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Original Article

The pressure dependence of the critical temperature of MgB_2

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Abstract

The dependence of the critical temperature T_c on the pressure P in the magnesium diboride MgB_2 has been studied in the two-band model. In each band consists of two pairing interaction, electron-phonon interaction and non-electron-phonon interaction. This research derived the exact equation of the critical temperature dependence on pressure for magnesium diboride superconductor. It was found that increasing electron-phonon coupling constant and non-electron-phonon coupling constant of 1st and 2nd band will increase the T_c. The critical temperature decreased as pressure increased and can be fitted well to the experimental T_c versus P in magnesium diboride.

Keywords: pressure effect, magnesium diboride, two-band superconductor, weak-coupling interaction, high- T_c superconductor

1. Introduction

The superconductor, MgB_2 was superconducting at 39K with a big surprise which was discovered by Nagamatsu in 2001 (Nagamatsu, Nakagawa, Muranaka, Zenitani, & Akimitsu, 2001). Although, the structure $MgB2$ is regarded as a conventional superconductor based on the Bardeen-Cooper-Schrieffer (BCS) theory, its high critical temperature (Vinod, Varghese, & Syamaprasad, 2007), anomalous temperature behavior of the specific heat (Hardy *et al.*, 2010) and shift from 0.5 isotope exponent (Budko *et al.*, 2001) cannot be explained by the BCS theory. Because of the absence of grain-boundary weak links, MgB_2 is more similar to conventional superconductor than to high temperature superconductors (Larbalestier *et al.*, 2001). Liu, Mazin, and Kortus (2001) predicted the existence of two-band in MgB_2 and it has been observed in experimental studies (Lavarone *et al.*, 2002). It is concluded that MgB_2 is a superconductor with two energy gaps, the σ band energy gap originating from σ bonding and the π band energy gap originating from π bonding (Xi, 2008); the σ band energy gap of 6.8MeV opens on cylindrical Fermi surfaces while the π band energy gap of 1.8 MeV is associated to the three dimensional Fermi surfaces (Choi, Roundy, Sun, Cohen, & Louie, 2002).

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The principal parameters determining the superconducting properties and used to tune the critical temperature can be varied by applying external pressure to the superconductors. The electronic and magnetic properties of superconductors can be altered via changes in lattice parameters. Some materials such as AVO_4 orthovanadates undergo the structural change into different phases under applied pressure (Errandonea & Garg, 2018). Hodder investigated the pressure dependence of T_c on the conventional superconductor and showed that T_c decreased as the pressure increased (Hodder, 1969). For Tl-based and Bi-based superconductors, the critical temperature increased as pressure is increased (Chanpoom, 2020). At high pressure some elements or compounds, the structural transitions onto metallic and superconductivity phase and showed superconductivity state under pressure (Buzea & Robbie, 2005). The investigation of pressure dependence on the critical temperature in high temperature superconductors is useful in the search for new superconductors with highly T_c values. In the first high temperature superconductor $La_{2-x}Ba_xCuO_4$, it was found that the critical temperature increased with the external pressure to superconductors. The critical temperature of $HgBa_2Ca_2Cu_3O_{8+\delta}$ can increase to 160K under high pressure (Gao *et al.*, 1994). Krzyosiak *et al.* (2018) studied the effect of high pressure on the critical temperature of superconductors. They suggested that the dependence of the critical temperature on high external pressure varied with parameters and showed four types of curve change in response to applied pressure. The pressure could induce the formation of a super-lattice in MgB_2 (Tschauner, Errandonea, & Serghiou, 2006). In MgB_2, hydrostatic pressure can reduce the density of state and can lead to a reduction in the transition temperature from 39.7K at $P = 0GPa$ to 37.7K at $P = 1.2GPa$ (Shabbir, wang, Ghorbani, Dou, & Xiang, 2015).The hydrostatic pressure of $1.2GPa$ can significantly enhance flux pinning or the critical current density of optimally doped $Ba_{0.6}K_{0.4}Fe_2As_2$ from $5\times10^5 A/cm^2$ to nearly $10^6 A/cm^2$ at 2T, and from $2\times10^5 A/cm^2$ to nearly $5.5\times10^5 A/cm^2$ at 12T (Shabbir, wang, Ma, Dou, Yan, & Mei, 2016). The pressure induced a transition from the regime where pinning is controlled by spatial variation in the critical transition temperature to the regime controlled by spatial variation in the mean free path (Shabbir, wang, Ghorbani, Dou, & Xiang, 2015). For $Sr_4V_2O_6Fe_2As_2$ superconductor, at $1.2GPa$, the transition temperature can increase from 15K to 22K, as well as the critical current density, J_c up to 30 times at both low and high fields (Shabbir, wang, Ghorbani, Shekhar, Dou, & Srivastava, 2015). In $Sr_{0.6}K_{0.4}Fe_2As_2$ tape, hydrostatic pressure induced pinning centers are the main source of J_c enhancement, along with a fractional contribution from geometric changes around the grain boundaries under pressure (Shabbir *et al*., 2017).

After the existence of superconductivity in two-band superconductor MgB_2 studies about the dependence on pressure of the critical temperature reported that the critical temperature decreases as the pressure increases but there is a different value of on pressure coefficient (Goncharov *et al.*, 2001; Tang *et al.*, 2001; Tomita, Hamlin, & Schilling, 2001). Kononenko *et al.* (2015) studied the effect of two-band in MgB_2 under hydrostatic pressure that showed the underestimation of effect of pressure on the interband scattering. The effect of pressure on the critical temperature of MgB_2 can be explained with two-band BCS model incorporating interband interactions; increasing interband electron-phonon (electron-electron) coupling will increase (decrease) the critical temperature (Ogbuu & Abah, 2015). Ummario (2005) studied the pressure dependence of the critical temperature in MgB_2 and two-band Eliashberg theory found that T_c decreases as the pressure increases and can be fitted very well with the experimental T_c versus P. The pressure dependence of T_c is complex and depends on various parameters such as the phonon frequency and the density of state.

This research studied the pressure dependence on the critical temperature by using BCS-like model. This study also sets up the theoretical model to investigate the pressure dependence on the critical temperature. The exact formula of T_c's equation depending on pressure is derived. The comparison with the experimental data is shown.

2. Materials and Methods

Experiments suggest that MgB_2 is a two-band s-wave superconductor. The multiband superconductors were first introduced by Suhl, Matthias, and Walker (Suhl, Matthias, & Walker, 1959) and Moskalenke, Palistrant, and Vakalyuk (Moskalenke, Palistrant, & Vakalyuk, 1991) showing that a two-gap superconductor was described by a two band mechanism with an interband pairing channel. The pairing interaction consists of two parts, an attractive electron-phonon interaction and an attractive non-electron phonon interaction in σ-band, π-band and $\pi-\sigma$ scattering of interband pairs. The pressure dependence of T_c can be derived from weak-coupling BCS model (Bardeen, Cooper, & Schrieffer, 1957) and strong-coupling Eliashberg model (Eliashberg, 1961).

The linearized Hamiltonian of a two-band superconductor with the interband scattering and intraband pairs is used (Kristofeffel & Rubin, 2001; Udomsamuthirun, Kumvongsa, Burakorn, Changkanarth, & Yoksan, 2005).

$$H = H_\pi + H_p + H_{p\pi} \tag{1}$$

here

$$\left.\begin{aligned}
H_\pi &= \sum_{k\sigma} \varepsilon_{\pi k\sigma} \pi^+_{k\sigma} \pi_{k\sigma} + \sum_{kk'} V_{\pi\pi kk'} \pi^+_{k\uparrow} \pi^+_{-k\downarrow} \pi_{-k'\downarrow} \pi_{k'\uparrow} \\
H_p &= \sum_{k\sigma} \varepsilon_{pk\sigma} p^+_{k\sigma} p_{k\sigma} + \sum_{kk'} V_{ppkk'} p^+_{k\uparrow} p^+_{-k\downarrow} p_{-k'\downarrow} p_{k'\uparrow} \\
H_{p\pi} &= \sum_{kk'} V_{p\pi kk'} (p^+_{k\uparrow} p^+_{-k\downarrow} \pi_{-k'\downarrow} \pi_{k'\uparrow} + \pi^+_{k\uparrow} \pi^+_{-k\downarrow} p_{-k'\downarrow} p_{k'\uparrow})
\end{aligned}\right\} \tag{2}$$

here H_π, H_p are the Hamiltonian of π-band and σ-band respectively, $H_{p\pi}$ is the Hamiltonian of interband scattering.

Following the two-band Hamiltonian of superconductivity and applying standard techniques, the linearized gap equations as

$$\Delta_{pk} = -\sum_{k'} V_{ppkk'} \left(\frac{\Delta_{pk'}}{2\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}} \right) \tanh\left(\frac{\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}}{2T} \right) - \sum_{k'} V_{p\pi kk'} \left(\frac{\Delta_{\pi k'}}{2\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}} \right) \tanh\left(\frac{\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}}{2T} \right) \tag{3}$$

$$\Delta_{\pi k} = -\sum_{k'} V_{\pi\pi kk'} \left(\frac{\Delta_{\pi k'}}{2\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}} \right) \tanh\left(\frac{\sqrt{\varepsilon^2_{\pi k'} + \Delta^2_{\pi k'}}}{2T} \right) - \sum_{k'} V_{\pi pkk'} \left(\frac{\Delta_{pk'}}{2\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}} \right) \tanh\left(\frac{\sqrt{\varepsilon^2_{pk'} + \Delta^2_{pk'}}}{2T} \right) \tag{4}$$

here $\varepsilon_{ik'}(i = p,\pi)$ is the band dispersion measured from the Fermi energy, $\Delta_{ik'}(i = p,\pi)$ is the superconducting gap and $V_{ikk'}(i = p,\pi)$ is pairing interaction potential. The two-band model, the paring interaction consists of two parts (Daemen & Overhauser, 1990; Yoksan, 1991), an attractive electron-phonon interaction V_{ph} and an attraction non-Electron-phonon interaction U_c. The ω_D and ω_c are the characteristic energy cutoff of the Debye phonon and non-phonon respectively. The interaction potential $V_{ikk'}$ may be written as

$$V_{ikk'} = \begin{cases} -V_{ph}^{i} - U_C^{i} & , for \quad 0 < |\varepsilon_k| < \omega_D \\ -U_C^{i} & , for \quad \omega_D < |\varepsilon_k| < \omega_c \end{cases} \tag{5}$$

$i = p,\pi, p\pi$. The interactions of the superconducting order parameter are

$$\Delta_{jk} = \begin{cases} \Delta_{j1} & , for \quad 0 < |\varepsilon_k| < \omega_D \\ \Delta_{j2} & , for \quad \omega_D < |\varepsilon_k| < \omega_c \end{cases} \tag{6}$$

$j = p,\pi$. Substituting Equation (5),(6) in Equation (3) and (4) and replacing the summation over k' by integration over energy $\varepsilon_{ik'}$ (using $k_B = h = 1$) and constant density of state $N(\varepsilon_k) = N(0)$, at $T = T_c$, yields

$$\begin{pmatrix} (\lambda_1+\mu_1)I_1 - 1 & (\lambda_{12}+\mu_{12})I_1 & \mu_1 I_2 & \mu_{12} I_2 \\ (\lambda_{12}+\mu_{12})I_1 & (\lambda_2+\mu_2)I_1 - 1 & \mu_{12} I_2 & \mu_2 I_2 \\ \mu_1 I_1 & \mu_{12} I_1 & \mu_1 I_2 - 1 & \mu_{12} I_2 \\ \mu_{12} I_1 & \mu_2 I_1 & \mu_{12} I_2 & \mu_2 I_2 - 1 \end{pmatrix} \begin{pmatrix} \Delta_{11} \\ \Delta_{21} \\ \Delta_{12} \\ \Delta_{22} \end{pmatrix} = 0 \tag{7}$$

here $I_1 = \int_0^{\omega_D} \frac{\tanh\left(\frac{\varepsilon}{2T_c}\right)}{\varepsilon} d\varepsilon \qquad I_2 = \int_{\omega_D}^{\omega_c} \frac{\tanh\left(\frac{\varepsilon}{2T_c}\right)}{\varepsilon} d\varepsilon$

$\lambda_1 = N(0)V_{ph}^{1}, \lambda_2 = N(0)V_{ph}^{2}, \lambda_{12} = N(0)V_{ph}^{12} = N(0)V_{ph}^{21}$

$\mu_1 = N(0)U_c^{1}, \mu_2 = N(0)U_c^{2}, \mu_{12} = N(0)U_c^{12} = N(0)U_c^{21}$

λ_1, λ_2 are the phonon coupling constant of 1^{st} and 2^{nd} band

μ_1, μ_2 are the non-phonon coupling constant of 1^{st} and 2^{nd} band

λ_{12}, μ_{12} are the interband phonon and non-phonon coupling constant respectively.

Solving the secular equation of Equation (7), It gets

$$I_1 = \frac{1 - \mu_t I_2}{\lambda_t + \mu_t + (2b_m - \mu_t \lambda_t) I_2} \tag{8}$$

here $\lambda_t = \lambda_1 + \lambda_2, \mu_t = \mu_1 + \mu_2$ and $b_m = \mu_{12}^2 - \mu_1 \mu_2$

Let λ_t and μ_t depended on pressure P, differentiation of Equation (8) with respect to P yield

$$\frac{dI_1}{dP} = \frac{\lambda_t \phi_{\lambda_t} + \mu_t \phi_{\mu_t} - 2\mu_t \lambda_t \phi_{\lambda_t} \ln\left(\frac{\omega_c}{\omega_D}\right)}{(\lambda_t + \mu_t)\left(\lambda_t + \mu_t + (4b_\mu - 2\lambda_t \mu_t)\ln\left(\frac{\omega_c}{\omega_D}\right)\right) B_0} \tag{9}$$

here the bulk modulus $B_0 = -\frac{dP}{d\ln V}, \frac{d\ln\mu_t}{d\ln V} = \phi_{\mu_t}, \frac{d\ln\lambda_t}{d\ln V} = \phi_{\lambda_t}$.

The T_c's equation can be derived from differentiation of $I_1 = \int_0^{\omega_D} \frac{\tanh\left(\frac{\varepsilon}{2T_c}\right)}{\varepsilon} d\varepsilon$ with respect to pressure; in case $\omega_D >> T_c$, the variation of the critical temperature on pressure is

$$\frac{d\ln T_c}{dP} = \frac{d\ln \omega_D}{dP} - \frac{dI_1}{dP}$$
$$= \frac{d\ln \omega_D}{d\ln V}\cdot\frac{d\ln V}{dP} - \frac{dI_1}{dP}$$
$$= \frac{r_G}{B_0} - \frac{dI_1}{dP} \tag{10}$$

here $r_G = -\frac{d\ln \omega_D}{d\ln V}$ is the mode Gruneisen parameter. By substituting Equation (9) in Equation (10) the exact formula of T_c's equation of two-band superconductors can be written as

$$T_c = Exp\left[\frac{r_G}{B_0} - \left(\frac{\lambda_t\phi_{\lambda_t} + \mu_t\phi_{\mu_t} - 2\mu_t\lambda_t\phi_{\lambda_t}\ln\left(\frac{\omega_c}{\omega_D}\right)}{(\lambda_t+\mu_t)\left[\lambda_t+\mu_t+\left(4b_\mu - 2\lambda_t\mu_t\right)\ln\left(\frac{\omega_c}{\omega_D}\right)\right]B_0}\right)\right]P \tag{11}$$

Equation (11) shows the formula of pressure dependence on the critical temperature, varying on parameters $\lambda_t, \mu_t, \phi_{\lambda_t}, \phi_{\mu_t}, b_\mu, r_G, B_0, \omega_D$ and ω_c.

3. Results and Discussion

The pressure dependence of the critical temperature of two-band superconductor in weak-coupling limit is derived analytically as shown in Equation (11). This study adjusted parameters $\lambda_t, \mu_t, \phi_{\lambda_t}, \phi_{\mu_t}, b_\mu, r_G, B_0, \omega_D$ and ω_c to get desired experimental result. The critical temperature at zero pressure is $T_c(0) = 37.4K$ (Lorenz, Meng, & Chu, 2001); this research used the set of parameters as $\phi_{\lambda_t} = 2.2, \phi_{\mu_t} = 1.8, b_\mu = 0.1, \omega_c = 800K, \omega_D = 745K, B_0 = 90GPa$ and $r_G = 1$. The calculation of Equation (11) varied on P, λ_t and μ_t is shown in Figure 1. It was found that the T_c decreased as pressure increased.

This research numerically evaluates the critical temperature as a function of pressure order the range $0-2GPa$ for different values of $\lambda_t = 0.2, 0.3$ and $\mu_t = 0.1, 0.2$. It was found that increasing λ_t and μ_t will increase the T_c. The variation of the critical temperature with the pressure corresponded to the experimental data of MgB_2 (Lorenz *et al.*, 2001). It is observed that the case of $\lambda_t = 0.3$ and $\mu_t = 0.1$ fits well with the data of MgB_2 over the range $0-2GPa$.

In case of pressure range $0-30GPa$, this study numerically evaluates the dependence on pressure of T_c values at $T_c(0) = 37.3K$ (Tissen, Nefedova, Kolesnikov, & Kulakov, 2001). The results uses parameters as $\phi_{\lambda_t} = 2.6, \phi_{\mu_t} = 1.8, b_\mu = 0.1, \omega_c = 800K$ and $\omega_D = 745K, B_0 = 90GPa$ and $r_G = 1$. The calculation using Equation (11) are shown in Figure 2. It was found that the T_c decreases as pressure increases and the critical temperature approaches to zero at very high pressure.

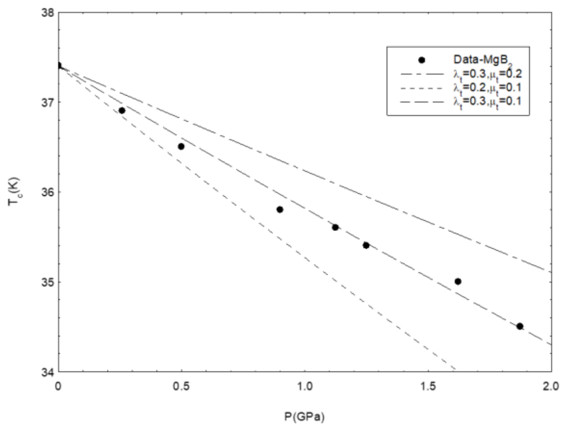

Figure 1. The variation of Tc versus P for different value of λ_t and μ_t based on Equation (11). On pressure range $0-20GPa$.

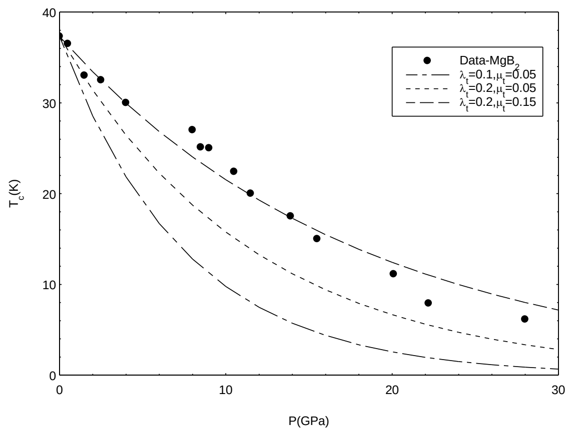

Figure 2. The variation of Tc versus P for different value of λ_t and μ_t based on Equation (11). On pressure range $0-30GPa$.

For this case, over the range $0-30GPa$ and values of $\lambda_t = 0.1, 0.2$ and $\mu_t = 0.05, 0.15$ it was found that the critical temperature increases as λ_t and μ_t increase. The result agreed with the experimental data of MgB_2 (Tissen, Nefedova, Kolesnikov, & Kulakov, 2001).

It is observed that the critical temperature vanished at very high pressure. The influence of the coupling constant of 1st and 2nd band, both coupling constant λ_t and μ_t can increase T_c; the non-phonon coupling constant μ_t showed more effect on the critical temperature than the phonon coupling constant λ_t at very high pressure.

4. Conclusions

This research has investigated the pressure dependence of the critical temperature and focused on MgB_2 superconductor. The exact equation for the critical temperature using the two-band BCS model is derived. It was found that the critical temperature decreased as the pressure increased and can be fit well with the experimental data of MgB_2 over the entire pressure range. Both the electron-phonon coupling constant λ_t and the non-electron-phonon coupling constant μ_t showed effect on the critical temperature of MgB_2, increasing the electron-phonon coupling constant and the non-electron-phonon coupling constant will increase the T_c. The effect of pressure on the critical temperature of MgB_2 can be explained within the two-band BCS model taking into account the electron-phonon and non-electron-phonon attractive interaction with the weak-coupling limit.

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