

THERMODYNAMIC MAGNETIC FIELD AND SPECIFIC HEAT JUMP OF IRON-BASED SUPERCONDUCTOR BY TWO-BAND GINZBURG-LANDAU APPROACH

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Abstract

In this research, temperature-dependent thermodynamic magnetic field and specific heat jump of Fe-based superconductor were studied by two-band Ginzburg-Landau theory. The analytical form of the thermodynamic magnetic field was investigated by four temperature-dependent models; Chen's model, Zhu's model, Shanenko's model and Changjan & Udomsamuthirun's model. For the calculation of specific heat jump, we use the Ruthgers expression. Calculation findings indicate an inverse relationship between the critical temperature and the specific heat jump. When compared with various models, the results from Changjan and Udomsamuthirun's models suit experimental data of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x = 0.4$) and KFe_2As_2 superconductors better

Keywords: Thermodynamic magnetic field, Specific heat jump, Fe-based superconductor, Ginzburg-Landau theory

Introduction

A lot of attention has been given to the discovery of superconductivity in Fe-based superconductors from both experimental and theoretical perspectives. Iron, as a ferromagnet, is not commonly thought to be compatible with superconductivity. Because, all the locally polarized spins on iron point toward the same direction and produce a magnetic field that prevents the creation of cooper pairs (Day, 2009). Therefore, it was very exciting discovery when Hosono and colleague

discovered superconductivity in fluorine-doped LaFeAsO (Kamihara *et al.*, 2008). In addition to these materials' unusual coupling methods, their potential for high field applications is intriguing. Fe-based superconductors have an extremely high upper critical field (H_{c2}) of over 100 T (Hunte *et al.*, 2008; Tarantini *et al.*, 2011) and comparatively little anisotropy (Baily *et al.*, 2009; Yamamoto *et al.* 2009).

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The multiband structure of the superconducting state is related to the main uniqueness properties of Fe-based superconductors (Khasanov *et al.*, 2009; Askerzade, 2012). Barzykin and Gor'kov (Barzykin and Gor'kov, 2008) studied pairing symmetry in oxypnictides multiband Bardeen-Cooper-Schrieffer (BCS) theory. The comparison between BCS and Eliashberg theory to describe two-band iron pnictide superconductors was proposed by Dolgov and colleauge (Dolgov *et al.*, 2009). Umrinino (Ummarino, 2011) used three-band $s \pm$ wave Eliashberg theory with antiferromagnetic spin fluctuations to explained the phenomenology of iron pnictide superconductors. The thermodynamic properties of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ were measured by four-band Eliashberg model in the intermediate coupling regime (Benfatto *et al.*, 2009). The two-band GL theory was also applied to explain the anomalous behavior of Fe-based superconductors. The lower critical field (H_{c1}) and upper critical field (H_{c2}) of LiFeAs superconductors were analyzed by anisotropy Ginzburg-Landau equations for layered systems (Askerzade, 2013). Changjan and Udomsamuthirun (Changjan and Udomsamuthirun, 2011) investigated the critical magnetic field ratio (H_{c2}/H_{c1}) of magnetic superconductor by anisotropic two-band Ginzburg-Landau approach. In addition, the two-band Ginzburg-Landau theory was implemented to examine the london penetration depth (Changjan and Udomsamuthirun, 2014) and the critical temperature (Changjan and Udomsamuthirun, 2013) of Fe-based superconductors.

KFe_2As_2 is a distinctive material among the numerous Fe-based superconductors. This compound distinguishes itself from previous iron-based superconductors in a wide range of ways, e.g., a realization of the Pauli limit or a manifestation of the superconducting gap with nodal lines. Additionally, experimental observations reveal that the isostructural phase transition from the tetragonal to collapsed tetragonal phase develops with increasing pressure (Ptok *et al.*, 2020). The maximum temperature of doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ systems is 38 K for $x = 0.4$. It belongs to a family of materials known as the '122' compounds, which are characterized by their chemical formula AFe_2As_2 (where A is a alkaline earth metal such as Ba or Sr). The replacement of potassium (K) for barium (Ba) has been shown to improve the material's superconducting characteristics (Rotter *et al.*, 2008).

One of the superconducting critical parameter of superconductors is the specific heat jump, which refers to the sudden increase in specific heat that occurs when a material becomes superconducting (Ginzburg and Andryushin, 2004). The specific heat jump is an unique characteristic of superconductors that can be utilized to understand the mechanism of

an unconventional superconductor (Wen, 2020). Fangying (Fangying, 2014) investigated the specific heat in two-band superconductors via two-bands Ginzburg-Landau model. When the two bands are in close connection, the finite interband Josephson coupling is negative repulsive. The specific heat jump of MgB_2 was calculated by first-principles calculations (Golubov *et al.*, 2002), BCS model (Askerzade, 2002) and Ginzburg-Landau model (Askerzade and Gencer, 2002; Askerzade, 2004). The thermodynamic magnetic field and specific heat jump of KFe_2As_2 and $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x = 0.4$) superconductors were conducted with the two-gap GL theory (Askerzade, 2014). In this work temperature-dependent thermodynamic magnetic field and specific heat jump of Fe-based superconductor were studied by two-band Ginzburg-Landau theory. Finally, the results of the calculations were compared with the experimental data of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x = 0.4$) and KFe_2As_2 superconductors.

Materials and Methods

We can formulate the Ginzburg-Landau free energy functional for two band magnetic superconductors in the presence of two band in Fe-based superconductors as follows (Hampshire, 1998; Changjan and Udomsamuthirun, 2011; Changjan *et al.*, 2017)

$$F_{sc}[\psi_1, \psi_2] = \int d^3r f_{sc} = \int d^3r (F_1 + F_2 + F_{12} + \int H_s dB) \quad (1)$$

With

$$F_{i(i=1,2)} = \frac{1}{2m_i} |(-i\hbar\vec{\nabla} - 2e\vec{A})\psi_i|^2 + \alpha_i |\psi_i|^2 + \frac{1}{2} \beta_i |\psi_i|^4, \quad (2)$$

$$F_{12} = \varepsilon (\psi_1^* \psi_2 + c.c.) + \varepsilon_1 \left\{ (i\hbar\vec{\nabla} - 2e\vec{A})\psi_1^* (-i\hbar\vec{\nabla} - 2e\vec{A})\psi_2 + c.c. \right\} \quad (3)$$

Here, F_i and F_{12} are the free energy density of band i ($i=1, 2$) and the interaction between bands.

The effective mass of the carriers in band i was indicated by m_i . ψ_i is the order parameter of band i and $|\psi_i|^2$ is proportional to the density of carriers, the coefficient α_i depends on the temperature, while coefficient β_i is independent of temperature. ε and ε_1 describe the interaction between the band order parameters and their gradients. $c.c.$ represents the previous term's complex conjugate. $\int H_s dB$

accounts for the energy stored in the local magnetic fields. For small change in B-field, rewrite the free energy of two-band magnetic superconductors from Equation (1) as (Hampshire, 1998; Changjan and Udomsamuthirun, 2011)

$$F_{sc}[\psi_1, \psi_2] = \int d^3r f_{sc} = \int d^3r \left(F_1 + F_2 + F_{12} + \gamma_0 + \gamma_1 B + \gamma_2 \frac{B^2}{2\mu_0} \right). \quad (4)$$

Here γ_0, γ_1 and γ_2 are coefficient parameters and $\gamma_2 = 1$ for non-magnetic superconductors. The coefficient parameter γ_1 depends on the gradient of field and $\gamma_1 = 0$ for the uniform applied field, $B = \mu_0 H + \mu_0 M_{sc} + \mu_0 M_{ions}$,

When the magnetic superconductors place in magnetic field, there are the field produced by ions ($\mu_0 M_{ions}$), the applied field ($\mu_0 H$) and the field produced by the carriers ($\mu_0 M_{sc}$). Minimization Equation (4) with respect to ψ_i^* ($i = 1, 2$), the 1st GL equations of two-band magnetic superconductor can be found as

$$\frac{1}{2m_1} (-i\hbar \nabla - 2e\vec{A})^2 \psi_1 + \alpha_1 \psi_1 + \beta_1 (\psi_1^* \psi_1) \psi_1 + \varepsilon \psi_2 - \varepsilon_1 (-i\hbar \nabla - 2e\vec{A})^2 \psi_2 = 0, \quad (5)$$

$$\frac{1}{2m_2} (-i\hbar \nabla - 2e\vec{A})^2 \psi_2 + \alpha_2 \psi_2 + \beta_2 (\psi_2^* \psi_2) \psi_2 + \varepsilon \psi_1 - \varepsilon_1 (-i\hbar \nabla - 2e\vec{A})^2 \psi_1 = 0. \quad (6)$$

In the absence of magnetic field. Let $\alpha_1 = \alpha_2 = \alpha$ and $\beta_1 = \beta_2 = \beta$, the modulus of order parameter can be obtained as

$$|\psi_1|^2 = \frac{\varepsilon^2 (\varepsilon^2 - \alpha^2)}{\alpha \beta (\varepsilon^2 + \alpha^2)} = |\psi_2|^2. \quad (7)$$

Free-energy difference between normal and superconducting states can be written as (Askerzade, 2014)

$$\Delta F = \frac{\beta_1}{2} |\psi_1|^4 + \frac{\beta_2}{2} |\psi_2|^4 - 2\varepsilon |\psi_1|^2 |\psi_2|^2. \quad (8)$$

Then, we get

$$\Delta F = (\beta - 2\varepsilon) \left[\frac{\varepsilon^2 (\varepsilon^2 - \alpha^2)}{\alpha \beta (\varepsilon^2 + \alpha^2)} \right]^2. \quad (9)$$

For calculated the specific heat jump, we use

$$\frac{\Delta C}{T_c} = \frac{1}{4\pi} \cdot \left(\frac{\partial H_c}{\partial T} \right)^2 \bigg|_{T_c} \quad (10)$$

Where H_c represent for a thermodynamic magnetic field that related to free energy differences as (Abrikosov, 1985)

$$\Delta F = \frac{H_c^2}{8\pi}. \quad (11)$$

Using Equation (9) and (11), the thermodynamic magnetic field can be rewritten as

$$H_c = \sqrt{8\pi(\beta - 2\varepsilon)} \left[\frac{\varepsilon^2 (\varepsilon^2 - \alpha^2)}{\alpha \beta (\varepsilon^2 + \alpha^2)} \right]. \quad (12)$$

From Equation (10) and (12) we can obtain the following expression for the specific heat jump of two-band Fe-based superconductor

$$\Delta C = T_c \left[\frac{\varepsilon^4 (\beta - 2\varepsilon)^{\frac{1}{2}}}{\beta (\varepsilon^2 + \alpha^2)} \right]^2 \left(\frac{\partial \alpha}{\partial T} \right)^2. \quad (13)$$

We consider the temperature dependent function, α from the 4 model to examine the specific heat jump.

Model 1: Chen's model (Chen *et.al*, 2011) consider the supposition that $\alpha = \left(1 - \frac{T}{T_c}\right)$ The specific heat jump is provided by

$$\Delta C = \left[\frac{\beta - 2\varepsilon}{\beta^2} \right] \left(\frac{1}{T_c} \right). \quad (14)$$

Model 2: Zhu's model (Zhu *et.al*, 2008) consider the supposition that $\alpha = \left[\left(1 - \left(\frac{T}{T_c}\right)^2\right) / \left(1 + \left(\frac{T}{T_c}\right)^2\right) \right]$ The specific heat jump is provided by

$$\Delta C = \left[\frac{\beta - 2\varepsilon}{\beta^2} \right] \left[-4T / T_c^2 \left[1 + \left(\frac{T}{T_c} \right)^2 \right]^2 \right]^2. \quad (15)$$

Model 3: Shanenko's model (Shanenko *et al*, 2011) consider the supposition that $\alpha = \left[\left(1 - \left(\frac{T}{T_c}\right)^2\right) / \left(1 + \left(\frac{T}{T_c}\right)^2\right) \right]$

The specific heat jump is provided by

$$\Delta C = \left[\frac{\beta - 2\varepsilon}{\beta^2} \right] \left(\frac{2T_c - T}{T_c^2} \right). \quad (16)$$

Model 4: Changjan and Udomsamuthirun's model (Changjan and Udomsamuthirun, 2013) consider the supposition that $\alpha = \left[p \left(1 - \left(\frac{T}{T_c} \right)^2 \right) + \frac{q}{2} \left(1 - \left(\frac{T}{T_c} \right)^2 \right)^2 \right]$

where p and q are arbitrary constant. The specific heat jump is provided by

$$\Delta C = \left[\frac{\beta - 2\varepsilon}{\beta^2} \right] \left(\frac{\left[p + q \left(1 - \frac{T}{T_c} \right) \right]^2}{T_c} \right). \quad (17)$$

Results and Discussion

The specific heat jump in a superconductor is a unique characteristic that is observed when a material transitions into the superconducting state (Figure 1). This jump in specific heat is caused by the sudden loss of normal electron excitations, known as quasiparticles, in the material. This loss of quasiparticles results in a decrease in the thermal energy of the material, leading to a sharp increase in the specific heat. The specific heat jump is a useful tool for identifying superconductors and determining the critical temperature at which a material becomes superconducting.

Two-band GL equations in non-magnetic model were solved analytically to calculate the specific heat jump of non-magnetic borocarbide: MgB₂ (Askerzade and Gencer, 2002; Askerzade, 2004) and Fe-based superconductors: KFe₂As₂ and Ba_{1-x}K_xFe₂As₂ (x = 0.4) (Askerzade, 2014). In this work, we use two-band GL equations for magnetic superconductor to investigated the specific heat jump (ΔC) of Fe-based superconductors. The result of calculation as shown in Equation (13). To analyzed the relationship between the specific heat jump and the critical temperature, we take into account the temperature dependent function, α from the 4 model as shown in Equations (14-17). At critical temperature ($T=T_c$) ($T=T_c$), the relationship between the specific heat jump and the critical temperature of model 1, model 2 and model 3 display the same outcome as

$$\Delta C_{1-3} = \left[\frac{\beta - 2\varepsilon}{\beta^2} \right] \left(\frac{1}{T_c} \right). \quad (18)$$

While the correlation between (ΔC) and T_c of model 4 is

$$\Delta C_4 = \left[\frac{\beta - 2\varepsilon}{\beta^2} \right] \left(\frac{p^2}{T_c} \right) \quad (19)$$

Where p implied the arbitrary constant.

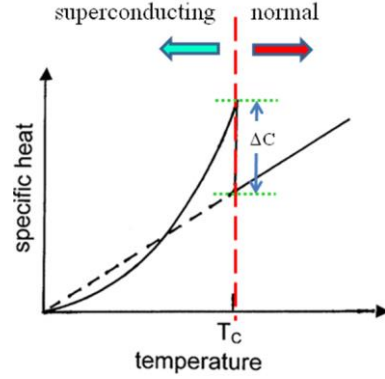


Figure 1. Shows the specific heat jump at critical temperature (T_c)

Equations (18) and (19) were used to calculate the specific heat jump at the critical temperature of the KFe₂As₂ superconductor. The following parameter values were utilized in these calculations: $T_c=3.5K$, $\beta=0.5$, $\varepsilon=-0.1$ and $p=0.96$. The calculation approach the specific heat jump at the critical temperature to the value $\Delta C_{1-3}=0.82$ and $\Delta C_4=0.75$ which is close to the value 0.76 obtained from the experimental study (Abdel-Hafiez *et al*, 2012). Similar calculations for Ba_{1-x}K_xFe₂As₂ (x=0.4) compound were conducted with the two-band GL equations for magnetic superconductor by using the parameters: $T_c=32.2K$, $\beta=0.5$, $\varepsilon=-0.006$ and $p=1.04$. The specific heat jump calculated using Equation (18) and (19) with these parameters is $\Delta C_{1-3}=0.77$ and $\Delta C_4=0.83$. while the corresponding experimental data is around 0.81 (Bud'ko *et al*, 2009). According to the single-band GL theory, this superconductor's normalized specific heat jump is equal to 1 (Abrikosov, 1985). This finding demonstrates that the specific heat jump is smaller in two-order parameter superconductors than in single-order parameter superconductors.

Conclusions

Two-band GL theory for magnetic superconductor was employed in this study to determine the Fe-based superconductor's specific heat jump at the critical temperature. The findings demonstrate that the specific heat jump is lower than in single-band superconductors. It has been shown that our model

is in good agreement with experimental data for KFe_2As_2 and $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ($x = 0.4$) superconductors. Focusing on four models, Changjan and Udomsamuthirun's model's calculation fit the experimental data more accurately than the other models since it contained arbitrary constants that could be adjusted. However, every model show inverse variation between the specific heat jump and the critical temperature, $\Delta C\alpha\frac{1}{T_c}$. By carefully selecting the appropriate parameters, the provided theory can be utilized to predicted the critical temperature in many band superconductors.

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