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Pressure dependence of T_c and H_{c2} of a dirty two-gap superconductor, carbon-doped MgB₂

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Abstract

We have measured T_c and $H_{c2}(T)$ of carbon-doped MgB₂ 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 MgB₂, $dH_{c2}/dP = -0.036$ T/kbar. By analyzing our results within the theoretical framework of a dirty two-gap supersonductor, 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 σ band to be d ln n/dP = -0.013/kbar.

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1. Introduction

MgB₂ [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 MgB₂ can dramatically alter the temperature dependence of H_{c2} and, in some instances, lead to significant enhancement of $H_{c2}(0)$ due to its twogap nature [12–17]. Previously we reported on $H_{c2}(T)$ of carbon-doped MgB₂ 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 HgBa₂Ca₂O_{8+ δ} 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 MgB₂, up to

15.6 kbar. We use two quantities relevant in the context of twogap superconductivity as fitting parameters for $H_{c2}(T)$. We then extract ξ_{σ} and ξ_{π} the coherence lengths associated with the σ band. Finally, under the assumption that the σ 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 σ band.

2. Experiment

The synthesis of carbon-doped MgB₂ is described in Ref. [21]. It has been determined to have two phases. The majority phase, having the MgB₂ structure with 10% of the B-sites replaced by carbon atoms, is the superconducting phase. The minority phase, MgB₂C₂, 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 pistoncylinder self-clamping pressure cell that can generate pressures up to 20 kbar. The pressure medium used is Fluorinert. Pressure

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Fig. 1. Pressure dependence of T_c . The dashed line is a linear fit to the data, $dT_c/dP = -0.20$ K/kbar. The inset shows R vs. T at P = 0, 2, 6 and 15.6 kbar.

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 is about twice as large as the average value for bulk MgB₂, but is comparable to the steepest slopes of $T_c(P)$ at low P (up to 20 kbar) measured for supposedly pure MgB₂ [22]. It could simply be that those slopes correspond to samples with impurities.

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 onset or resistive 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 MgB₂ has not been measured. However, X. Chen et al. calculated $dH_{c2}(T = 0)/dP$ for pure MgB₂, 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 λ matrix is defined by $\lambda_{mm'} = \lambda_{mm'}^{(ep)} - \mu_{mm'}$, m, m' = 1, 2, where $\lambda_{mm'}^{(ep)}$



Fig. 2. $H_{c2}(T)$ of MgB_{1.8}C_{0.2} at (a) 6 kbar and (b) 15.6 kbar. The squares are generated by using the resistive onset criterion and the disks are generated by using the resistive midpoint criterion. The long-dash curve is the WHH fit using the onset data near T_c and short-dash curve is the WHH fit using the midpoint data near T_c . The solid curve is the best fit based on the model of a two-gap dirty superconductor of Ref. [10] for the onset data and the long-short-dash curve is the best fit for the midpoint data. The insets show R vs. T in different magnetic fields.



Fig. 3. The dependence of $H_{c2}(T = 0)$ on pressure for MgB_{1.8}C_{0.2}. The error bars come from the difference between $H_{c2}(T = 0)$ determined by the resistive midpoint and onset criteria. The result is consistent with the theoretical prediction for pure MgB₂, $dH_{c2}(T = 0)/dP = -0.036$ T/kbar [23], shown as a solid line.





Fig. 4. $H_{c2}/H_{c2}(0)$ vs. reduced temperature T/T_c at (a) P = 6 kbar and (b) P = 15.6 kbar. The data generated by the midpoint criterion are plotted with triangles and those by the onset criterion with squares. Also shown are the best theoretical fits. Due to the small spread in the data points, there are uncertainties in both η and a_2 and they are shown in the insets.

is the matrix of electron-phonon coupling constants, μ_{mm} is the Coulomb pseudo-potential matrix and $1 = \sigma$ band and $2 = \pi$ band. Some related quantities are defined as follows $\lambda_{\pm} = \lambda_{11} \pm \lambda_{22}, \lambda_0 = (\lambda_{-}^2 + 4\lambda_{12}\lambda_{21})^{1/2}, w = \lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21}$ and $a_0 = 2w/\lambda_0, a_1 = 1 + \lambda_-/\lambda_0$ and $a_2 = 1 - \lambda_-/\lambda_0$. For pure MgB₂, the λ matrix is calculated by Golubov et al. [24] to be $\lambda_{\sigma\sigma} = 0.81, \lambda_{\pi\pi} = 0.285, \lambda_{\sigma\pi} = 0.119$ and $\lambda_{\pi\sigma} = 0.09$. Since the off-diagonal elements of the λ matrix are a measure of how strongly the two bands couple, so is a_2 . For pure MgB₂, using the values for the λ matrix listed above, a_2 is computed to be 0.07. Finally, D_1 and D_2 are diffusivities for the two bands and the ratio of these two is $\eta = D_2/D_1$.

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 η . Good fits to our data are achieved by employing the values of a_0 obtained from the λ matrix calculated for pure MgB₂. 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 η , 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 η that enclose all the data points. The widths of the ranges are considered uncertainties in a_2 and η . The best fit for ambient pressure is shown in Ref. [17].

Table 1						
The values of a_2 , η , ξ_{σ}	and ξ_{π}	at P	= 0,	6 and	15.6	kbar

Parameters of two gap superconductivity	P = 0 kbar	6 kbar	15.6 kbar
a ₂ η ξσ ξπ	0.57 ± 0.10 0.029 ± 0.005 $5.0 \pm 0.8 \text{ (nm)}$ $0.9 \pm 0.2 \text{ (nm)}$	0.70 ± 0.10 0.018 ± 0.005 $6.0 \pm 0.6 \text{ (nm)}$ $0.8 \pm 0.2 \text{ (nm)}$	$\begin{array}{c} 0.40 \pm 0.10 \\ 0.053 \pm 0.005 \\ 4.0 \pm 0.7 \ (nm) \\ 0.9 \pm 0.2 \ (nm) \end{array}$

In Table 1, we have listed the values of best fitting a_2 and η at the three different pressures.

The coherence length of the σ band can be extracted from how H_{c2} depends on T near T_c . In the context of two gap superconductivity, $H_{c2} = 8\phi_0(T_c - T)/\pi^2(a_1D_1 + a_2D_2)$ [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 MgB₂ since $\eta = D_{\pi}/D_{\sigma}$ was determined to be between 0.013–0.058, $H_{c2} = 8\phi_0(T_c - T)/\pi^2 a_1 D_\sigma$. 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_{σ} . The difference between the slopes from the onset and midpoint data contributes to the uncertainty of our estimation of D_{σ} . From this and $2\pi T_c \xi^2 = D$, we deduce the coherence length of the σ band. Because the values of $\eta = D_2/D_1 = D_\pi/D_\sigma$ are also known, ξ_{π} can be calculated at the three pressures as well. The results for ξ_{σ} and ξ_{π} are also listed in Table 1. Since we have not systematically changed the λ matrix and only used a_2 as a fitting parameter, the values for ξ_{σ} and ξ_{π} 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 MgB₂. 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:

$$H_{c2}(0) = \frac{\phi_0 T_c}{2\gamma D_2} e^{-(\lambda_- + \lambda_0)/2w}, \quad D_2 \ll D_1 e^{-\lambda_0/w}, \tag{1}$$

$$H_{c2}(0) = \frac{\phi_0 T_c}{2\gamma D_1} e^{(\lambda_- - \lambda_0)/2w}, \quad D_1 \ll D_2 e^{-\lambda_0/w},$$
(2)

where, $\ln \gamma = -0.577$ 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 λ matrix.

We now turn to the extraction of the carrier density. J.J. Scholtz 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 MgB₂, the Fermi surface of the dominant band, the σ band, also has a cylindrical shape. Assuming the σ 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 σ 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 σ 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 $d \ln T_c/dP = 1/T_c dT_c/dP = -0.0062/kbar$ and from independent measurements on the compressibility of MgB₂ along the *c*-axis [21], and assuming it is essentially the same after carbon doping, $d \ln c/dP = 1/c dc/dP = -0.00025/kbar$. ξ_{σ} , however, is relatively pressure-insensitive up to 15.6 kbar. Hence,

$$\frac{\mathrm{d}\ln n}{\mathrm{d}P} = -0.013/\mathrm{kbar},\tag{4}$$

which is about three times the value for YBa₂Cu₄O₈, 0.0045/kbar [25,26] and has the opposite sign. We see that in MgB₂ the decrease in T_c under pressure is mainly caused by the decrease of carrier concentration.

In summary, we have measured T_c and $H_{c2}(T)$ at pressures up to 15.6 kbar for carbon-doped MgB₂. By fitting the 2gap theoretical curves to $H_{c2}(T)$ at three different pressures we have extracted the four parameters in the context of 2-gap superconductivity, a_2 , which is a measure of how strongly the two bands are coupled, η , the ratio of the diffusivities in the π and σ bands, and the coherence lengths in these two bands, ξ_{σ} and ξ_{π} . Finally, from the pressure dependence of the *c*axis lattice constant, T_c and $H_{c2}(0)$, we have estimated that the fractional change of the carrier density is -0.013/kbar.

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