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Anisotropy of the Sommerfeld Coefficient in Magnesium Diboride Single Crystals

Z. Pribulova,[1,2,*] T. Klein,[1,2] J. Marcus,[1] C. Marcenat,[3] F. Levy,[3] M. S. Park,[4] H. G. Lee,[4] B. W. Kang,[4] S. I. Lee,[4] S. Tajima,[5] and S. Lee[6]

[1]Institut Néel–CNRS, F-38042 Grenoble Cedex 9, France
[2]Université Joseph Fourier, F-38041 Grenoble, France
[3]CEA-Grenoble, Département de Recherche Fondamentale sur la Matière Condensée, F-38054 Grenoble, France
[4]NVCRICS and Department of Physics, Pohang University, Pohang 790-784 Republic of Korea
[5]Department of Physics, Osaka University, Osaka 560-0043, Japan
[6]Superconductivity Research Laboratory, ISTEC, Shinonome 1-10-13, Koto-ku, Tokyo 135-0062, Japan
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The anisotropic field dependence of the Sommerfeld coefficient γ has been measured down to $B \to 0$ by combining specific heat and Hall probe magnetization measurements in MgB_2 single crystals. We find that $\gamma(B, \theta)$ is the sum of two contributions arising from the σ and π band, respectively. We show that $\gamma_\sigma(B, \theta) = B/B_{c2}(\theta)$ where $B_{c2}(\theta) = B_{c2}^{ab}/\sqrt{\sin^2\theta + \Gamma^2\cos^2\theta}$ with $\Gamma \sim 5.4$ (θ being the angle between the applied field and the c axis) and $\gamma_\pi(B, \theta) = \gamma_\pi(B) = B/B_\pi(B)$. The "critical field" of the π band B_π is fully isotropic but field dependent increasing from $\sim$0.25 T for $B \leq 0.1$ T up to 3 T $\sim B_{c2}^c$ for $B \to 3$ T. Because of the coupling of the two bands, superconductivity survives in the π band up to 3 T but is totally destroyed above for any orientation of the field.

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It is now well established that the anisotropy parameter (Γ) of magnesium diboride (MgB_2) is strongly field and temperature dependent [1,2]. This is a direct consequence of the coexistence of two weakly coupled superconducting bands. As suggested by point contact spectroscopy [3] or small angle neutron scattering [4] experiments, the so-called π band is very sensitive to magnetic field and, above some "crossover" field on the order of 0.5–1 T, the anisotropy is then mainly given by the parameters of the quasi-2D σ band leading to $\Gamma = \Gamma_{H_{c2}} = H_{c2}^{ab}/H_{c2}^{c}$ ($\sim$5–6 at low temperature, H_{c2}^{ab} and H_{c2}^{c} being the upper critical fields parallel to the ab planes and c axis, respectively). On the other hand, at low field, the anisotropy has to be averaged over the entire Fermi surface [5] leading to $\Gamma \sim \Gamma_{H_{c1}} \sim 1$ in good agreement with H_{c1} measurements [2].

Similarly, as a consequence of this suppression of the π band, preliminary measurements of the Sommerfeld coefficient $\gamma = \lim C_{el}/T|_{T\to 0}$ (C_{el} being the electronic contribution, to the specific heat) by Bouquet *et al.* [6] clearly showed that its field dependence is highly nonlinear. However, the details of the nature of the superconducting state remained unknown. We will show here that, above $\sim$0.3 T, superconductivity is induced in the π band by coupling with the σ band leading to a shrinking of the vortex core from $\xi_\pi(0) \sim 350$ Å down to $\xi_\pi = \xi_\sigma^c \sim 100$ Å for $B \sim 3$ T. Superconductivity is completely destroyed in this band above 3 T for any orientation of the magnetic field.

We present the first detailed analysis of the angular and field dependence of γ by combining specific heat and Hall probe magnetization measurements. In classical superconductors, the angular dependence of γ is determined by the B/B_{c2} ratio with $B_{c2} = B_{c2}^{ab}/\sqrt{\sin^2\theta + \Gamma^2\cos^2\theta}$ (θ being the angle between the c axis and the field). We show that, in MgB_2, the contribution of the σ band to γ is directly proportional to $B/B_{c2}(\theta)$, whereas the contribution of the π band is isotropic but highly nonlinear in field. For $T \geq 10$ K, the influence of the small gap is smeared out by the temperature and $\Delta C_p/T = f(B/B_{c2}(T, \theta))$. Specific heat measurements have been performed on single crystals of MgB_2 grown under high pressure [7,8] (with typical dimensions of few hundred microns) using an ac technique. This high sensitivity technique is very well adapted to measure C_p of very small samples and to carry continuous measurements during field sweeps at a given temperature. We were thus able to obtain the field dependence of the Sommerfeld coefficient continuously on the entire field range for different θ values. A precise *in situ* calibration of the thermocouple used to record the temperature oscillations was obtained from measurements on ultrapure silicon.

Figure 1 displays this field dependence for $H \parallel c$ and $H \parallel$ ab (at $T = 2$ K). As previously observed by Bouquet *et al.*, the γ vs H_a curve is nonlinear. Those measurements suggested that γ is isotropic below 0.2 T, becoming anisotropic for $H \geq 0.5$ T. However, for fields up to a few H_p, the first penetration field, the measurements are strongly hysteretic reflecting different vortex distributions in the sample [see [9] and inset of Fig. 1(a)]. The proximity of H_p may thus cast some doubt on the field dependence of γ observed in [6] at low field. As shown in the inset of Fig. 1(a), the first penetration field H_p can be clearly identified on the ascending branch of zero field cooled cycles as $\gamma = 0$ up to $H_a = H_p$ and rises sharply above this field due to the fast proliferation of vortices in the sample. Vortices remain pinned in the samples for decreasing fields and $\gamma \neq 0$ down to $H_a = 0$. To clearly identify the field dependence of γ in this region it was important to

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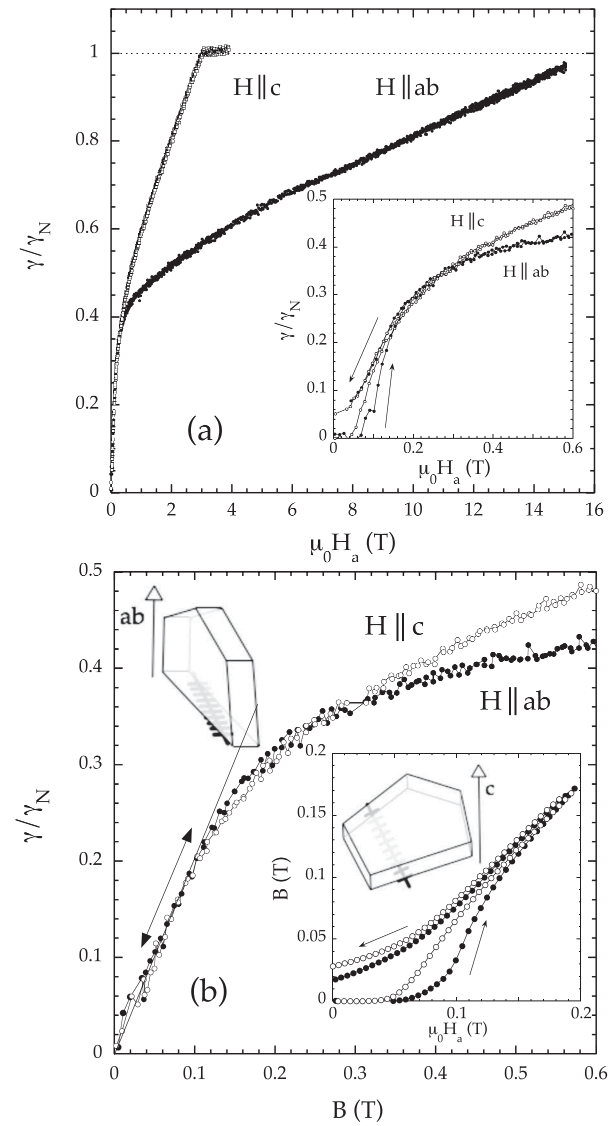

FIG. 1. Magnetic field dependence of the Sommerfeld coefficient γ at $T = 2.5$ K for $H \parallel c$ and $H \parallel$ ab. In the inset: low field dependence showing the hysteretic behavior related to flux penetration and pinning. (b) Sommerfeld coefficient γ for $H \parallel c$ and $H \parallel$ ab as a function of the average field B. In the inset: average field B deduced by Hall probe magnetometry (see sketches) as a function of the applied field H_a.

determine the *true* induction B in the sample. We thus performed Hall probe magnetization measurements on the same sample for both field directions using a miniature Hall probe array [see sketches in Fig. 1(b)]. The induction B at the surface of the sample has been averaged over $\sim$25 points for $H \parallel c$ and $\sim$10 points for $H \parallel$ ab (the average field is hereafter noted B). The B vs H_a curves are displayed in the inset of Fig. 1(b) and the corresponding γ vs B curves in Fig. 1(b). As shown, γ is perfectly linear and isotropic at low field (note that, as expected γ vs B is completely reversible). However, the linear regime is only visible up to $\sim$0.1 T and γ remains isotropic up to $B \sim 0.3$ T.

As discussed in [6], in MgB_2 the nonlinear behavior can be qualitatively understood by writing $\gamma = \omega\gamma_\pi + (1-\omega)\gamma_\sigma$, where ω is the relative weight of the π band (on the order of $\frac{1}{2}$ [10]). Assuming that all excitations are localized in the vortex cores, i.e., that $\gamma_i \propto \gamma_N(\xi_i/a_0)^2$ for $B < B_i = \Phi_0/2\pi\xi_i^2$ and $\gamma_i = \gamma_N$ for $B > B_i$ (with $i = \pi$ or σ), one gets two linear behaviors corresponding to $B < B_\pi$ and $B > B_\pi$, respectively [introducing $a_0 \sim \sqrt{(\Phi_0/B)}$]. The low field linear behavior is hence clearly visible but limited on a very restricted field range and, as discussed below, the high field linear behavior is only observed for $\theta \neq 0$ (for $B > 3$ T).

To get a better description of $\gamma(B, \theta)$, we measured the angular dependence of the Sommerfeld coefficient for various applied fields [see inset of Fig. 2(a), at $T = 2$ K]. In a classical single gap superconductor γ is fully determined by the B/B_{c2} ratio. In clean systems, deviations from the above mentioned linear behavior may be expected [11], but γ still remains a function of B/B_{c2}. Obviously such a simple behavior does not hold in MgB_2 since γ is isotropic up to ≈ 0.3 T and its anisotropy then rises up to 5–6 for $B \rightarrow B_{c2}$. However, as shown in Fig. 2(a), substracting from $\gamma(\theta)$ a constant for each H_a value, i.e., taking $[\gamma/\gamma_N - \omega a(B)]/(1-\omega)$ instead of γ/γ_N, leads to a collapse of all the data on a single curve when plotted as a function of $B/B_{c2}(\theta) \propto B\sqrt{\sin^2\theta + \Gamma^2\cos^2\theta}$ [12] with $\Gamma = \Gamma_{H_{c2}} = 5.4$. We here assumed that $\gamma_\pi(B, \theta)$ is isotropic and hence depends only on B $[\gamma_\pi/\gamma_N = a(B)]$ and that $\gamma_\sigma(B, \theta)/\gamma_N = [\gamma/\gamma_N - \omega a(B)]/(1-\omega) = f(B/B_{c2}(\theta))$. It is important to note that we made *no assumption* on the form of the function f and directly got $\gamma_\sigma(B, \theta) = [B/B_{c2}(\theta)]\gamma_N$ as expected in classical (dirty) superconductors. Note also that γ appears to be fully isotropic below 0.3 T but, in this field range, the contribution of the σ band is less than a few percent and the corresponding variation is at the limit of our experimental resolution [13].

The $a(B) = \gamma_\pi/\gamma_N$ values are displayed in the inset of Fig. 2(b) (solid symbols) together with direct determinations from magnetic field sweeps for the indicated θ values: $\gamma_\pi/\gamma_N = [\gamma/\gamma_N - (1-\omega)B/B_{c2}(\theta)]/\omega$ (open symbols). For $B \geq 3$ T, $\gamma_\pi = \gamma_N$ showing that superconductivity is completely destroyed in this band at high field. This is further emphasized in the field dependence of γ at fixed $\theta \neq 0$ values [Fig. 2(b)] which clearly shows that γ becomes perfectly linear for $B \geq 3$ T in all directions. Note that the linear fits intercept the $B = 0$ axis at $\omega \sim 0.5$ in good agreement with numerical calculations [10]. With this ω value, we did *not* observe any linear high field behavior for $H \parallel c$ but γ can be rather described by a $(B/B_{c2}^c)^\alpha$ law (with $\alpha \sim 0.4$–0.5). As discussed in [14], it is then possible to introduce an *effective* field dependent ξ_{eff} value: $\xi_{\text{eff}}(B) = \sqrt{\omega\xi_\pi(B)^2 + (1-\omega)\xi_\sigma^2}$ with $a(B) = [\xi_\pi(B)/a_0]^2$ (for $B \leq 3$ T). This effective value, combined with a field dependent penetration depth can then be used to described all physical properties (see also

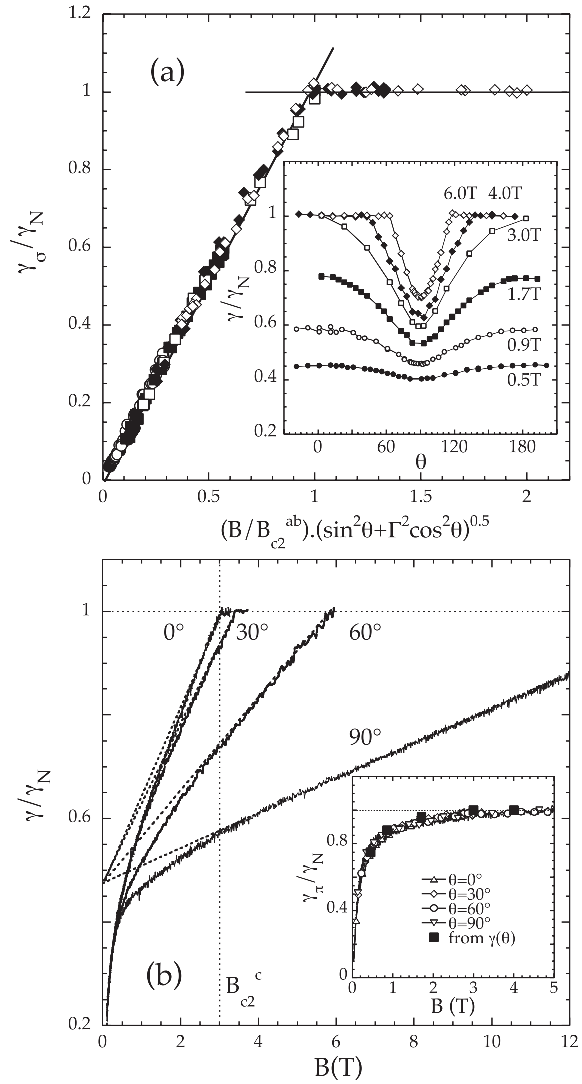

FIG. 2. (a) $[\gamma/\gamma_N - \omega a(B)]/(1-\omega)$ as a function of B/B_{c2} with $B_{c2} = B_{c2}^{ab}/\sqrt{\sin^2\theta + \Gamma^2\cos^2\theta}$ (with $\omega \sim \frac{1}{2}$ and $\Gamma \sim 5.4$), in the inset γ/γ_N as a function of θ for the indicated values of the applied field. (b) Field dependence of the Sommerfeld coefficient for the indicated field directions showing that γ becomes linear for $B \geq 3$ T. In the inset: field dependence of the contribution of the π band: $\gamma_\pi/\gamma_N = a(B)$ deduced from the angular measurements (solid squares) and magnetic sweeps at the indicated angles (open symbols, see text for details).

[15]). The $\xi_\pi(0)$ value would correspond to a critical field for the π band on the order of $B_\pi(0) = 0.25$ T but superconductivity still survives in this band due to the coupling with the σ band leading to a shrinking of the vortex core from $\xi_\pi \approx 350$ Å below 0.1 T down to $\xi_\pi = \xi_\sigma^{ab}$ for $B \sim 3$ T $= B_{c2}^c$. However, it is important to note that, since the π band is isotropic, it can have only one θ independent B_{c2} value and superconductivity is hence destroyed in this band in all direction for $B \geq 3$ T.

As expected the $\xi_\sigma^{ab} \sim 100$ Å and $\xi_\sigma^c \sim 20$ Å values are very close to the BCS single band estimate: $\hbar v_{F,\sigma}/\pi\Delta_\sigma \sim 130$ Å and $\sim$20 Å in the ab planes and along the c direction, respectively ($v_{F,\sigma}$ being the Fermi velocity of the σ band $\sim 4.6 \times 10^7$ cm/s and $\sim 0.7 \times 10^7$ cm/s for the two crystallographic directions and Δ_σ the large gap value $\sim$7.0 meV). More surprisingly, the as-deduced ξ_π value ($\sim$350 Å) is also quite close to $\hbar v_{F,\pi}/\pi\Delta_\pi \sim 400$–500 Å [taking an average $v_{F,\pi}$ value on the order of $(5–6) \times 10^7$ m/s [5,16] and $\Delta_\pi \sim 2.4$ meV]. Indeed, it has been suggested by Zhitomirsky *et al.* [16] that this single band estimate should not be applicable in MgB_2 and that in the clean limit $\xi_\pi^c/\xi_\sigma^c \leq \sqrt{\omega\langle v_{F,\pi}^2\rangle/(1-\omega)\langle v_{F,\sigma}^2\rangle} \sim 1-2$ for reasonable $\langle v_{F,\pi}^2\rangle/\langle v_{F,\sigma}^2\rangle$ values [5,16]. Similarly, it has been shown that, in the dirty limit, $\xi_\pi^c/\xi_\sigma^c \sim 3$ for $D_\pi/D_\sigma \sim 4$ [17] (where D_i is the diffusivity of the i band), i.e., for a σ band which would be much dirtier than the π band. This numerical ξ_π value obviously deserves further theoretical investigation.

As discussed in [6], an effective anisotropy ratio can be defined as the ratio of the magnetic fields in the ab plane and c axis which correspond to the same γ value but, as pointed out in [6], the choice of the corresponding field is then arbitrary and an almost linear increase of Γ with field was proposed. However, we have seen that superconductivity is completely destroyed in the π band for $B \geq 3$ T and Γ is hence expected to be equal to 5.4 above 3 T. We have calculated this field dependent anisotropy $\Gamma(B)$, writing $\gamma(B,\theta) = \gamma(B\sqrt{\sin^2\theta + \Gamma(B)^2\cos^2\theta}, \theta = 90°)$, i.e., introducing an effective field dependent $B_{c2}^* = B_{c2}^{ab}/\sqrt{\sin^2\theta + \Gamma(B)^2\cos^2\theta}$ and writing that $\gamma = f(B/B_{c2}^*)$. The corresponding $\Gamma(B)$ values have been reported on Fig. 3 (open symbols and lines) for $\theta = 0°$, 30°, and 60° together with the $\Gamma_\lambda = \frac{\lambda_c}{\lambda_{ab}}$ values deduced from

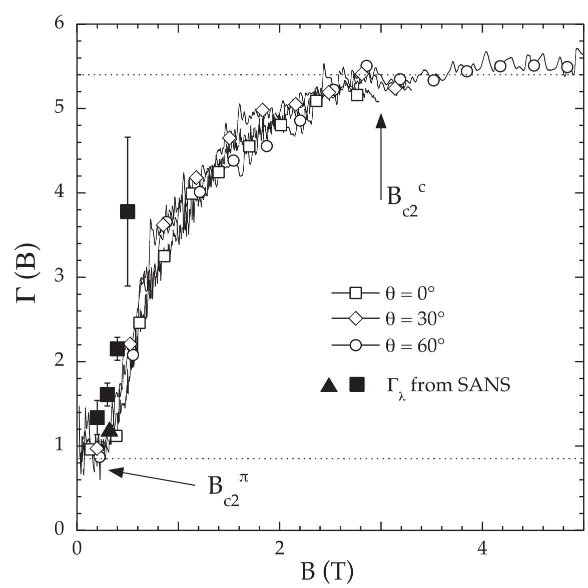

FIG. 3. Field dependence of the anisotropy ratio (see text for details) together with $\Gamma_\lambda = \frac{\lambda_c}{\lambda_{ab}}$ values deduced from small angle neutron scattering data (closed squares: from [4], closed triangle: from [16].

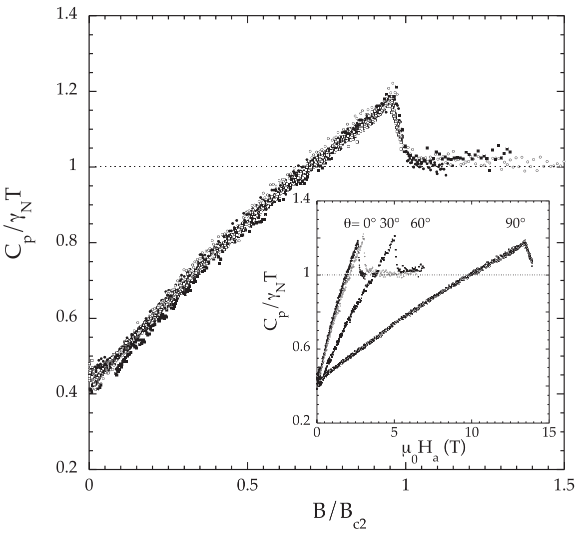

FIG. 4. (a) Magnetic field dependence of the specific heat at $T = 9$ K showing that, at high temperature, C_p/T scales as $B/B_{c2}(\theta)$. In the inset: same dependence plotted as a function of the applied field H_a for $\theta = 0°$, $30°$, $60°$, and $90°$.

small angle neutron scattering data (closed squares: from [4], closed triangle: from [18]). As shown the same effective anisotropy (saturating at 5.4 for $B \geq 3$ T) is obtained for all angles and a very reasonable agreement is obtained between specific heat and SANS data confirming that $\Gamma_\lambda = \Gamma = \Gamma_\xi$. Note that Γ stays on the order of 1 up to B_π and then sharply increases reaching $\Gamma_{H_{c2}}$ for $B \geq B_{c2}^c$.

Finally, we have investigated the influence of the temperature on the field and angular dependence of C_p. The inset of Fig. 4 displays the field dependence of C_p/T at $T = 9$ K for the indicated θ values. In this temperature range superconductivity in the π band is reduced due to thermal activation over the small gap and, as shown in the main panel of Fig. 4, all curves can then be rescaled directly as a function of $B/B_{c2}(\theta)$ clearly showing that a *classical* behavior is recovered at high temperature (except that Γ is temperature dependent).

We have shown that, the contribution of the σ band to the specific heat $\gamma_\sigma(B, \theta) = [B/B_{c2}(\theta)]\gamma_N$ whereas the contribution of the π band is isotropic but highly nonlinear in field: $\gamma_\pi(B, \theta) = \gamma_\pi(B) = [B/B_\pi(B)]\gamma_N$ for $B \leq 3\ \mathrm{T} \sim B_{c2}^c$ and $\gamma_\pi = \gamma_N$ for $B \geq 3$ T. We hence show that superconductivity can be induced in the π band by coupling with the σ band but only up to B_{c2}^c and no superconductivity is observed in this band for $B \geq 3$ T.

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*Present address: Centre of Low Temperature Physics IEP SAS & FS UPJS, Watsonova 47, SK-04001 Kosice, Slovakia.

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