TEMPERATURE DEPENDENCE OF THE LONDON PENETRATION DEPTH OF YNi₂B₂C BOROCARBIDS USING TWO-BAND GINZBURG-LANDAU THEORY

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Temperature dependence of London penetration depth of nonmagnetic borocarbides YNi_2B_2C is studied in the framework two-band Ginzburg-Landau theory. Its temperature dependence is non-linear near T_c . The strength of the non-linearity is mainly dependent on the interaction coupling between the order parameters of two separate bands. In addition, the inter-gradient interaction as well as the ratio of effective masses of two separate bands was also found to be important in determining its temperature dependence. The results of the calculations are in good agreement with the experimental data for bulk YNi_2B_2C

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1 Introduction

The new class of rare-earth transition-metal borocarbides with the general formula RNi_2B_2C attracted the interest of many scientist, because of their wide variety of physical properties: compounds with R=Y,Lu exhibit fairly high superconducting transition temperatures, T_c, of about 15-16 K [1]; magnetism coexist with superconductivity for R=Dy, Ho, Er and Tm [2] whereas only antiferromagnetic order occurs for R=Pr,Nd, Sm, Gd and Tb [3]. This compounds show a layered structure and therefore, they considered as possibly close to quasi-2D cuprates. However, various local density approximation (LDA) band structure calculations [4-7] clearly demonstrated their 3D electronic structure. Quantum oscillation measurements of nonmagnetic botocarbides with R=Lu,Y give evidence for a clear multiband character in the normal state [8].

Two-band Eliashberg theory for borocarbideswas first proposed by Shulga et al [9] for the study upper critical field $H_{c2}(T)$ and such calculations were successfully applied to compounds with R=Lu,Y. Recently, the similar two-band Eliashberg theory has been applied [10] to MgB₂, which also reveal two-band nature of superconductivity [11,12]. Although extensive theoterical studies at microscopic level were carried out after the discovery of borocarbides, it is necessary to provide addional information on its superconducting properties bu using the macroscopic Ginzburg-Landau (G-L) theory. Regardless of the origin of superconductivity, G-L theory has been found adequate for explaining the measurable macroscopic quantities. The temperature

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dependence of fundamental measurable quantities like the lower critical field H_{c1} and the upper critical field H_{c2} are expected to help understanding the mechanism of superconductivity.

A two-band (TB) G-L description for the reentrant behavior of the upper critical field H_{c2} in magnetic borocarbides with Dy and Ho has been used in [13]. In last work magnetic order parameter terms was included into free energy functional. Calculations of upper critical field and their derivatives for nonmagnetic borocarbides using TB GL theory was reported in [14]. More recently similar calculations of $H_{c2}(T)$ [15], $H_{cm}(T)$ and specific heat jump $\frac{\Delta C}{C_N}$ [16] for magnesiume diboride MgB₂ has been conducted in framework TB GL theory.

The lower critical magnetic field of nonmagnetic borocarbides YNi₂B₂C are determined [17,18] by magnetization measurements. As followed from this measurements, the temperature dependence of London penetration depth λ (T) in borocarbides is close to quadratic relation, rather than the s-wave Bardeen-Cooper-Schrieffer (BCS) model behavior. So the London penetration depth in BCS model approximately follows exponential laws [19], which is the same as low-temperature single band (SB) superconductors. The different temperature dependence may indicate a slight difference in pairing state of different superconductor. In this paper, we study TB G-L theory and apply it to determine the temperature dependence of $\lambda^{-2}(T)$ for nonmagnetic borocarbide YNi₂B₂C. We show that the presence of two- order parameter in the theory gives a non-linear temperature dependence, which is shown to be in a good agreement with experimental data for YNi₂B₂C.

2 Theory

The TB G-L free energy functional with coupled superconducting order parameters can be written similarly as in [13-16],

$$F_{SC}[\Psi_1, \Psi_2] = \int d^3r \left(F_1 + F_{12} + F_2 + H^2 / 8\pi \right)$$
(1)

with

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

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

Here m_i^* are the effective masses of electron pairs belonging to the band i (i=1,2). F_i is the free energy of individual bands. F_{12} is the coupling energy term between the bands. α is determined by $\alpha_i = \gamma_i (T - T_{ci})$, while the coefficient β_i is independent of temperature, γ_i being proportionality constant. The quantities ε and ε_1 describe the coupling of two order parameters and their gradients, respectively. \vec{H} is the external magnetic field, Φ_0 is the magnetic flux quantum and \vec{A} is the vector potential.

By minimization of the free energy of Eq.(1)

$$\frac{\partial F}{\partial \Psi_1^*} = 0 \qquad \frac{\partial F}{\partial \Psi_2^*} = 0 \tag{4}$$

we then obtain the usual basic equation for the description of the two-band superconductivity. Here we assume that the order parameters $|\Psi_i|^2$ have weak spatial dependence. This approximation implicitly assumes isotropic s-wave superconductivity. To proceed further in one dimension for simplicity, we write a vector potential $\vec{A} = (0, Hx, 0)$ and with this, Eqs.(4) gives two set of equations of the following form:

$$-\frac{\hbar^2}{2m_1^*}(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2})\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2})\Psi_2 + \beta_1\Psi_1^3 = 0$$
(5)

$$-\frac{\hbar^2}{2m_2^*}\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2}\right)\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^2}\right)\Psi_1 + \beta_2\Psi_2^3 = 0.$$
(6)

Here $l_s^2 = (\hbar c/2eH)$ is the so-called magnetic length. The signs of the coefficients ε_1 and ε can be taken arbitrarily, which are related to the electronic configuration of the superconductor. Note that we ignore the magnetic field dependence of these coefficients. If the inter-band interaction is ignored, the Eqs. (4) and (5) are decoupled into two ordinary G-L equations with two different critical temperatures. In general, independent of the sign of ε , the superconducting phase transition results at a well-defined temperature exceeding both T_{c1} and T_{c2} , which is determined from the equation

$$\alpha_1(T_c)\alpha_2(T_c) = \varepsilon^2 \quad . \tag{7}$$

In the absence of any magnetic field, we can obtain an equilibrium value of the order parameters from Eqs.(5) and (6) with the solutions,

$$|\Psi_1|^2 = -\frac{\varepsilon^2 \left(\alpha_1(T)\alpha_2(T) - \varepsilon^2\right)}{\varepsilon^2 \beta_1 \alpha_2(T) + \beta_2 \alpha_1^3(T)} \tag{8}$$

$$|\Psi_{2}|^{2} = -\frac{\alpha_{1}^{2}(T)\left(\alpha_{1}(T)\alpha_{2}(T) - \varepsilon^{2}\right)}{\varepsilon^{2}\beta_{1}\alpha_{2}(T) + \beta_{2}\alpha_{1}^{3}(T)}.$$
(9)

At temperatures in the vicinity of T_c and the magnetic fields slightly larger than H_{c1} , the field dependence can be neglected. In this case, $|\Psi_1|$ and $|\Psi_2|$ can be considered as constants. The wave function is $\Psi_i(\vec{r}) = |\Psi_i| \exp(i\phi_i(\vec{r}))$. Here, $\phi_j(r)$ are the phases of the order parameters and the G-L free energy functional (1) can be rewritten as

$$F_{SC}[\phi_2,\phi_2] = \int d^3r \begin{pmatrix} \frac{\hbar^2}{4m_1^*} n_1(T) (\frac{d\phi_1}{dr} - \frac{2\pi}{\phi_0} \vec{A})^2 + \frac{\hbar^2}{4m_2^*} n_2(T) (\frac{d\phi_2}{dr} - \frac{2\pi}{\phi_0} \vec{A})^2 \\ + \varepsilon (n_1(T)n_2(T))^{1/2} \cos(\phi_1 - \phi_2) \\ + \varepsilon_1 (n_1(T)n_2(T))^{1/2} \cos(\phi_1 - \phi_2) (\frac{d\phi_1}{dr} - \frac{2\pi}{\phi_0} \vec{A}) \\ (\frac{d\phi_2}{dr} - \frac{2\pi}{\phi_0} \vec{A}) + \frac{H^2}{8\pi} \end{pmatrix}$$
(10)

Here, $n_1(T) = 2 |\Psi_1|^2$ and $n_2(T) = 2 |\Psi_2|^2$ are the densities of superconducting electrons for the corresponding bands, respectively. The temperature dependences of n_1 (T), n_2 (T) are defined by the equilibrium value of order parameters $|\Psi_1|$ and $|\Psi_2|$, which satisfy the G-L

equations (see Eqs. (8-9). In Eq. (10), the phase differences in equilibrium are determined by the following conditions

$$\cos(\phi_1 - \phi_2) = 1 \text{ or } \phi_1 - \phi_2 = 2\pi n, \quad \text{if} \quad \varepsilon < 0$$
 (11)

$$\cos(\phi_1 - \phi_2) = -1 \text{ or } \phi_1 - \phi_2 = (2n+1)\pi, \quad \text{if} \quad \varepsilon > 0$$
(12)

The equations determining the equilibrium values of magnetic field and phases of the orderparameters would be obtained by the minimising the free energy functional Eq.(10) with respect of the vector potential \vec{A} and the phases ϕ_1 , ϕ_2 . The equation for the vector potential \vec{A} takes the form

$$\frac{\nabla x \nabla x \vec{A}}{4\pi} = \frac{2\pi}{\phi_0} \left\{ \frac{\hbar^2}{2m_1^*} n_1(T) (\frac{d\phi_1}{dr} - \frac{2\pi}{\phi_0} \vec{A})^+ \frac{\hbar^2}{2m_2^*} n_2(T) (\frac{d\phi_2}{dr} - \frac{2\pi}{\phi_0} \vec{A})^+ \varepsilon_1 (n_1(T) n_2(T))^{1/2} \cos(\phi_1 - \phi_2) [(\frac{d\phi_1}{dr} - \frac{2\pi}{\phi_0} \vec{A}) + (\frac{d\phi_2}{dr} - \frac{2\pi}{\phi_0} \vec{A})] \right\}$$
(13)

We use the relevant Maxwell equation, $\nabla x \vec{H} = \frac{4\pi}{c} \vec{J}$, and Eq. (9) to find the London equation (by taking into account the equilibrium value of phase differences $\phi_1 - \phi_2$, see Eqs. (11) and (12)) of the form

$$\lambda^2 \frac{d^2 H}{dr^2} - H = 0 \quad , \tag{14}$$

Where λ is the London penetration depth, which can be written in the following form

$$\lambda(T) = \left\{ \frac{8\pi e^2}{c^2} \right\}^{-1/2} \left(\frac{n_1(T)}{m_1^*} + \varepsilon_1 (n_1(T)n_2(T))^{1/2} + \frac{n_2(T)}{m_2^*} \right)^{-1/2}$$
(15)

The dimensionless parameter $\frac{\lambda^{(T)}}{\lambda^{(0)}}$ is introduced with $\lambda(0) = \left(\frac{8\pi e^2 T_c}{c^2} \left(\frac{\gamma_1}{\beta_1 m_1^*} + \frac{\gamma_2}{\beta_2 m_2^*}\right)\right)^{1/2}$. One can then derive the following expression in the framework of TB GL theory

$$\frac{\lambda^{-2}(T)}{\lambda^{-2}(0)} = -\frac{2}{x+D^{-1}} \left(\tilde{\varepsilon}^2 + x(\tau - \tau_{c1})^2 + 2x\eta \tilde{\varepsilon}^2(\tau - \tau_{c1}) \right) \\
\left\{ \frac{\theta^2 + (2 - \tau_{c1} - \tau_{c2})\theta}{\tilde{\varepsilon}^2 D(\tau - \tau_{c2}) + (\tau - \tau_{c1})^3} \right\}$$
(16)

with

$$D = \frac{\beta_1 \gamma_2^2}{\beta_2 \gamma_1^2} , \tau_{c1,c2} = \frac{T_{c1,c2}}{T_c} , \tau = \frac{T}{T_c} , x = \frac{\gamma_1 m_1^*}{\gamma_2 m_2^*}, \theta = \tau - 1 , \tilde{\varepsilon}^2 = \frac{\varepsilon^2}{T_c^2 \gamma_1 \gamma_2}, \eta = \frac{\varepsilon_1 T_c \gamma_2 m_2^*}{2\varepsilon \hbar^2}$$
(17)

3 Results and discusion

Ghosh et al. [17] and da Rocha et al [18] found that the lower critical magnetic field $H_{c1}(T)$ data seem to be fit to te relation $H_{c1}(T) = H_{c1}(0)[1-(T/T_c)^2]$. As shown by calculations in SB BCS theory, the Ginzbutg-Landau parameter $\kappa(T) = \frac{\lambda(T)}{\xi(T)}$ [19] varies little with temperature. Due to this argument, the London penetration depth of YNi₂B₂C follows approximately also a quadratic law dependence of the form $\lambda^2(0)/\lambda^2(T) \approx 1 - (T/T_c)^2$. Solid circles in the graph of Fig.1 show this results [17]. The full line denotes the results of calculations from TB G-L theory. Here we used the equations (12) and (13) with the parameters: T_{c1} =9.8 K, T_{c2} =1.825 K, coupling coefficient $\tilde{\varepsilon}^2 = 0.33$ with D=1.5 and integradient interaction parameter $\eta = -0.11$. The same parameters were also used in [14] to determine the temperature dependence of upper critical field H_{c2} . With this choice of parameters and using equation (6), the critical temperature T_c results in about 16 K. According to the calculations [9], the average Fermi velocity in the first band equals v_{F2} =3.8 10⁷ cm/s, while in the second band v_{F1} =0.8 10⁷ cm/s. This yields that the parameter of effective mass ratio x can be taken as approximately 5 as in [14]. In choosing mass ratio parameter as inverse ratio of Fermi velocity parameters we use the following arguments.

The velocity of the superconducting electrons in different bands is given by (see Ref.[20])

$$v_{1,2} = \frac{1}{m_{1,2}^*} \left(\frac{\hbar}{2} \frac{d\phi_{1,2}}{dr} - \frac{2e}{\hbar}A\right).$$
(18)

Then for the quantity $m_1^* v_1 - m_2^* v_2$ we can write

$$m_1^* v_1 - m_2^* v_2 = \frac{\hbar}{2} \frac{d}{dr} (\phi_1 - \phi_2)$$
⁽¹⁹⁾

As a consequence of the relations (11) and (12), we can get

$$m_1^* v_1 = m_2^* v_2 \quad . \tag{20}$$

Note that the temperature dependence of $\lambda(T)$ in the TB G-L theory is dominantly determined by the interaction parameters ε_1 and ε . When the carriers have different effective masses $m_1^* >> m_2^*$ in different bands; the penetration depth can more effectively be determined by the small mass m_2^* . The contribution to $\lambda(T)$ from the larger mass is ignorable in such a case. As shown in Fig.1, the theoretical data of TB G-L theory are in agreement with experimental data [17]. It is well know that, the SB G-L theory [19,20] gives a well-known linear temperature dependence of the penetration depth as $\lambda^2(0)/\lambda^2(T) = 1 - T/T_c$. The two-fluid model gives temperature dependence $\lambda^2(0)/\lambda^2(T) = 1 - (T/T_c)^4$ [19,20]. For comparision results of SB GL theory and two-fluid model also presented in Fig.1. In addition to our previous report [14], we claim that the TB GL theory can successfully be applied to determine the temperature dependence of $\lambda(T)$.

In summary, we have shown that experimental data of penetration depth λ (T) for nonmagnetic borocarbide YNi₂B₂C can be described well in the framework of TB GL theory at temperatures close to T_c. Presence of two-order parameters and their coupling play significant role in determining its temperature dependence.



Fig. 1. Temperature dependence of London penetration depth $\lambda(T)$ of nonmagnetic borocarbide YNi₂B₂C versus reduced temperature, T/T_c. Full circles show the experimental data [17], while the lines are for theoretical expectations of $\lambda(T)$ for SB GL, TB GL, two-fluid theory calculations.

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