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Physica C 459 (2007) 56–61
PHYSICA C
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Angular dependence of upper critical field in two-band Ginzburg–Landau theory

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Received 29 November 2006; received in revised form 11 March 2007; accepted 17 April 2007
Available online 3 May 2007

Abstract

Generalization of two-band Ginzburg–Landau (GL) theory to the case of anisotropic mass is presented. The temperature dependence of the anisotropy parameter of upper critical field $\gamma_{c2}(T) = H^{\parallel}_{c2}(T)/H^{\perp}_{c2}(T)$ and angular dependence of $H_{c2}(\theta, T)$ are calculated using anisotropic mass two-band Ginzburg–Landau theory of superconductors. It is shown that, with decreasing temperature anisotropy parameter $\gamma_{c2}(T)$ is increased. Results of our calculations are in agreement with experimental data for single crystal MgB_2.

PACS: 74.20.De; 74.25.Ha; 74.70.Ad; 74.20.Mn

Keywords: Two-band superconductivity; Angular dependence; Upper critical field; Mass anisotropy

1. Introduction

Recently discovered [1] superconducting compound MgB_2 has led to a growing amount of both experimental and theoretical works due to the fact that it holds the highest superconducting transition temperature of about $T_c = 39$ K for a binary compound of a relatively simple crystal structure. Calculations of the band structure and the phonon spectrum predict a double energy gap [2,3], a larger gap attributed to two-dimensional p_{x-y} orbitals (σ-band) and smaller gap attributed to three-dimensional p_z bonding and anti-bonding orbitals (π-band). As a superconductor the electron–phonon mechanism of superconductivity [4] in MgB_2 involves giant anharmonicity and nonlinear electron–phonon coupling [5]. Two-band characteristic of the superconducting state in MgB_2 is clearly evident in the recently performed tunneling measurements [6,7] and specific heat measurement [8]. Another class of two-band superconductors are the nonmagnetic borocarbides [9] $Lu(Y)Ni_2B_2C$.

Magnetic phase diagram for bulk samples of MgB_2 and nonmagnetic borocarbides $Lu(Y)Ni_2B_2C$ has been of interest to researchers. In contrast to common superconductors, the upper critical field for bulk samples of MgB_2 and borocarbides $Lu(Y)Ni_2B_2C$ have a positive curvature near T_c. To understand the nature of the unusual behavior at a microscopic level, a two-band Eliashberg model of superconductivity was first proposed by Shulga et al. [9] for $LuNi_2B_2C$ and YNi_2B_2C and recently [10] for MgB_2. Two-band Ginzburg–Landau (GL) model for bulk MgB_2 was successfully applied to fit the experimental results of the temperature dependence of upper and lower critical fields for MgB_2 and nonmagnetic borocarbides [11–13].

Systematic deviation from single-band anisotropic GL behavior was observed in recent experimental works (see below) on angular dependence of upper critical field in MgB_2 single crystals. It is necessary to take into account different characteristics of anisotropy in different bands. Motivated by these experiments, in this paper we extend our previous analysis of the two-band effects [11–13] on

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0921-4534/$ - see front matter © 2007 Published by Elsevier B.V.
doi:10.1016/j.physc.2007.04.218

angular dependence of the upper critical field $H_{c2}(\theta, T)$. We also study the temperature dependence of anisotropy parameter $\gamma_{c2} = H_{c2}^{\parallel}/H_{c2}^{\perp}$ of upper critical field H_{c2} in single crystals of MgB_2. Within the two-band GL theory our calculations yield good agreement with experiments on the angle dependence of $H_{c2}(\theta, T)$.

The rest of this paper is organized as follows. In the next section, we outline the two-band Ginzburg–Landau theory and derive the expressions for the upper critical field $H_{c2}(T)$. In Section 3, we concentrate on the angle dependence of H_{c2} and obtain expressions valid in the vicinity of the critical temperature T_c. Our results for MgB_2 are presented in Section 4 and discussed in the light of available experimental data.

2. Basic equations

In the presence of two order parameters Ψ_1 and Ψ_2 in a superconductor, GL free energy functional $\mathscr{F}$ can be written as [11–13]

$$\mathscr{F}[\Psi_1, \Psi_2] = \int \mathrm{d}^3r\big(F_1 + F_{12} + F_2 + H^2/8\pi\big), \tag{1}$$

with

$$F_i = \frac{\hbar^2}{4m_i}\left|\left(\nabla - \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_i\right|^2 + \alpha_i(T)\Psi_i^2 + \frac{\beta_i}{2}\Psi_i^4 \tag{2}$$

and

$$F_{12} = \varepsilon(\Psi_1\Psi_2^* + c.c.) + \varepsilon_1\left[\left(\nabla + \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_1^*\left(\nabla - \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_2 + c.c.\right]. \tag{3}$$

In the above equations, m_i denotes the effective mass of the carriers belonging to band i ($i = 1, 2$), F_i is the free energy of the ith band, and $\Phi_0 = hc/2e$ is the flux quantum. The coefficient α is given as $\alpha_i = \gamma_i(T - T_{ci})$, which depends on temperature linearly, γ_i is the proportionality constant, while the coefficient β is independent of temperature. $\vec{H}$ is the external magnetic field related to the vector potential $\vec{A}$ by $\vec{H} = \nabla \times \vec{A}$. The quantities ε and ε_1 describe inter-band interaction of two order parameters and their gradients, respectively. Intergradient interaction term is equal to zero in the free energy employed by Zhitomirsky and Dao [14]. However, the intergradient term as introduced by Doh et al. [15] and Affleck et al. [16] seems to be crucial. As shown by Askerzade [11–13] presence of this term leads to measurable effects in the study of H_{c1} and H_{c2}. For instance, the effect of positive curvature in H_{c2} is enhanced due to the inclusion of intergradient interaction term. In a very recent work [17] it is shown that this term is also important in the case of inclusion of anisotropic order parameters.

Minimization of the free energy functional with respect to the order parameters yields GL equations for two-band superconductors with the choice $\vec{A} = (0, Hx, 0)$

$$-\frac{\hbar^2}{4m_1}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^4}\right)\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^4}\right)\Psi_2 + \beta_1\Psi_1^3 = 0, \tag{4}$$

$$-\frac{\hbar^2}{4m_2}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^4}\right)\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^4}\right)\Psi_1 + \beta_2\Psi_2^3 = 0, \tag{5}$$

where $l_s^2 = \hbar c/2eH$ is the square of the so-called magnetic length. In the derivation of the GL equations above, small spatial variation of the gap function is assumed. Thus, the higher order derivatives are not significant in the calculation of upper critical field. As shown by Zhitomirsky and Dao [14] higher order derivatives become important for the study of the orientation of the vortex lattice along c-axis in MgB_2 crystals. In this work, sixth order gradient terms were included to the free energy functional.

For the calculation of upper critical field H_{c2}, the system of Eqs. (4a) and (4b) can be linearized in the vicinity of T_c and solved using the ansatz [11] $\Psi_{1,2} \propto \mathrm{e}^{-x^2/2l_s^2}$. Equation that determines the upper critical field in the isotropic case has the form

$$\left(\frac{eH\hbar}{2m_1c} + \alpha_1(T)\right)\left(\frac{eH\hbar}{2m_2c} + \alpha_2(T)\right) = \left(\varepsilon - \varepsilon_1\frac{2eH}{\hbar c}\right)^2 \tag{6}$$

and the solution for $H_{c2}(T)$ can be written as

$$H_{c2}(T) = \frac{\Phi_0}{2\pi\xi^2}, \tag{7}$$

where the coherence length ξ of two-band superconductors is given by the expression

$$\xi^2 = \frac{\hbar^2}{4}\left[-\left(m_1\alpha_1(T) + m_2\alpha_2(T) + \frac{8\varepsilon\varepsilon_1 m_1 m_2}{\hbar^2}\right) + \sqrt{\left(m_1\alpha_1(T) + m_2\alpha_2(T) + \frac{8\varepsilon\varepsilon_1 m_1 m_2}{\hbar^2}\right)^2 - 4m_1m_2(\alpha_1(T)\alpha_2(T) - \varepsilon^2)}\right]^{-1}. \tag{8}$$

In the vicinity of the critical temperature T_c, we may neglect terms of order H^2 in Eq. (5) and obtain the approximate expression for the upper critical field

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

We note [11–13] that the critical temperature T_c of a two-band superconductor as a result of inter-band interaction is higher than T_{c1} and T_{c2}, i.e., $(T_c - T_{c1})(T_c - T_{c2}) = \varepsilon^2/\gamma_1\gamma_2$.