

THE STUDY ON TEMPERATURE-DEPENDENT SURFACE CRITICAL MAGNETIC FIELD OF IRON-BASED SUPERCONDUCTORS

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Abstract

The upper critical magnetic field (H_{c2}) is one of the important properties of superconductors in external magnetic field. The higher magnetic field strength, the more superconductivity is maintained. However, the surface critical magnetic field (H_{c3}) is larger than upper critical magnetic field which the ratio of H_{c3} to H_{c2} is constant. In this study, we investigated the surface critical magnetic field of the iron-based superconductor using Ginzburg-Landau's anisotropic two-band method. The surface critical magnetic field was calculated with four temperature-dependent models. Our analytical formula of the surface critical magnetic field obtains the temperature parameters. Finally, the numerical calculation was applied to the experimental data of iron-based superconductors

Keywords: Surface Critical Magnetic Field, Temperature-Dependent, Iron-Based Superconductors, Ginzburg-Landau Theory

Introduction

Superconductors can lose their superconductivity when subjected to a magnetic field. The maximal magnetic field that causes a superconductors to transition from superconducting to a normal conductors is referred to as the critical magnetic field (H_c). Three types of critical magnetic fields exist: lower critical magnetic field (H_{c1}), upper

critical magnetic field (H_{c2}), and surface critical magnetic field (H_{c3}). Each magnetic field is classified as type II superconductors (Kittel, 2005). When the external magnetic field is below the H_{c1} , the magnetic flux cannot enter through the superconductor. Consequently, the area has a superconducting state. When the external

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magnetic field exceeds the H_{c1} but falls short of the H_{c2} , a portion of the magnetic flux can pass through the superconductor. When the external magnetic field reaches the H_{c2} , the superconductor allows all magnetic flux to pass through. Superconductivity has been lost, yet the surface remains superconducting. When the external magnetic field exceeds the surface critical magnetic field, the superconductor loses all superconductivity and changes into a normal conductor. In other words, the surface critical magnetic field is the maximum magnetic field at which a superconductor may sustain its superconductivity (Fournais and Helffer, 2006). Meissner and Ochsenfeld (Ketterson and Song, 1999) investigated the magnetic properties of superconductors in 1933. They found the Meissner effect and established that superconductors exhibited perfect diamagnetism in the superconducting state. F. and H. London (Buckel, 1991) used Maxwell's equation for the superconductor system to describe the Meissner effect and the magnetic properties of superconductors in 1935. Saint-James and de Gennes theoretically demonstrated in 1963 that the critical magnetic field of isotropic one band of superconductors near the surface of materials is greater than the upper critical magnetic field of bulk superconductors as $H_{c3} = 1.66 H_{c2}$ (Saint-James and Gennes, 1963). In 1964, Abrikosov confirmed the theory of Saint-James and de-Gennes that thin film superconductors have $H_{c3} \approx 1.7H_{c2}$ (Abrikosov, 1965). In 2003, Askerzade studied the MgB_2 superconductor's surface critical magnetic field (Askerzade, 2003). He found that H_{c3} to H_{c2} is equal to a well-known single-band superconductor by Saint-James and de-Gennes. Iron-based superconductors were discovered in 2008 by Kamihara *et al.*, who showed that the solid-state reaction in LaSeAsO superconductor had a very high upper critical magnetic field of 55 K (Kamihara *et al.*, 2008). In 2011, Tsindlekht *et al.* published the ratio of H_{c3} to H_{c2} for the iron-based superconductor: KFeSe is 4.4 (Tsindlekht *et al.*, 2011). In 2014, Meakniti *et al.* evaluated magnetic properties' effects on the surface critical magnetic field (Meakniti *et al.*, 2014). Paramagnetism and antiferromagnetism have a H_{c3} to H_{c2} ratio of 1.66. In 2017, Changjan *et al.* utilized four temperature-dependent models for lead bismuth superconductor (Changjan *et al.*, 2017).

In this research, we study the surface critical magnetic fields of two-band magnetic superconductors dependent on the temperature and the anisotropy. We use a 4-model function including Chen's model (Chen *et al.*, 2011), Zhu's model

(Zhu *et al.*, 2008), Shanenko's model (Shanenko *et al.*, 2011), and Changjan and Udomsamuthirun's model (Changjan and Udomsamuthirun, 2013) to consider the cross-temperature-dependent and employ anisotropic functions (Fetter and Walecka, 1995) with the elliptical shape of Haas and Maki's model (Haas and Maki, 2001) and the pancake shape of Posazhennikova's model (Posazhennikova *et al.*, 2003).

Materials and Methods

Based on the Ginzburg-Landau theory, we can use the anisotropic two-band free energy to figure out the surface critical magnetic field for magnetic superconductors (Hampshire, 1998; Hampshire, 2001; Changjan and Udomsamuthirun, 2011). We are particularly interested in the anisotropy and temperature dependence. The two-band free energy expressed as

$$F_{sc}[\psi_1, \psi_2] = \int d^3r \left(F_1 + F_2 + F_{12} + \gamma_0 + \gamma_1 + \gamma_2 \frac{B^2}{2\mu_0} \right) \quad (1)$$

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

$$F_{12} = \varepsilon(\psi_1^* \psi_2 + c.c.) \langle f_1(\hat{k}) f_2(\hat{k}) \rangle + \varepsilon_1 \left\{ (i\hbar\nabla - 2e\vec{A})\psi_1^* (-i\hbar\nabla - 2e\vec{A})\psi_2 \right\} \langle f_1(\hat{k}) f_2(\hat{k}) \rangle + c.c. \quad (3)$$

The anisotropic free energy of the different bands is denoted by F_i , while the interaction between the first and second bands is denoted by F_{12} , where the first, second, and third terms of F_i represent kinetic energy, temperature dependence, and temperature independence, respectively, m_i specifies the effective mass of electron carriers. ψ_i is the order parameter, The coefficients α_i and β_i represent temperature-dependent and temperature-independent properties, respectively. $f_i(\hat{k})$ is the anisotropic function (Haas and Maki, 2001; Posazhennikova *et al.*, 2003), where the variables in the first and second bands are represented by the subscripts $i(i = 1, 2)$, ε and ε_1 represent the interaction of the two order parameters and their gradient, the complex conjugate appears as $c.c.$, $\vec{A}$ is the vector potential, a series of $\gamma_0 + \gamma_1 B + \gamma_2 \frac{B^2}{2\mu_0}$ is the magnetic field, when γ_0, γ_1 and γ_2 are coefficient of a magnetic field series (Hampshire, 1998; Hampshire, 2001).

$$\begin{aligned} & \frac{\langle f_1^2(\hat{k}) \rangle}{2m_1} (-i\hbar\nabla - 2e\vec{A})^2 \psi_1 \\ & + \alpha_1 \langle f_1^2(\hat{k}) \rangle \psi_1 + \varepsilon \langle f_1(\hat{k}) f_2(k) \rangle \psi_2 \\ & + \varepsilon_1 \langle f_1(\hat{k}) f_2(k) \rangle (-i\hbar\nabla - 2e\vec{A})^2 \psi_2 = 0 \end{aligned} \quad (4)$$

$$\begin{aligned} & \frac{\langle f_2^2(\hat{k}) \rangle}{2m_2} (-i\hbar\nabla - 2e\vec{A})^2 \psi_2 \\ & + \alpha_2 \langle f_2^2(\hat{k}) \rangle \psi_2 + \varepsilon \langle f_1(\hat{k}) f_2(\hat{k}) \rangle \psi_1 \\ & + \varepsilon_1 \langle f_1(\hat{k}) f_2(\hat{k}) \rangle (-i\hbar\nabla - 2e\vec{A})^2 \psi_1 = 0 \end{aligned} \quad (5)$$

Determine $\psi_1(x) = C\psi_2(x)$, $\psi_1(x) = e^{-\frac{\delta x^2}{2}}$ and $m_1 = m_2 = m$ to reduce the 1st Ginzburg-Landau equation and simplify to obtain the second-order formula as follows

$$\begin{aligned} & -\frac{\hbar^2}{2m} [C^2 \langle f_1^2(\hat{k}) \rangle - \langle f_2^2(\hat{k}) \rangle] \frac{d^2 \psi_1}{dx^2} \\ & + \frac{4e^2 A^2}{2m} [C^2 \langle f_1^2(\hat{k}) \rangle - \langle f_2^2(\hat{k}) \rangle] \psi_1 \\ & + [\alpha_1 C^2 \langle f_1^2(\hat{k}) \rangle - \alpha_2 \langle f_2^2(\hat{k}) \rangle] \psi_1 = 0 \end{aligned} \quad (6)$$

Where $\vec{A} = (0, B_0(x - x_0), 0)$ is the one-dimensional vector potential that represents the magnetic field in the z-direction, the equation can be rewritten as

$$\frac{d^2 \psi_1}{dx^2} - \lambda^2 B_0^2 (x - x_0)^2 \psi_1 = \frac{\lambda^2 [\alpha_1 C^2 \langle f_1^2(k) \rangle - \alpha_2 \langle f_2^2(k) \rangle]}{\alpha_0 [C^2 \langle f_1^2(k) \rangle - \langle f_2^2(k) \rangle]} \psi_1 \quad (7)$$

When $\vec{B}_0 = B_0 \vec{z}$, $B_0 = \mu_0(\chi - \chi')H_{c2} + \mu_0(1 + \chi')(H + M_{sc})$, $\lambda = \frac{2e}{\hbar}$ and $\alpha_0 = -\frac{2e^2}{m}$. Then, assigning $\psi = \exp(-\frac{1}{2}b\xi^2)$, $\xi = (\lambda B_0)^{\frac{1}{2}}x$, $\xi_0 = (\lambda B_0)^{\frac{1}{2}}x_0$ and $\beta = \frac{\lambda^2 [\alpha_1 C^2 \langle f_1^2(k) \rangle - \alpha_2 \langle f_2^2(k) \rangle]}{\alpha_0 [C^2 \langle f_1^2(k) \rangle - \langle f_2^2(k) \rangle]}$, we can obtain $-\frac{d^2 \psi_1}{d\xi^2} + (\xi - \xi_0)^2 \psi_1 = \beta \psi_1$ and solve the issue using the variation method (Abrikosov, 1965) by assigning $\psi = \exp(-\frac{1}{2}b\xi^2)$, which gives the value $b = \left(1 - \frac{2}{\pi}\right)^{\frac{1}{2}}$, $\beta = \left(1 - \frac{2}{\pi}\right)^{\frac{1}{2}}_{min}$.

Finally, the surface critical magnetic field depends on the anisotropic and temperature of the two-band magnetic superconductor as follows.

$$H_{c3} = \frac{\frac{1.66}{\alpha_0} \left[\frac{\alpha_1(T)C^2 \langle f_1^2(\hat{k}) \rangle - \alpha_2(T) \langle f_2^2(\hat{k}) \rangle}{C^2 \langle f_1^2(\hat{k}) \rangle - \langle f_2^2(\hat{k}) \rangle} \right] H_{c2} - (\chi - \chi') H_{c2}}{(1 + \chi')} \quad (8)$$

We used four temperature dependency models to understand more about the temperature dependence of the surface critical magnetic field (Changjan *et al.*, 2017), including M1: $\alpha_1 = \left(1 - \frac{T}{T_c}\right)$, (Chen *et al.*, 2011), M2: $\alpha_2 = \left(\frac{1 - \left(\frac{T}{T_c}\right)^2}{1 + \left(\frac{T}{T_c}\right)^2}\right)$, (Zhu *et al.*, 2008), M3: $\alpha_3 = \left(1 - \frac{T}{T_c}\right) + \frac{1}{2} \left(1 - \frac{T}{T_c}\right)^2$, (Shanenkov *et al.*, 2011) and M4: $\alpha_4 = p \left(1 - \frac{T}{T_c}\right) + \frac{q}{2} \left(1 - \frac{T}{T_c}\right)^2$, (Changjan and Udomsamuthirun, 2013). Each of the four models is based on empirical theories that determine the temperature dependence of α_1 and α_2 based on experimental data and assumptions, but they lack theoretical validation. Chen *et al.* assume a linear function, whereas Zhu *et al.*, Shanenko *et al.*, and Changjan and Udomsamuthirun assume a non-linear relationship for the temperature dependence function in order to explain the critical temperature behavior. The linear term can be validated from the BCS theory, but it does not fit the experimental results, in contrast to the non-linear term. Changjan and Udomsamuthirun introduce arbitrary constants p and q to the assumption of Shanenko *et al.* and modify it accordingly. Each model can only be justified in the temperature range near the critical temperature. Then consider the anisotropic functions of the ellipse and pancake models (Haas and Maki, 2001; Posazhennikova *et al.*, 2003).

Table 1. Shows the possible term of temperature dependence and anisotropy. Here e=ellipse, p=pancake.

1 st and 2 nd band parameters		M1		M2		M3		M4	
		e	p	e	p	e	p	e	p
M1	e	M11-e-e	M11-e-p	M12-e-e	M12-e-p	M13-e-e	M13-e-p	M14-e-e	M14-e-p
	p	M11-p-e	M11-p-p	M12-p-e	M12-p-p	M13-p-e	M13-p-p	M14-p-e	M14-p-p
M2	e	M21-e-e	M21-e-p	M22-e-e	M22-e-p	M23-e-e	M23-e-p	M24-e-e	M24-e-p
	p	M21-p-e	M21-p-p	M22-p-e	M22-p-p	M23-p-e	M23-p-p	M24-p-e	M24-p-p
M3	e	M31-e-e	M31-e-p	M32-e-e	M32-e-p	M33-e-e	M33-e-p	M34-e-e	M34-e-p
	p	M31-p-e	M31-p-p	M32-p-e	M32-p-p	M33-p-e	M33-p-p	M34-p-e	M34-p-p
M4	e	M41-l-e	M41-e-p	M42-e-e	M42-e-p	M43-e-e	M43-e-p	M44-e-e	M44-e-p
	p	M41-p-e	M41-p-p	M42-p-e	M42-p-p	M43-p-e	M43-p-p	M44-p-e	M44-p-p

There are four types of temperature dependent function and four types of anisotropic functions employed in response to the two-band surface critical magnetic field so there are $[4 \times 4 \text{ (temperature-dependent)}] \times [2 \times 2 \text{ (anisotropy)}] = 64$ events of temperature dependence and anisotropy in our model on the Table 1. After calculation, we found that only the terms related to M4 provided calculation results that were most consistent with the experimental results. So, to show numerical results, we will use only M1-M4 (M14), M2-M4 (M24), M3-M4 (M34), and M4-M4 (M44).

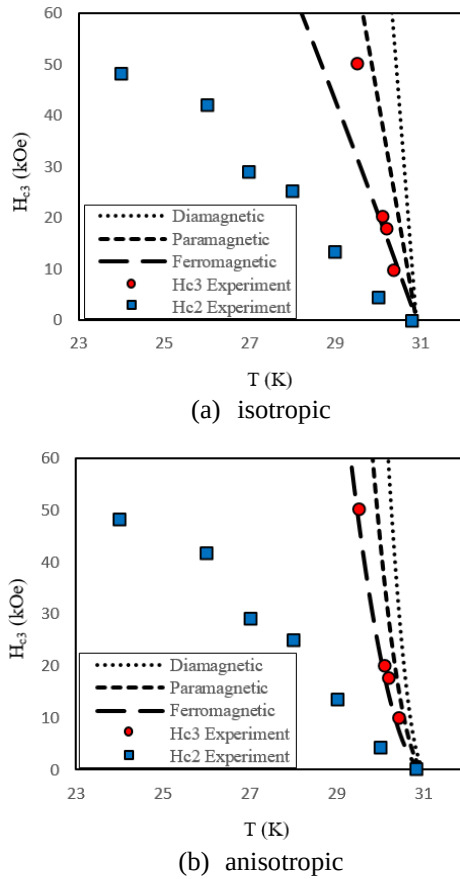


Figure 1. Shows the H_{c3} versus temperature for paramagnetism, ferromagnetism and diamagnetism of Fe-based superconductors.

Results and Discussion

The study of the surface critical magnetic field of iron-based superconductors revealed that they have ferromagnetic properties. We firstly investigate the basics properties that the magnetic properties of

this superconductor should be diamagnetism, paramagnetism or ferromagnetism. The magnetic parameters χ and χ' were trial into Equation. (8) and comparing with the experimental result of $K_{0.73}Fe_{1.68}Se_2$ superconductor (Tsindlekht *et al.*, 2011). The experiment data on a $K_{0.73}Fe_{1.68}Se_2$ superconductor were compared on H_{c3} with isotropic case and with anisotropic case in Figure 1-(A) and 1-(B), respectively. Figure 1, our results revealed that the ferromagnetism with anisotropy properties was the most suitable for further study on $K_{0.73}Fe_{1.68}Se_2$ superconductor. Here, the parameter used are Figure 1-(A) the isotropic case with $p_1 = 15$, $q_1 = 15$, $p_2 = 15$ and $q_2 = 15$ and: $\chi = 1$, $\chi' = 0.93$ (Ferromagnetism); $\chi = 0$, $\chi' = -0.08$ (Paramagnetism); $\chi = -0.5$, $\chi' = -0.58$ (Diamagnetism). Figure 1-(B) the anisotropic case with $p_1 = 1$, $q_1 = 0.5$, $p_2 = 1$, $a = 40$, $b = 0.1$ and: $\chi = 1$, $\chi' = 1$ (Ferromagnetism); $\chi = 0$, $\chi' = 0$ (Paramagnetism); $\chi = -0.5$, $\chi' = -0.5$ (Diamagnetism)

The effect of the cross-temperature-dependent model between the first band and second band and the anisotropic model on the surface critical magnetic field has been investigated. The first, second, third, and fourth cases is shown in the graph of H_{c3} versus temperature (T), as illustrated in Figure 2. Our findings indicated that the cross-temperature dependent of all four cases (M14, M24, M34, and M44) have an anisotropic function with a pancake shape in the first band and an elliptical shape in the second band. The first case is a cross-model of M14, Figure. 2-(A). the parameters are used as $\chi = 1$, $\chi' = 1$, $p = 1$ and $q = 11$; M14-ellipse- ellipse: $a = 0.5$, $b = 0.1$; M14-ellipse-pancake: $a = 0.5$, $b = 1$; M14-pancake-ellipse: $a = 40$, $b = 0.1$ and M14-pancake-pancake: $a = 40$, $b = 1$. The second case is a cross-model of M24, Figure. 2-(B). the parameters are used as $\chi = 1$, $\chi' = 1$, $p = 1$ and $q = 11$; M24- ellipse- ellipse $a = 0.5$, $b = 0.1$; M24- ellipse- pancake $a = 0.5$, $b = 1$; M24- pancake-ellipse $a = 40$, $b = 0.1$ and M24- pancake-pancake $a = 40$, $b = 1$. The third case is a cross-model of M34, Figure. 2-(C). the parameters are used as $\chi = 1$, $\chi' = 1$, $p = 1$ and $q = 11$; M34-ellipse-ellipse $a = 0.5$, $b = 0.1$; M34-ellipse-pancake $a = 0.5$, $b = 1$; M34-pancake-ellipse $a = 40$, $b = 0.1$, and M34-pancake-pancake $a = 40$, $b = 1$. The fourth case is a cross-model of M44, Figure. 2-(D). the parameters are used as $\chi = 1$, $\chi' = 1$, $p_1 = 1$, $q_1 = 0.5$, $p_2 = 1$ and $q_2 = 11$; M44-ellipse- ellipse $a = 0.5$, $b = 0.1$; M44-ellipse-pancake $a = 0.5$, $b = 1$; M44-pancake-ellipse $a = 40$, $b = 0.1$; M44-pancake-pancake $a = 40$, $b = 1$. Here, solid line is ellipse-ellipse, big-dashed line is ellipse-pancake, small-

dashed line is pancake-ellipse and dotted line is pancake-pancake, red circle is H_{c3} experiment and blue square is H_{c2} experiment. The study provided evidence that the band structure of the $K_{0.73}Fe_{1.68}Se_2$ superconductor is influenced by both temperature and anisotropy, resulting in the emergence of a pancake-ellipse shape. In this study, the two-band model was used for the calculation of H_{c3} as in equation (8), the H_{c3} curve with $T_c = 31$ K. Figures 2-(A) to 2-(D) show the anisotropy of the four cross-temperature-dependent models, M14, M24, M34, and M44, respectively. The results of all four models only identified a pancake shape in the first band and an ellipse shape in the second band.

The anisotropic function of H_{c3} with a pancake shape in the first band and an elliptical shape in the second band and H_{c2} from experimental data from Ref. (Tsindlekht *et al.*, 2011) was used to investigate the surface critical magnetic field to upper critical magnetic field ratio (H_{c3}/H_{c2}). Figure 3 illustrates the relationship between the H_{c3}/H_{c2} and T/T_c ratios. As the T/T_c ratio increases, the H_{c3}/H_{c2} ratio for all four cases (M14, M24, M34, and M44) decreases and approaches around 4.4 in the critical temperature range. This result is consistent with the experimental findings on $K_{0.73}Fe_{1.68}Se_2$ by

(Tsindlekht *et al.*, 2011), which also showed an H_{c3}/H_{c2} ratio of approximately 4.4. Furthermore, our study revealed that the H_{c3}/H_{c2} ratios were higher than those reported for conventional superconductors, as described by (Saint-James and Gennes, 1963), with a ratio of approximately 1.66.

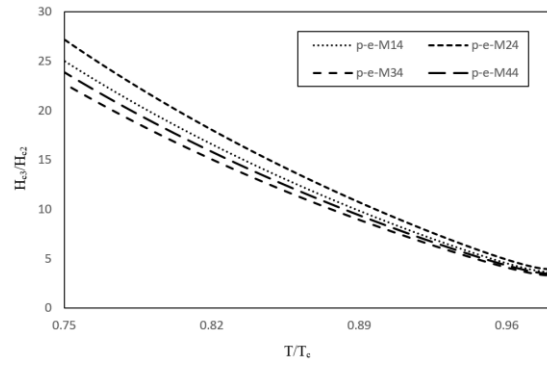


Figure 3. Shows the relationship between H_{c3}/H_{c2} versus T/T_c of cross-temperature-dependent for pancake-ellipse of M14, M24, M34 and M44.

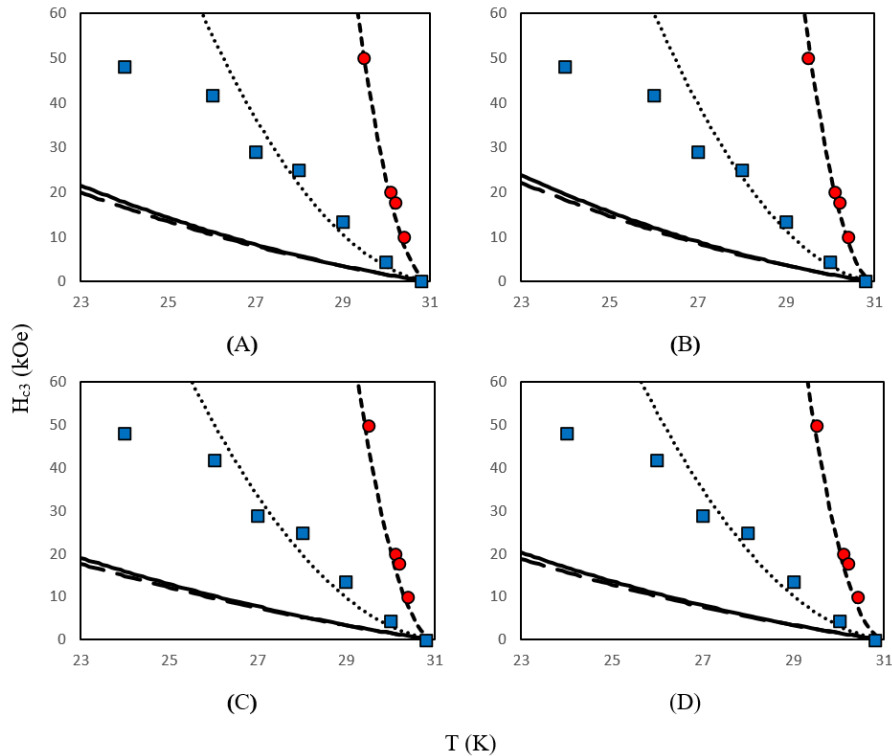


Figure 2. Shows the relationship between H_{c3} versus T of cross-temperature-dependent for (A) M14, (B) M24, (C) M34 and (D) M44.

Conclusions

In this work, the Ginzburg-Landau theory are used to study the surface critical magnetic field (H_{c3}). Our computations start with the anisotropic two-band free energy equation. Minimize free energy with respect to order parameters (ψ_1 and ψ_2); the result is the first Ginzburg-Landau equation, which consists of two equations. The first Ginzburg-Landau equation is then simplified, and the H_{c3} is found using the variation method, for which the H_{c3} of two-band magnetic superconductors is dependent on the temperature and the anisotropy. We employ four temperature-dependent functions and two anisotropic functions by considering cross-temperature dependence and cross-anisotropy: there are $[4 \times 4 \text{ (temperature-dependent)}] \times [2 \times 2 \text{ (anisotropy)}] = 64$ events, classified into 4 cases, consisting of Case 1: M11, M12, M13 and M14, case 2: M21, M22, M23 and M24, case 3: M31, M32, M33 and M34 and case 4: M41, M42, M43 and M44. There are 16 events in total, each of them based on 4 anisotropic types: ellipse-ellipse, ellipse-pancake, pancake-ellipse and pancake-pancake bringing the total to 64 events. According to our results from the trial method, the terms related to M4, including M14, M24, M34 and M44, with anisotropy in the pancake first band and elliptical second band (M14-p-e, M24-p-e, M34-p-e, and M44-p-e), produced the most consistent calculation results with the experimental data of $\text{K}_{0.73}\text{Fe}_{1.68}\text{Se}_2$ superconductor. In addition, the ferromagnetism ($\chi = 1$) of H_{c3} were found in the $\text{K}_{0.73}\text{Fe}_{1.68}\text{Se}_2$ superconductor. This corresponds to the FeSe superconductor (Nouailhetas *et al.*, 2021). Moreover, The H_{c3}/H_{c2} ratio for all four cases (M14-p-e, M24-p-e, M34-p-e, and M44-p-e) was approximately 4.4 in the critical temperature range. This result is consistent with the experimental findings on $\text{K}_{0.73}\text{Fe}_{1.68}\text{Se}_2$, which also showed an $\frac{H_{c3}}{H_{c2}} \sim 4.4$ (Tsindlekht *et al.*, 2011). These experimental results are higher than the value predicted by the well-known formula (Saint-James and Gennes, 1963). When $\langle f_1^2(\hat{k}) \rangle = 1$, $\langle f_2^2(\hat{k}) \rangle = 1$ and $\alpha_1 = \alpha_2 = \alpha_0$ are set, the surface critical magnetic field in equation (8) can be reduced to an isotropic one-band magnetic superconductor (Meakniti *et al.*, 2014). The discovery of the shape of the band structure, specifically the Fermi surface form, and the H_{c3}/H_{c2} ratio in relation to temperature dependence in the iron-based superconductor will greatly benefit researchers.

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