted. In Fig. 4, we show the best fits for \( P = 6 \) and 15.6 kbar and the range of \( a_2 \) and \( \eta \) that enclose all the data points. The widths of the ranges are considered uncertainties in \( a_2 \) and \( \eta \). The best fit for ambient pressure is shown in Ref. [17].

### Table 1

<table>
<thead>
<tr>
<th>Parameters of two gap superconductivity</th>
<th>( P = 0 ) kbar</th>
<th>6 kbar</th>
<th>15.6 kbar</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_2 )</td>
<td>0.57 ± 0.10</td>
<td>0.70 ± 0.10</td>
<td>0.40 ± 0.10</td>
</tr>
<tr>
<td>( \eta )</td>
<td>0.029 ± 0.005</td>
<td>0.018 ± 0.005</td>
<td>0.053 ± 0.005</td>
</tr>
<tr>
<td>( \xi_{\sigma} )</td>
<td>5.0 ± 0.8 (nm)</td>
<td>6.0 ± 0.6 (nm)</td>
<td>4.0 ± 0.7 (nm)</td>
</tr>
<tr>
<td>( \xi_{\pi} )</td>
<td>0.9 ± 0.2 (nm)</td>
<td>0.8 ± 0.2 (nm)</td>
<td>0.9 ± 0.2 (nm)</td>
</tr>
</tbody>
</table>

In Table 1, we have listed the values of best fitting \( a_2 \) and \( \eta \) at the three different pressures.

The coherence length of the \( \sigma \) band can be extracted from how \( H_{c2} \) depends on \( T \) near \( T_c \). In the context of two gap superconductivity, \( H_{c2} = \frac{8\phi_0(T_c - T)}{\pi^2(a_1 D_1 + a_2 D_2)} \) [10]. Here the subscripts of the \( D \)'s correspond to the two bands, \( 1 = \sigma \) band and \( 2 = \pi \) band. In the case of \( D_1 \gg D_2 \), or \( D_\sigma \gg D_\pi \) which is true for carbon-doped MgB\(_2\) since \( \eta = D_\sigma / D_\pi \) was determined to be between 0.013–0.058, \( H_{c2} = \frac{8\phi_0(T_c - T)}{\pi^2 a_1 D_\sigma} \). Recall that \( a_1 = 2 - a_2 \) and we use the values of \( a_2 \) determined in Fig. 4 and in Ref. [17]. From the slopes of the linear region near \( T_c \) of the \( H_{c2}(T) \) plots at \( P = 0, 6 \) and 15.6 kbar we have extracted \( D_\sigma \). The difference between the slopes from the onset and midpoint data contributes to the uncertainty of our estimation of \( D_\sigma \). From this and \( 2\pi T_c \xi^2 = D_\sigma \), we deduce the coherence length of the \( \sigma \) band. Because the values of \( \eta = D_2/D_1 = D_\sigma / D_\pi \) are also known, \( \xi_\sigma \) can be calculated at the three pressures as well. The results for \( \xi_{\sigma} \) and \( \xi_{\pi} \) are also listed in Table 1. Since we have not systematically changed the \( \lambda \) matrix and only used \( a_2 \) as a fitting parameter, the values for \( \xi_{\sigma} \) and \( \xi_{\pi} \) represent reasonable estimates.

The well-known Ginzberg–Landau relation of \( 2\pi \xi^2 H_{c2}(0) = \phi_0 \) does not hold true for a two-band superconductor. This is not unique to carbon-doped MgB\(_2\). As discussed in Ref. [10], generally, \( H_{c2}(0) \), is related to both \( D_1 \) and \( D_2 \), and hence the coherence length in each band. When \( D_1 = D_2 \), the one-band dirty limit result is recovered, but in the case of very different diffusivities:

\[
H_{c2}(0) = \frac{\phi_0 T_c}{2\gamma D_2} e^{-(\lambda--\lambda_0)/2\gamma}, \quad D_2 \ll D_1 e^{-\lambda_0/\gamma}, \tag{1}
\]

\[
H_{c2}(0) = \frac{\phi_0 T_c}{2\gamma D_1} e^{-(\lambda--\lambda_0)/2\gamma}, \quad D_1 \ll D_2 e^{-\lambda_0/\gamma}, \tag{2}
\]

where, in \( \gamma = -0.577 \) is the Euler constant. Clearly the relation between \( H_{c2}(0) \) and the shorter of the two coherence lengths is dictated by the details of the \( \lambda \) matrix.

We now turn to the extraction of the carrier density. J.J. Schottel et al. have measured \( T_c(P) \) and \( H_{c2}(T = 0, P) \) for two types of high-temperature superconducting (HTSC) material [25,26] and because of the cylindrical shape of the Fermi surface of the material they studied, they were able to extract the pressure dependence of the carrier concentration. In the case of MgB\(_2\), the Fermi surface of the dominant band, the \( \sigma \) band, also has a cylindrical shape. Assuming the \( \sigma \) band is still the dominant band and still has a cylindrical Fermi surface after carbon doping, we can extract the carrier density in that band.
From the uncertainty principle, $\xi \sim \hbar v_F / k_B T_c$ and thus $k_F \sim m^* k_B T_c / \xi \hbar^2$. Assuming the $\sigma$ band has a cylindrical Fermi surface, the charge carrier density can be written as $n = k_F^2 / 2\pi c$, where $c$ is the $c$-axis lattice constant. We therefore have $n \sim (m^* k_B T_c \xi^2) / 2\pi \hbar^4 c$.

If we assume the change of $m^*$ with pressure negligible, $n \sim T_c^2 \xi^2 / c$. Applying this to the $\sigma$ band, we obtain:

$$\frac{d \ln n}{dP} = 2 \frac{d \ln T_c}{dP} + 2 \frac{d \ln \xi}{dP} \frac{d \ln c}{dP}.$$  

(3)

From our measurements $d \ln T_c / dP = 1 / T_c$ and $d T_c / dP = -0.0062 / \text{kbar}$ and from independent measurements on the compressibility of MgB$_2$ along the $c$-axis [21], and assuming it is essentially the same after carbon doping, $d \ln c / dP = 1 / c \cdot d c / dP = -0.00025 / \text{kbar}$. $\xi_0$, however, is relatively pressure-insensitive up to 15.6 kbar. Hence,

$$\frac{d \ln n}{dP} = -0.013 / \text{kbar},$$  

(4)

which is about three times the value for YBa$_2$Cu$_4$O$_8$, 0.0045 / kbar [25,26] and has the opposite sign. We see that in MgB$_2$ the decrease in $T_c$ under pressure is mainly caused by the decrease of carrier concentration.

In summary, we have measured $T_c$ and $H_c(2)$ at pressures up to 15.6 kbar for carbon-doped MgB$_2$. By fitting the 2-gap theoretical curves to $H_c(2)$ at three different pressures we have extracted the four parameters in the context of 2-gap superconductivity, $\omega_2$, which is a measure of how strongly the two bands are coupled, $\eta$, the ratio of the diffusivities in the $\pi$ and $\sigma$ bands, and the coherence lengths in these two bands, $\xi_\pi$ and $\xi_\sigma$. Finally, from the pressure dependence of the $c$-axis lattice constant, $T_c$ and $H_c(2)$, we have estimated that the fractional change of the carrier density is $-0.013 / \text{kbar}$.

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References