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Anisotropy of the upper critical field in MgB_2: the two-band Ginzburg–Landau theory

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The temperature dependence of the anisotropy parameter of upper critical field $\gamma_{H_{c2}}(T) = H_{c2}^{\parallel}(T)/H_{c2}^{\perp}(T)$ is calculated using two-band Ginzburg–Landau theory for layered superconductors. It is shown that, with decreasing temperature anisotropy parameter $\gamma(T)$ is increased. Result of calculations are in agreement with experimental data for single crystals of MgB_2 and with other calculations.

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Introduction: Three years ago superconductivity in magnesium diboride MgB_2 was discovered with critical temperature, $T_c = 39K$, which is the highest critical temperature for a simply binary compound [1]. The origin of superconductivity in this compound can be explained in the framework of ordinary e-ph mechnanism. The material shows a pronounced isotope effect [2]. Measurement of the nuclear spin-lattice relaxation rate also indicate that MgB_2 is phonon mediated superconductor [3]. Unusual superconductivity in this compound is related with two distinct energy gap assosiated with different part of the Fermi surface. The larger gap ($\Delta_\sigma = 7$ meV) originates from holelike carriers residing on two cylindrical Fermi surface sheets, derived from σ bonding of the p_{xy} boron orbital (σ-*band*). The smaller gap ($\Delta_\pi = 2$ meV) originates from the two 3D sheets of electrons and holes derived from π bonding of the p_z orbitals (π -*band*) [4 – 6].

In magnesium diboride MgB_2, the crystal structure as well as the electronic and phononic band structure are all far from isotropic [7]. This should lead to anisotropic superconducting state properties. The corresponding electron transport is very anisotropic ($\rho_c/\rho_{ab} = 3.5$ [8]) with the plasma frequency for the σ band along c (or z) axis being much smaller than that in the ab (xy) direction [9]. In a clean material the layered structure dictates srtong anisotropy of the upper magnetic critical field $H_{c2}^{\parallel} \gg H_{c2}^{\perp}$.Their ratio at low temperatures reaches to about 6, while $H_{c2}^{\perp}$ is as low as $2–3T$ [10]. On the other hand, for a dirty material the anisotropy is decreased, but both the magnititudes of $H_{c2}^{\parallel}$ and $H_{c2}^{\perp}$ are strongly increased [11].

A pronounced temperature dependence of the anisotropy parameter γ_H of the upper critical field was calculated based on the microscopic two-band (TB) model [12 – 15]. It is well known that Ginzburg–Landau (GL) theory remains powerful istrument for the study of magnetic phase diagram of superconductors. Isotropic GL theory with two s-wave order parameters was used for the calculation of H_{c2} [16], H_{c1} [17] and other superconducting state parameters [18] and achieved good agreement for bulk MgB_2 samples. In this study we firstly present calculations of the anisotropy parameter γ of the upper critical field using TB GL theory for layered superconductors. It is shown that, in contrast to (SB) layered superconductors, TB superconductors reveal temperature dependent anisotropy of the upper critical field.

Basic equations: Free energy functional for TB layered superconductors can be written as [16 – 19]:

$$F[\Psi_{1n}, \Psi_{2n}] = \sum_n \int d^2r (F_{1n} + F_{1n,2n} + F_{2n} + \\ + F_{1n,1(n+1)} + F_{2n,2(n+1)} + H^2/8\pi), \quad (1)$$

with

$$F_{in} = \frac{\hbar^2}{4m_i} \left| \left(\nabla_{2d} - \frac{2\pi i A}{\Phi_0} \right) \Psi_{in} \right|^2 + \\ + \alpha_{i,n}(T)\Psi_{i,n}^2 + \frac{\beta_{i,n}}{2}\Psi_{i,n}^4, \quad (2)$$

$$F_{1n,2n} = \varepsilon(\Psi_{1,n}\Psi_{2,n}^* + c.c.) + \\ + \varepsilon_1((\nabla_{2d} + \frac{2\pi i A}{\Phi_0})\Psi_{1,n}^*(\nabla_{2d} - \frac{2\pi i A}{\Phi_0})\Psi_{2,n} + c.c.), \quad (3)$$

$$F_{in,i(n+1)} = \frac{\hbar^2}{4m_i^c d^2} \left| \Psi_{in} - \Psi_{i,(n\pm1)} \exp\left(-i\frac{2\pi d A_z}{\Phi_0}\right) \right|^2, \quad (4)$$

where we choose x, y, z lying along the a, b and c crystallographic axes, respectively. Here, m_i denotes the effective mass of the carriers in the plane belonging to band i ($i = 1; 2$). F_{in} is the free energy of separate bands in the plane. The coefficient α is given as $\alpha_{in} = \gamma_i(T - T_{ci})$, which depends on temperature linearly, γ is the proportionality constant, while the coefficient β_{in} is independent of temperature. $\mathbf{H}$ is the external magnetic field and $\mathbf{H} = \mathrm{curl}\, A$. The quantities ε and ε_1 describe interband interaction of two order parameters and their gradients, respectively. Due to identical character of planes we can write: $\alpha_{in} = \alpha_i, \beta_{in} = \beta_i$. d is the distance between planes.

The choice of the vector potential $\mathbf{A}$ as $\mathbf{A} = (0, Hx, 0)$ corresponds to the perpendicular component of the magnetic field $\mathbf{H} = (0, 0, H)$. In this case GL equations for TB layered superconductors can be reduced to:

$$-\frac{\hbar^2}{4m_1}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_1 + \alpha_1(T)\Psi_1 + + \varepsilon\Psi_2 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_2 = 0, \tag{5}$$

$$-\frac{\hbar^2}{4m_2}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_2 + \alpha_2(T)\Psi_2 + + \varepsilon\Psi_1 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4})\Psi_1 = 0, \tag{6}$$

where $l_s^2 = \hbar c/2eH$ is the so-called magnetic length. Calculation $H_{c2}^{\perp}$ in similar manner to [18] leads to

$$H_{c2}^{\perp}(T) = \Phi_0/2\pi\xi_{\perp}^2, \tag{7}$$

where effective coherent lenght ξ_{eff} of TB superconductors is given by the expression

$$\xi_{\perp}^2 = \frac{\hbar^2}{4}\Big[-(m_1\alpha_1(T) + m_2\alpha_2(T) + 8\varepsilon\varepsilon_1 m_1 m_2/\hbar^2) + +\sqrt{(m_1\alpha_1(T) + m_2\alpha_2(T) + 8\varepsilon\varepsilon_1 m_1 m_2/\hbar^2)^2 - 4m_1 m_2(\alpha_1(T)\alpha_2(T) - \varepsilon^2)}\Big]^{-1}. \tag{8}$$

At small values for the upper critical field $H_{c2}^{\perp}(T)$ is true:

$$H_{c2}^{\perp}(T) = -\frac{\hbar c}{2e}\frac{(\alpha_1(T)\alpha_2(T) - \varepsilon^2)}{\frac{\hbar^2}{4}\left[\frac{\alpha_1(T)}{m_2} + \frac{\alpha_2(T)}{m_1} + \frac{8\varepsilon\varepsilon_1}{\hbar^2}\right]}. \tag{9}$$

For the calculation $H_{c2}^{\parallel}$, we choose $\mathbf{H} = (0, H, 0)$ and $\mathbf{A} = (0, 0, -Hx)$. Then GL equations for TB superconductors are reduced to the following form:

$$-\frac{\hbar^2}{4m_1}\frac{d^2\Psi_1}{dx^2} + \alpha_1\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1\frac{d^2\Psi_2}{dx^2} + 2\frac{\hbar^2}{4m_1^c d^2}(1 - \cos\frac{2\pi dHx}{\Phi_0})\Psi_1 = 0, \tag{10}$$

$$-\frac{\hbar^2}{4m_2}\frac{d^2\Psi_2}{dx^2} + \alpha_2\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1\frac{d^2\Psi_1}{dx^2} + 2\frac{\hbar^2}{4m_2^c d^2}(1 - \cos\frac{2\pi dHx}{\Phi_0})\Psi_2 = 0, \tag{11}$$

By elimination we can get equations for Ψ_1 and Ψ_2 from (10) and (11), which turn out to be identical (see [18])

$$\frac{\hbar^2}{4m_1}\frac{\hbar^2}{4m_2}\frac{d^4\Psi_1}{dx^4} - \left(\frac{\hbar^2}{4m_2}\alpha_1 + \frac{\hbar^2}{4m_1}\alpha_2\right)\frac{d^2\Psi_1}{dx^2} + \alpha_1\alpha_2\Psi_1 + \left(1 - \cos\frac{2\pi dHx}{\Phi_0}\right) \times \times\left(2\frac{\hbar^2}{4m_1^c d^2}\left[-\frac{\hbar^2}{4m_2}\frac{d^2}{dx^2} + \alpha_2\right] + 2\frac{\hbar^2}{4m_2^c d^2}\left[-\frac{\hbar^2}{4m_1}\frac{d^2}{dx^2} + \alpha_1\right]\right)\Psi_1 = (\varepsilon^2 + 2\varepsilon\varepsilon_1\frac{d^2}{dx^2} + \varepsilon_1^2\frac{d^4}{dx^4})\Psi_1. \tag{12}$$

By neglecting high derivatives of order parameter ($d^4\Psi_1/dx^4$) and small terms, we can obtain the Mathieu equation for the calculation of upper critical field $H_{c2}^{\parallel}$:

$$-\left(\frac{\hbar^2}{4m_2}\alpha_1 + \frac{\hbar^2}{4m_1}\alpha_2 + 2\varepsilon\varepsilon_1\right)\frac{d^2\Psi_1}{dx^2} + 2\left(\frac{\hbar^2}{4m_1^c d^2}\alpha_2 + \frac{\hbar^2}{4m_2^c d^2}\alpha_1\right)\left(1 - \cos\frac{2\pi dHx}{\Phi_0}\right)\Psi_1 = (\varepsilon^2 - \alpha_1\alpha_2)\Psi_1. \tag{13}$$

At small magnetic field $H \ll \Phi_0/2\pi d^2$ and after expansion of cosines in Eq.(13), we can get the final expression for anisotropy parameter of upper critical field

$$\gamma_{H_{c2}} = \frac{H_{c2}^{\parallel}}{H_{c2}^{\perp}} = \left[\frac{x(T-T_{c1}) + (T-T_{c2}) + 8\varepsilon^2 x\eta T_c}{\dfrac{m_2}{m_2^c}x(T-T_{c1}) + \dfrac{m_1}{m_1^c}(T-T_{c2})} \right]^{1/2}. \tag{14}$$

At high magnetic field $H > \Phi_0/2\pi d^2$ upper critical field $H_{c2}^{\parallel}$ can be defined from the lowest eigenvalue of Mathieu equation [20] and is given by the following expression

$$H_{c2}^{\parallel} = \frac{\Phi_0}{2\pi d} \frac{\alpha_2 \dfrac{\hbar^2}{4m_1^c d^2} + \alpha_1 \dfrac{\hbar^2}{4m_2^c d^2}}{\left(\left(\dfrac{\hbar^2}{4m_2}\alpha_1 + \dfrac{\hbar^2}{4m_1}\alpha_2 + 2\varepsilon\varepsilon_1 \right) \left(\alpha_2 \dfrac{\hbar^2}{4m_2^c d^2} + \alpha_1 \dfrac{\hbar^2}{4m_1^c d^2} - \dfrac{\varepsilon^2 - \alpha_1\alpha_2}{2} \right) \right)^{1/2}}. \tag{15}$$

It means that

$$H_{c2}^{\parallel} \prec \frac{1}{(T-T^*)^{1/2}}, \tag{16}$$

where T^* is given by the following expression:

$$T^* = T_c - \frac{\hbar^2}{4m_1^c d^2 \gamma_1} - \frac{\hbar^2}{4m_2^c d^2 \gamma_2}.$$

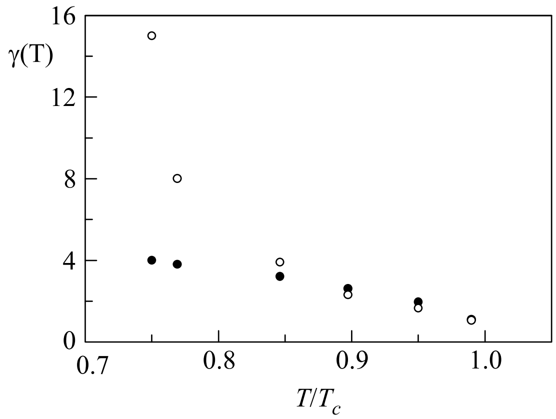
Result and discussion. In Figure we plot anisotropy parameter γ versus reduced temperature T/T_c. Experimental results from of Lyard [21] is given by the full symbols. The full points denote the results of calculations from above presented TB layered GL theory. Here we used parameters: $T_{c1} = 20$ K, $T_{c2} = 10$ K, $\varepsilon^2 = 3/8$, $x = 3$, $\eta = -0.16$. The same parameters were also used in Ref.[16–18] to determine temperature dependence of SC state parameters in the framework of isotropic TB GL theory. Anisotropy mass parameters for single crystals $m_2/m_2^c = 1.3$ and $m_1/m_1^c = 0.03$ are the same as in Ref. [22]. As shown in Ref.[16–18] isotropic GL theory gives good description of temperature dependences of measureable parameters of bulk samples of MgB_2. As followed from Eq.(14) influence of π (weak) band is effectively "switched of" and anisotropy parameter mainly defined by the σ (srtong) band. As a consequence at small magnetic field there is good agreement with experimental data on investigation of anisotropy of upper critical field. Increasing of γ with decreasing of temperature was observed experimentally by many groups [7, 10, 23, 24]. Thus, there are consensus with understanding of temperature behavior of γ.

At high magnetic field $H_{c2}^{\parallel}$ goes to infinity as $(T - T^*)^{1/2}$. It means that, the orbital depairing effect of a magnetic field parallel to the layers does not destroy the superconductivity. This correspond to the case where the cores of the vortices fit between the SC layers and external magnetic field has no effects on the superconductivity. In fact other magnetic mechanisms will limit the divergence. The divergence of $H_{c2}^{\parallel}$ at T^* will be removed by taking into account spin-orbit scattering [25] and paramagnetic effect [26, 27]. Similar anisotropy of upper critical field was observed for the other possible class of TB superconductors -nonmagnetic borocarbides $Y(Lu)Ni_2B_2C$ [28, 29].

Here it is necessary to remark that similar two-band GL equations recently was discussed in [30]. However, in equations presented in Ref.[30], terms similar to intergradient interaction in Eqs.(5), (6) and (10), (11) are absent. As shown in [16–18], maximal positive curvature of upper critical field of bulk samples can be achieved by inclusion of a intergradient interaction. In the case of no intergradients of order parameters $\eta = 0$, the curvature reaches maximum at the point of $0.5T_c$. Intergradient interaction shifts this maximum to the region close to critical temperature. Such behavior is in good agreement with experimental data for a bulk samples. As we can see from Eq.(14), in the case of anisotropic GL equations, intergradient term also play a crucial role in temperature dependence of anisotropy parameter $\gamma_{H_{c2}}$.

Another version of GL approximation was presented in Ref.[31]. This approach corresponds to an effective SB GL theory. In the framework of theory [31] , the ratio of order parameters is temperature and field independent, i.e. is constant. It means that two-band GL theory is equivalent to effective single band approximation. In contrast to [31], in our consideration the ratio of order parameters is temperature and field dependent [16–18] (see also Eqs.(5), (6) and (10), (11)).

As shown by Bulaevskii [32] in the case of SB layered superconductors upper critical field is defined by expressions: $H_{c2}^{\parallel} = \Phi_0/2\pi\xi_\perp\xi_\parallel, H_{c2}^{\perp} = \Phi_0/2\pi\xi_\parallel^2$. Note, that in this case anisotropy parameter γ_{Hc2} is tempera-



Temperature dependence of the anisotropy parameter γ_{Hc2}. The full line is a TB GL theory for layered superconductors, full symbols experimental data from Ref.[21]

ture independent. As stated in begining, all coefficients α and β in GL model is field-independent. Other generalization of considered model is related with introducing field dependent parameters α and β. Possible inclusion field-dependent coefficients in the framework TB GL is subject of future investigations.

Conclusions: In summary, we have shown that experimental data of anisotropy parameter $\gamma_{H_{c2}}(T)$ for MgB_2 can be described in the framework of TB layered GL theory at temperatures close to T_c in contrast SB layered superconductors, where anisotropy parameter is temperature independent. Presense of two order parameter with different dimensionality play significant role in determining temperature dependence of anisotropy parameter $\gamma_{H_{c2}}(T)$.

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