Superconductivity in two-band systems with variable charge carrier density. The case of $MgB_2$.

M.E. Palistrant and V.A. Ursu

Institute of Applied Physics of Moldavian Academy of Science
MD 2028, Chisinau, Moldova.

The theory of thermodynamic properties of two-band superconductor with reduced density charge carriers is developed on the base of phonon superconducting mechanism with strong electron-phonon interaction.

This theory is adapted to describe the behavior of critical temperature $T_c$, energy gaps $\Delta_1$, $\Delta_2$, and the relative jump of electron specific heat $(C_S - C_N)/C_N$ in the point $T = T_c$ along with the variation of charge carrier density in the compound $MgB_2$ when substitutional impurities with different valence are introduced into the system. It is shown, that according to the filling mechanism of energy bands which overlap on Fermi surface, the quantities $T_c$, $\Delta_1$, $\Delta_2$ decrease when this compound is doped with electrons and remain constant or weakly change when the system is doped with holes. The theory qualitatively agrees with the experimental data.

Also is shown that the consideration of inter- and intraband scattering of electrons on impurity potential improves this agreement.

1. Introduction

The superconductivity in $MgB_2$ compound with transition temperature $T_c \approx 39K$ was discovered about five years ago [1]. This discovery has generated a big interest and has attracted the attention of many researchers. Such interest is caused by big values of $T_c$, high values of upper critical field $H_{c2}$ and critical current $j_c$ in this compound that put this relatively simply substance along with complex high temperature oxide compounds. As a result of many researches is clear that the superconducting properties of $MgB_2$ is impossible to describe using the BCS - Eliashberg theory. The properties of this substance are characterized by a whole series of the anomalies which cannot be framed into this theory (see, for example, [2], [3]). The anisotropy of the system plays an important role in this case, particularly the overlapping of energy bands on Fermi surface which leads to the appearance of two and more gaps in the energy spectrum. The band structure of the compound $MgB_2$ confirms such overlapping of energy bands [4], [5]. The possibility to describe this compound by applying the two-band theory of superconductivity was expressed by the authors of a number of works (see, for example, [6]). However, the model
of superconductor with the overlapped on the Fermi surface energy bands was proposed long time before the discovery of high-temperature superconductors [7], [8]. The history of the development of the theory of multiband superconductors can be traced, in particular, in the surveys [9] - [12]. The Moskalenko’s model for the two-band system [7] assumes the formation of Cooper pairs in each band and the tunneling of these pairs as a whole from one band into another. This model makes possible to obtain high values of $T_c$, two energy gaps $\Delta_1$ and $\Delta_2$ (in this case the conditions $2\Delta_1/T_c > 3.5$ and $2\Delta_2/T_c < 3.5$ can be satisfied (in the one-band case $2\Delta/T_c = 3.5$)), the low values of the relative jump of electronic specific heat in the point $T = T_c$ (for MgB$_2$ this jump is equal to 0.8, in one-band case - this is an universal value, equal to $= 1.43$), the anomalous temperature dependency of heat capacity in the superconducting phase, the positive curvature of temperature dependency of upper critical field $H_{c2}$ and other properties [9]. The compound MgB$_2$ possesses such properties, and the two-band model [7] describes the qualitative picture of the behavior of diverse physical characteristics of this compound.

Together with the pure MgB$_2$ the influence of chemical substitution of the atoms of boron and magnesium by other elements (for example, C, Li, Cu etc.) on thermodynamic properties of MgB$_2$ is of interest and is sufficiently intensively investigated [13], [14]. The thermodynamic properties of two-band superconductor with the lowered (variable) charge carrier density in the assumption of weak interaction in the case of non-phonon superconducting mechanism are investigated in the work [15]. A more general case, when all possible electron couplings (intra- and inter-band) are considered in the work [16], and also in the review [12].

At the present many works are published where the properties of the compound MgB$_2$ are investigated on the basis of the Eliashberg equation considering the presence of two energy gaps. Thus, this compound is examined from the point of view of strong electron-phonon interaction (see, for example, the works [17], [18] and references in them).

The purpose of this work is to develop the theory of thermodynamic properties of superconducting states of the compound MgB$_2$ with variable charge carrier density. The two-band model [15] and electron-phonon mechanism of superconductivity, inherent to this compound, are assumed. In this case the relative alignment of energy bands is considered, and the theory parameters are evaluated considering strong electron-phonon and Coulomb interactions. This approach makes possible to trace the energy bands filling and determine the influence on superconducting state in MgB$_2$ of chemical substitution of magnesium and boron by other elements. At the same time the interband scattering of charge carriers on impurity potential is considered [19].

The work is structured as follows. In the Section 2 on the basis of Frolich’s Hamiltonian the equations for temperature Green functions, diagonal $M(x, x')$ and non-diagonal
Σ(x, x′) mass operators are obtained. The transition to band representation \((n\vec{k}\Omega)\) is performed expanding the Green functions and mass operators on Bloch functions. The system of equations for order parameters \(\Delta_1\) and \(\Delta_2\) with renormalized constants of electron-phonon interaction \(\lambda_{nm}\) (n;m = 1, 2) considering the dependency of mass operator \(M_n(\vec{k}, \Omega)\) from these constants is obtained. This system of equations is completed with an expression, determining the chemical potential \(\mu\). In the Section 3 the limiting cases \(T \sim T_c\) and \(T = 0\) are examined. The basic equations of superconducting theory are defined in each of these temperature ranges. The analytical expressions for the critical temperature \(T_c\), energy gaps \(\Delta_1\) and \(\Delta_2\) are obtained for specific range of values of charge carriers (chemical potential \(\mu\)). The expressions for the jump of electronic specific heat \(C_S - C_N\) also are obtained in the point \(T = T_c\). In the Section 4 the theory parameters for \(MgB_2\) compound are evaluated and the dependency of thermodynamic quantities on charge carrier density is built on the basis of energy bands filling mechanism.

In the last section an additional mechanism of impurity influence on superconductivity, namely interband scattering of electrons on impurity potential, also is considered [19]. The dependency of \(T_c\) value from the concentration of the introduced substitutional impurity \(C, Li\) and \(Cu\) is studied. The obtained results are compared with experimental data.

2. The Hamiltonian of the system and the main equation

The Hamiltonian of the system has the form:

\[
H = H_0 + H_1
\]

(1)

where \(H_0\) is the Hamiltonian of non-interacting electrons and phonons, and \(H_1\) - the Hamiltonian of electron-phonon interaction, determined by the expression

\[
H_1 = g \sum \int d\vec{x}\psi_{\sigma}(\vec{x})\psi_{\sigma}(\vec{x})\varphi(\vec{x}).
\]

(2)

Here \(g\) - the electron - phonon interaction constant, \(\psi_{\sigma}(\vec{x})\) and \(\psi_{\sigma}(\vec{x})\) - the operators of appearance and annihilation of electrons with the spin \(\sigma\) in the point \(\vec{x}\), \(\varphi(\vec{x})\) - phonon operator.

Having using the diagrammatic method of the perturbation theory [20] for normal \(G(xx')\) and abnormal \(F(xx')\) temperature Green functions, we obtain the system of equations

\[
G(x, x') = G^0(x, x') + \int \int dx_1dx_2G^0(x, x_1)M(x_1, x_2)G(x_2, x').
\]
\[- \int \int dx_1 dx_2 G^0(x, x_1) \Sigma(x_1, x_2) \tilde{F}(x_2, x'), \tag{3}\]

\[\tilde{F}(xx') = \int dx_1 dx_2 G^0(x_1, x) \tilde{\Sigma}(x_1, x_2) G(x_2, x') + \]

\[+ \int dx_1 dx_2 G^0(x_1, x) M(x_2, x_1) \tilde{F}(x_2, x'), \tag{4}\]

where the sign \(\sim\) indicates the complex conjugation of the corresponding value, \(G^0(x, x_1)\) - the electronic Green function for free electrons.

The diagonal \(M(x_1, x_2)\) and non-diagonal \(\Sigma(x_1, x_2)\) mass operators take the form

\[M(x_1, x_2) = -g^2 D(x_1, x_2) G(x_1, x_2), \tag{5}\]

\[\Sigma(x_1, x_2) = -g^2 D(x_1, x_2) F(x_1, x_2). \tag{6}\]

Here \(D(x_1, x_2)\) - phonon propagator.

Let’s pass in the expressions (3) - (6) to the \(n\vec{k}\Omega\) representation, expanding the quantities from these formulas on Bloch functions [21]. Then, the system of equations for Green functions \(G_{nm}(\vec{k}, \vec{k}', \Omega)\) and \(F_{nm}(\vec{k}, \vec{k}', \Omega)\), and the expression for mass operators \(M_{mm'}(\vec{p}, \vec{p}', \Omega)\) and \(\Sigma_{mm'}(\vec{p}, \vec{p}', \Omega)\) is not difficult to obtain. Such approach makes possible to investigate the thermodynamic properties of two-band systems taking into account all possible intra- and inter-band electrons couplings. The limit of weak electron-phonon interaction in these systems was examined in the works [12], [16].

Here we will examine a much simpler case, considering only the approximation of Green’s functions diagonal on bands indices. This case leads to the two-band model, proposed in the works [7], [8]:

\[G_{n_1n_2}(\vec{k}_1, \vec{k}_2, \Omega) = G_{n_1}(\vec{k}_1, \Omega_1) \delta_{n_1n_2} \delta_{\vec{k}_1, \vec{k}_2}, \]

\[F_{n_1n_2}(\vec{k}_1, \vec{k}_2, \Omega) = F_{n_1}(\vec{k}_1, \Omega_1) \delta_{n_1n_2} \delta_{\vec{k}_1, -\vec{k}_2}, \]

\[M_{mm'}(\vec{p}, \vec{p}', \Omega) = M_{m}(\vec{p}, \Omega) \delta_{\vec{p}, \vec{p}'} \delta_{mm'}, \]

\[\Sigma_{mm'}(\vec{p}, \vec{p}', \Omega) = \Sigma_{m}(\vec{p}, \Omega) \delta_{\vec{p}, -\vec{p}'} \delta_{mm'}. \tag{7}\]

In this approximation the solutions of the system of equations (3) and (4) for Green functions have the form

\[G_n(\vec{k}, \Omega) = -\frac{i Z_n(\Omega) \Omega + \tilde{\varepsilon}_n}{A_n(\vec{k}, \Omega)}, \tag{8}\]

\[F_n(\vec{k}, \Omega) = \frac{\Sigma_n(\vec{k}, \Omega)}{A_n(\vec{k}, \Omega)}, \quad \tilde{F}_n(\vec{k}, \Omega) = \frac{\tilde{\Sigma}_n(\vec{k}, \Omega)}{A_n(\vec{k}, \Omega)}, \tag{9}\]

\[4\]
where

\[
A_n(\vec{k}, \Omega) = \Omega^2 Z_n^2(\Omega) + \tilde{\varepsilon}_n^2(\vec{k}) + \Sigma_n(\vec{k}, \Omega) \tilde{\Sigma}_n(\vec{k}, \Omega),
\]

\[
Z_n(\Omega) = 1 - \frac{1}{\Omega} \text{Im} M_n(\vec{k}, \Omega), \quad \tilde{\varepsilon}_n(\vec{k}) = \varepsilon_n(\vec{k}) + \text{Re} M_n(\vec{k}, \Omega).
\] (10)

The expressions for mass operators \(M_n(\vec{p}, \Omega)\) and \(\Sigma_n(\vec{p}, \Omega)\) can be written in the form:

\[
M_n(\vec{p}, \Omega) = -\frac{1}{\beta} \sum_{\vec{k}_1} \sum_{\Omega_1} \sum_{n_1} g^2_{mn}(\vec{p}, \vec{k}_1) D(\vec{p} - \vec{k}_1, \Omega - \Omega_1) G_{n_1}(\vec{k}_1, \Omega_1),
\] (11)

\[
\Sigma_n(\vec{p}, \Omega) = -\frac{1}{\beta} \sum_{\vec{k}_1} \sum_{\Omega_1} \sum_{n_1} g^2_{nn}(\vec{p}, \vec{k}_1) D(\vec{p} - \vec{k}_1, \Omega - \Omega_1) F_{n_1}(\vec{k}_1, \Omega_1),
\] (12)

where

\[
g^2_{mn}(\vec{p}, \vec{p}') = g^2 |\chi(m\vec{p}, n\vec{p}')|^2,
\]

\[
\chi(m\vec{p}, n\vec{p}') = \int_{V_0} d\vec{r} U^*_m(\vec{p}) U^n(\vec{r}),
\] (13)

\(U_{mp}(\vec{r})\) - the amplitude of Bloch function, \(\Omega\) - Matsubara frequency for the electrons, \(V_0\) - the volume of unit cell.

Let’s introduce the definition \(\Sigma_n(\Omega) = Z_n(\Omega) \Delta_n(\Omega)\) and simplify the equations (11) and (12) disregarding the delay effects. After that let’s integrate over \(\Omega_1\) and then let’s pass to the integration over energy according to the dispersion law of electrons energy from \(n\) - th band:

\[
\varepsilon_n(\vec{k}) = \zeta_n + \frac{k^2}{2m_n} - \mu.
\] (14)

Then, on the basis of relations (9)-(12) we obtain the system of equations

\[
\Delta_1 = \bar{\lambda}_{11} \int_{-d_1}^{d_1} d\varepsilon_1 \frac{th\beta E_1/2}{2E_1} \Delta_1 + \bar{\lambda}_{12} \int_{-d_2}^{d_2} d\varepsilon_2 \frac{th\beta E_2/2}{2E_2} \Delta_2,
\]

\[
\Delta_2 = \bar{\lambda}_{21} \int_{-d_1}^{d_1} d\varepsilon_1 \frac{th\beta E_1/2}{2E_1} \Delta_1 + \bar{\lambda}_{22} \int_{-d_2}^{d_2} d\varepsilon_2 \frac{th\beta E_2/2}{2E_2} \Delta_2,
\] (15)

where

\[
\lambda_{nm} = g^2_{nm} N_m, \quad E_n = \sqrt{(\varepsilon_n - \mu)^2 + \Delta_n^2}, \quad \bar{\varepsilon}_n = \frac{\varepsilon_n}{Z_n}, \quad \bar{\lambda}_{nm} = \frac{\lambda_{nm}}{Z_n},
\]
\[ d_n = \mu - \zeta_n, \quad d_{cn} = \zeta_{cn} - \mu, \quad (n; m = 1, 2), \quad (16) \]

\(N_m\) - the density of electron states on \(m\) - th cavity of Fermi surface, \(\zeta_{cn}\) - the cut-off energy in the \(n\)-th band. According to the definition (10) and the dispersion law (14), for the quantities \(Z_n\) we obtain:

\[ Z_1 = 1 + \lambda_{11} + \lambda_{12}, \quad Z_2 = 1 + \lambda_{22} + \lambda_{21}. \quad (17) \]

Since we examine a system with the variable (including low) charge carrier density, let’s supplement the system of equations (15) with a relation, determining the chemical potential \(\mu\) (charge carrier density \(\tilde{n}\)):

\[ \tilde{n} = \sum_m N_m \int_{-d_m}^{d_m} d\varepsilon_m \left[ \frac{E_m(k) - |\varepsilon_m(k) - \mu|}{E_m(k)} + \frac{2|\varepsilon_m(k) - \mu|}{1 + \exp \beta E_m(k)} \right]. \quad (18) \]

When we have low values of charge carrier density \(\tilde{n} \sim \Delta_n\) is necessary to correlate the solution of system (15) with the expression (18).

Let’s examine the phonon mechanism of superconductivity, which is inherent to \(MgB_2\).

The cut-off of integrals in the integration over energy in each band are carried out on the characteristic phonon frequency \((\mu_n = \mu - \zeta_n)\):

\[ d_n = \begin{cases} \omega_{0n} & (\mu_n \geq \omega_{0n}) \\ \mu_n & (\mu_n < \omega_{0n}) \end{cases}; \quad d_{cn} = \begin{cases} \omega_{0n} & (\zeta_{cn} - \mu \geq \omega_{0n}) \\ \zeta_{cn} - \mu & (\zeta_{cn} - \mu < \omega_{0n}) \end{cases}. \quad (19) \]

**3. The limiting cases** \(T \sim T_c\) and \(T = 0\)

Let’s study the system of equations (15) at \(T \sim T_c\). For this purpose we expand the parameters \(\Delta_n\) in terms of the difference \((\beta - \beta_c)\), where \(\beta = 1/T\):

\[ \Delta_n = c_n (\beta - \beta_c)^{1/2} + c_n^{(1)} (\beta - \beta_c)^{3/2} + ... \quad (20) \]

Introducing this expansion into equation (15) and equalizing the expressions with the same degrees of the difference \((\beta - \beta_c)\), we obtain a system of equations which determines the coefficients \(c_n\) and \(c_n^{(1)}\) (\(n = 1, 2\)):

\[ c_1 = -\bar{\lambda}_{11} I_1(\mu) c_1 - \bar{\lambda}_{12} I_2(\mu) c_2, \quad c_2 = -\bar{\lambda}_{21} I_1(\mu) c_1 - \bar{\lambda}_{22} I_2(\mu) c_2 \quad (21) \]

\[ c_1^{(1)} = \frac{\bar{\lambda}_{11}}{\beta_c} \left[ \theta_1(\mu) - \beta_c^3 F_1(\mu) c_1^2 \right] c_1 - \bar{\lambda}_{11} I_1(\mu) c_1^{(1)} + \frac{\bar{\lambda}_{12}}{\beta_c} \left[ \theta_2(\mu) - \beta_c^3 F_2(\mu) c_2^3 \right] c_2 - \bar{\lambda}_{12} I_2(\mu) c_2^{(1)}, \quad (1) \]
\[ c_2^{(1)} = \frac{\bar{\lambda}_{21}}{\beta_c} \left[ \theta_1(\mu) - \beta_c^3 F_1(\mu) c_1^2 \right] c_1 + \frac{\bar{\lambda}_n}{\beta_c} \left[ \theta_2(\mu) - \beta_c^3 F(\mu) c_2^2 \right] c_2 - \bar{\lambda}_{22} I_2(\mu) c_2^{(1)}. \]  

(22)

where

\[
I_n(\mu) = - \int_{-\bar{d}_n}^{\bar{d}_n} \frac{\beta_c \varepsilon / 2}{2\varepsilon} d \varepsilon, \quad F_n = \frac{1}{8} \int_{-\bar{d}_n \beta_c}^{\bar{d}_n \beta_c} dx \frac{\sinh x - x}{x^3 \cosh^2 x / 2},
\]

\[
\theta_n(\mu) = \frac{1}{2} \left[ th \frac{\beta_c d_n}{2} + th \frac{\beta_c d_n}{2} \right], \quad \bar{d}_n = \frac{d_n}{Z_n}, \quad \bar{d}_n = \frac{d_n}{Z_n}.
\]

(23)

Equalizing to zero the determinant \( D \) of the system (21), we obtain an equation for superconducting transition temperature \( T_c \), and on the basis of (18) - an expression, which ties \( \bar{n} \) and \( \mu \):

\[
1 + \bar{\lambda}_{11} I_1(\mu) + \bar{\lambda}_{22} I_2(\mu) + \bar{a} I_1(\mu) I_2(\mu) = 0,
\]

\[
\bar{n} = \sum_n N_n \left[ \bar{\zeta}_n - \bar{\zeta}_n - |\bar{\zeta}_n - \bar{\mu}| + |\bar{\zeta}_n - \bar{\mu}| \right],
\]

(24)

where

\[
\bar{a} = \bar{\lambda}_{11} \bar{\lambda}_{22} - \bar{\lambda}_{12} \bar{\lambda}_{21}.
\]

(25)

On the basis of the system of equations (21) is not difficult to determine the ratio of the parameters \( z_c = \Delta_1 / \Delta_2 \) at \( T = T_c \):

\[
z_c = \frac{c_1}{c_2} = \frac{\bar{\lambda}_{12} I_2(\mu)}{1 + \bar{\lambda}_{11} I_1(\mu)} = - \frac{1 + \bar{\lambda}_{22} I_2(\mu)}{\bar{\lambda}_{21} I_1(\mu)}
\]

(26)

The quantity \( z_c \) implicitly depends on charge carrier density (chemical potential) through the dependency of quantity \( T_c \) on this parameter, and also explicitly - due to the integration limits in formulas (23).

The solutions of the system of equations (22) can be represented in the form: \( c_1^{(1)} = D_1 / D \), \( c_2^{(1)} = D_2 / D \) where \( D \), \( D_1 \) and \( D_2 \) are the respective determinants of this system. The condition \( D = 0 \) corresponds to the solvability of the system of equations (21) for the superconducting transition temperature. Consequently, it is necessary to put the condition \( D_1 = D_2 = 0 \). From this condition the following relation results:

\[
c_1^2 = \frac{1}{\beta_c^3} \left( \frac{N_1 \theta_1(\mu) + N_2 \theta_2(\mu)}{N_1 F_1(\mu) + N_2 F_2(\mu)} \right) / z_c^2.
\]

(27)
For certainty let’s assume $\zeta_1 < \zeta_2 < \zeta_{c_1} < \zeta_{c_2}$. As it follows from the dispersion law of electrons energy (14), these parameters determine the mutual arrangement of energy bands.

In the range of values $\bar{d}_n/T_c$ and $\bar{d}_{cn}/T_c \gg 1$ the equation (23) allows to obtain analytical expression for superconducting transition temperature $T_c$. Considering $\omega_{01} = \omega_{02} = \omega_0$ and cutting off the integrals according to (19), on the base of (24) we obtain

$$T_c = \frac{2\omega_0\gamma}{\pi} e^{-\xi},$$

(28)

where

$$\xi = \bar{\lambda}_{11} + \bar{\lambda}_{22} - \bar{a}\varphi \pm \sqrt{(\bar{\lambda}_{11} + \bar{\lambda}_{22} - \bar{a}\varphi)^2 - 4\psi}. \quad (29)$$

Here the quantities $\varphi$ and $\psi$ are determined by chemical potential $\mu$:

1. At $\bar{\mu} - \bar{\zeta}_2 < \omega_0$ and $\bar{\zeta}_{c_1} - \bar{\mu} > \omega_0$

$$\varphi = \frac{1}{2} \ln \frac{\bar{\mu} - \bar{\zeta}_2}{\omega_0}, \quad \psi = 1 - \frac{1}{2} \ln \frac{\bar{\mu} - \bar{\zeta}_2}{\omega_0}; \quad (30)$$

2. $\bar{\mu} - \bar{\zeta}_2 > \omega_0$ and $\bar{\zeta}_{c_1} - \bar{\mu} > \omega_0$

$$\varphi = 0, \quad \psi = 1; \quad (31)$$

3. $\bar{\mu} - \bar{\zeta}_2 > \omega_0$ and $\bar{\zeta}_{c_1} - \bar{\mu} < \omega_0$

$$\varphi = \frac{1}{2} \ln \frac{\bar{\zeta}_{c_1} - \bar{\mu}}{\omega_0}, \quad \psi = 1 - \frac{1}{2} \ln \frac{\bar{\zeta}_{c_1} - \bar{\mu}}{\omega_0}, \quad \bar{\mu} = \frac{\mu}{Z_1}, \quad \bar{\mu}' = \bar{\mu}Z_1/Z_2. \quad (32)$$

In the points $\mu = \zeta_2$ and $\mu = \zeta_{c_1}$ we have respectively,

$$\xi = \frac{2\lambda_{11} + \bar{\lambda}_{22} \pm \sqrt{(2\lambda_{11} - \bar{\lambda}_{22})^2 + 8\lambda_{12}\bar{\lambda}_{21}}}{2\bar{a}}, \quad (33)$$

$$\xi = \frac{\bar{\lambda}_{11} + 2\bar{\lambda}_{22} \pm \sqrt{(\bar{\lambda}_{11} - 2\bar{\lambda}_{22})^2 + 8\lambda_{12}\bar{\lambda}_{21}}}{2\bar{a}} \quad (34)$$

At $\zeta_1 < \mu < \zeta_2$ and $\zeta_{c_1} < \mu < \zeta_{c_2}$ the value of $T_c$ is determined by electron - phonon interaction in the first and second bands, respectively. In this case the dependency from $\mu$ takes place at $\bar{\mu} - \bar{\zeta}_1 < \omega_0$ and $\bar{\zeta}_{c_2} - \bar{\mu}' < \omega_0$:

$$T_c = \frac{2\gamma}{\pi} \sqrt{(\bar{\mu} - \bar{\zeta}_1)\omega_0} e^{-1/\lambda_{11}}, \quad T_c = \frac{2\gamma}{\pi} \sqrt{(\bar{\zeta}_{c_2} - \bar{\mu}')\omega_0} e^{-1/\lambda_{22}}. \quad (35)$$
Hereinafter $\lambda_{11}^0 = \lambda_{11}$ at $N_2 = 0$, and $\lambda_{22}^0 = \lambda_{22}$ at $N_1 = 0$.

For the jump of specific heat in the point $T = T_c$ we have [15]

$$\frac{C_S - C_N}{V} = \beta_c^5 \sum_n N_n F_n(\mu) c_n^4. \quad (36)$$

Using the relations (27) and (28) we bring the jump of specific heat to the form:

$$\frac{C_S - C_N}{V} = T_c \frac{[N_1 \Theta_1(\mu) + N_2 \Theta_2(\mu)/z_c^2]^2}{N_1 F_1(\mu) + N_2 F_2(\mu)/z_c^4} \quad (37)$$

In this case the relative jump of specific heat takes the form:

$$\frac{C_S - C_N}{C_N} = \frac{[N_1 \Theta_1(\mu) + N_2 \Theta_2(\mu)/z_c^2]^2}{4[N_1 F_1(\mu) + N_2 F_2(\mu)/z_c^4][N_1 \varphi_1(\mu) + N_2 \varphi_2(\mu)]} \quad (38)$$

where

$$\varphi_n(\mu) = \int_{-\mu - \zeta_n}^{\infty} \frac{x^2 dx}{(1 + e^x)(1 + e^{-x})}. \quad (39)$$

At $T = 0$ on the basis of given above expressions (15) and (18) is not difficult to obtain the system of equations, which determine the order parameters $\Delta_m(0) = \Delta_m$ and chemical potential $\mu(0) = \mu$. This system takes the form

$$\Delta_m = \frac{1}{2} \sum_n \tilde{\lambda}_{mn} \Delta_m \tilde{n} \left[ \tilde{d}_{cn} + \sqrt{\tilde{d}_{cn}^2 + \Delta_n^2} \right] - \tilde{d}_n + \sqrt{\tilde{d}_n^2 + \Delta_n^2} \quad (40)$$

$$\tilde{n} = \sum_n N_n \left[ \tilde{\zeta}_{cn} - \tilde{\zeta}_n - \sqrt{(\tilde{\zeta}_{cn} - \tilde{\mu})^2 + \Delta_n^2} + \sqrt{(\tilde{\zeta}_n - \tilde{\mu})^2 + \Delta_n^2} \right]. \quad (41)$$

In the analytical studies we will examine the specific ranges of values of chemical potential, when the following inequalities are fulfilled: $\Delta_n/\tilde{d}_{cn}, \Delta_n/\tilde{d}_n \ll 1$. We use the definition of quantities $\tilde{d}_n$ and $\tilde{d}_{cn}$ in accordance with cutting of integrals over energy at electron-phonon interaction (19). On the basis of the system of equations (40) in the interval where energy bands overlap ($\zeta_2 < \mu < \zeta_{c1}$) is easy to get:

$$\Delta_1 = 2 D_0 e^{-\xi_0}, \quad \xi_0 = \frac{\lambda_{22} - \lambda_{12}/z}{\tilde{a}}, \quad z = \frac{\Delta_1}{\Delta_2}. \quad (42)$$
Here $D_0$ and $z$ are determined by the value of chemical potential $\mu$. In the interval $\zeta_2 < \mu < \zeta_{c1}$ we obtain the following relations: 1) $\bar{\mu}' - \bar{\zeta}_2 < \omega_0 \quad \bar{\zeta}_{c1} - \bar{\mu} > \omega_0, \quad D_0 = \omega_0$,

$$a \ln z = \bar{\lambda}_{11} - \bar{\lambda}_{22} - \bar{\lambda}_{21} z + \frac{\bar{\lambda}_{12}}{z} - a \frac{1}{2} \ln \left( \frac{\bar{\mu}' - \bar{\zeta}_2}{\omega_0} \right);$$  

(43)

2) $\bar{\mu}' - \bar{\zeta}_2 > \omega_0, \quad \bar{\zeta}_{c1} - \bar{\mu} > \omega_0, \quad D_0 = \omega_0$,

$$a \ln z = \bar{\lambda}_{11} - \bar{\lambda}_{22} - \bar{\lambda}_{21} z;$$  

(44)

3) $\bar{\mu}' - \bar{\zeta}_2 > \omega_0, \quad \bar{\zeta}_{c1} - \bar{\mu} < \omega_0, \quad D_0 = \sqrt{\omega_0 (\bar{\zeta}_{c1} - \bar{\mu})}$

$$a \ln z = \bar{\lambda}_{11} - \bar{\lambda}_{22} + \frac{\bar{\lambda}_{12}}{z} - \bar{\lambda}_{21} z - a \frac{1}{2} \ln \frac{\omega_0}{\bar{\zeta}_{c1} - \bar{\mu}}.$$  

(45)

In the interval where the overlapping of energy bands is absent $\mu < \zeta_2$ and $\mu > \zeta_{c1}$ one energy gap is present $\Delta_1$ and $\Delta_2$, respectively. In this case for low ($\bar{\mu}' - \bar{\zeta}_1 < \omega_0$) and high ($\bar{\zeta}_2 - \bar{\mu}') < \omega_0$ values of chemical potential we have

$$\Delta_1 = 2 \sqrt{\omega_0 (\bar{\mu} - \bar{\zeta}_1)} e^{-1/\bar{\lambda}_{11}}, \quad \Delta_2 = 2 \sqrt{\omega_0 (\bar{\zeta}_2 - \bar{\mu}')} e^{-1/\bar{\lambda}_{22}}.$$  

(46)

The formulae (46) show that the parameter $\Delta_1$ increases together with the chemical potential $\mu$ at the beginning of filling area of first energy band, and the parameter $\Delta_2$ diminishes in the end of second energy band filling area. In the energy bands overlapping area $\zeta_2 < \mu < \zeta_{c1}$ the picture is more complex and can be obtained as a result of numerical evaluation of given above expressions. In the case of low values of parameters $\bar{d}_n(\bar{d}_n \sim \Delta_n)$ is necessary to obtain numerically a self-consistent solution for the system of equations (40) and (41). Let’s note, that on the basis of these equations the analytical expressions for $\Delta_n$ and $\mu$ were obtained in the work [22] for the state of the deep Bose-condensation of local pairs ($\mu_n < 0, (\Delta_n/\mu_n)^2 \ll 1$).

4. Application of the model to the study of doped MgB2 superconducting properties

The obtained above equations for $T_c$ (24), (28) and for $\Delta_n$ (40) contain variable charge carrier density $\bar{n}$ (chemical potential $\mu$) and, consequently, can describe the behavior
of the corresponding values of two-band superconductor when its atoms are chemically substituted by other elements.

In particular, the compounds $MgB_{2-x}C_{x}$, $Mg_{1-x}Cu_{x}B_{2}$ and other [13], [14] are of great interest. Numerous theoretical and experimental studies prove, that the anomalies of the observed physical quantities in the superconductive compound $MgB_{2}$ can be understood basing on energy bands overlapping on the Fermi surface and the presence of two energy gaps (see for example, [3] - [6]). Diverse approaches in scientific literature there are to study the compound $MgB_{2}$. These approaches lead to ambiguous values of theory parameters.

According to the contemporary researches [2] - [6], [18], [23], the compound $MgB_{2}$ is a two-band superconductor with strong electron-phonon interaction. On the Fermi surface two energy bands overlap: a two-dimensional band $\delta$ and a three-dimensional one $\pi$. Hereinafter we will call the $\sigma$ - band the first band, and the $\pi$ - zone - the second band. In accordance with this let’s designate the electron-phonon interaction constants $\lambda_{11}$ and $\lambda_{22}$ intraband, $\lambda_{12}$ and $\lambda_{21}$ - as interband ones.

The table 1 gives the values of these parameters, and also the Coulomb interaction parameters $\mu^*$, obtained by the authors of works [18], [23] (a), [24](b) and [6] (c) on the basis of Eliashberg equations. As it can be seen from this table, the values of the quantities $\lambda_{nm}$ and renormalized quantities $\bar{\lambda}_{nm}$ aren’t single-valued ones. A common thing for them is the relation $\bar{\lambda}_{11} > \bar{\lambda}_{22}, \bar{\lambda}_{12}, \bar{\lambda}_{21}$ which tells about the significant role of two-dimensional $\sigma$ band in Cooper pair’s formation process in $MgB_{2}$.

Solving the Eliashberg equations for the pure $MgB_{2}$ on the basis of these parameters is possible to obtain values for superconducting transition temperature $T_c$, close to 40 K [18].

Here we put the problem to investigate the influence of substitutional impurity on thermodynamic properties of two-band superconductor. Since the impurity introduction cannot change the picture of phonon spectrum so, so that this change would radically affect superconductivity, to solve this problem we will use the given above renormalized equations of the two-band theory (24) and (40), in which the renormalized constants of electron-phonon interaction are determined by the relations:

$$\bar{\lambda}_{11} = \frac{\lambda_{11} - \mu_{11}^*}{1 + \lambda_{11} + \lambda_{12}}, \quad \bar{\lambda}_{22} = \frac{\lambda_{22} - \mu_{22}^*}{1 + \lambda_{22} + \lambda_{21}}, \quad \bar{\lambda}_{12} = \frac{\lambda_{12} - \mu_{12}^*}{1 + \lambda_{11} + \lambda_{12}},$$

$$\bar{\lambda}_{21} = \frac{\lambda_{21} - \mu_{21}^*}{1 + \lambda_{22} + \lambda_{21}},$$

where $\mu_{nm}^*$ is the parameter describing the Coulomb interaction of electrons.
The quantities $\lambda_{nm}$ we determine from the condition that the values of $T_c$ and $\Delta_1$, $\Delta_2$ would correspond to experimental data.

We select the values $T_c = 39.4K$, $\Delta_1 = 7.1meV$, $\Delta_2 = 2.7meV$, $z = \frac{\Delta_1}{\Delta_2} = 2.63$, $N_1/N_2 = 0.73$ and $\omega_0 = 75meV$, which were obtained in the work [23]. The obtained in such a way the effective constants of electron-electron interaction are given in the table 1 (case d). We use these values of $\bar{\lambda}_{nm}$ to calculate basing on (31) the ratio $z_c = \Delta_1/\Delta_2$ and the relative jump of electronic specific heat $(C_S - C_N)/C_N$ at $T = T_c$. We obtain: $z_c = 3.2; (C_S - C_N)/C_N = 0.79$. This, $z < z_c$, and the jump of specific heat is small in comparison with the one-band superconductors (1.43) and is close to the experimental values [2].

|   | $\lambda_{11}$ | $\lambda_{22}$ | $\lambda_{12}$ | $\lambda_{21}$ | $\mu_{11}^*$ | $\mu_{22}^*$ | $\mu_{12}^*$ | $\mu_{21}^*$ | $\bar{\lambda}_{11}$ | $\bar{\lambda}_{22}$ | $\bar{\lambda}_{12}$ | $\bar{\lambda}_{21}$ |
|---|----------------|----------------|----------------|----------------|--------------|--------------|--------------|--------------|----------------|----------------|----------------|--------------|
| a | 1.017          | 0.448          | 0.213          | 0.155          | 0.21         | 0.172        | 0.095        | 0.069        | 0.362          | 0.172          | 0.054          | 0.053        |
| b | 0.96           | 0.28           | 0.16           | 0.22           |              |              |              |              |                |                |                |              |
| c | 1.5            | 0.4            | 0.5            | 0.1            | 0.1          | 0.1          | 0.1          |              | 0.302          | 0.135          | 0.04           | 0.038        |

The given above theory allows to build the dependency of thermodynamic characteristics on the chemical potential $\mu$ (charge carrier density $\tilde{n}$) in the wide interval of its values.

However, within the study of doped MgB$_2$ is of interest to examine $\mu$ near the value of $\mu_0 \approx 0.74eV$, which corresponds to the case of the pure MgB$_2$.

As it follows from the band calculations [4], $\mu_0$ lies in the range of values, close to the complete filling of energy band $\sigma$. For certainty we select the parameters $\zeta_1 = \zeta_2 = 0$, $\zeta_{c1} = 0.8eV$, $\zeta_{c2} = 1.0eV$. The interval where two bands overlap on the Fermi surface $\zeta_2 < \mu < \zeta_{c1}$ gives the main contribution to superconductivity. It is convenient to represent the dependency of thermodynamic values from the value $\delta = (\mu - \mu_0)/\mu_0 = (\tilde{n} - \tilde{n}_0)/\tilde{n}_0$, which determines the relative change of charge carrier density as a result of substitutional impurity introduction into MgB$_2$. At $\delta > 0$ the density of electrons increases, and at $\delta < 0$ - the density of holes. This approach allows to compare the obtained results with the experimental data (see Fig. 4 in the work [13]), because from these data is possible to determine the relative change of charge density $\delta$. 

Table 1
In Fig. 1 the dependency of $T_c$ from the parameter $\delta$ is given. This dependency was obtained on the basis of developed above theory (curve 1). The same figure shows the points, which correspond to the experimental values of $T_c$ for diverse substitutions of atoms of $Mg$ and $B$, taken from Fig. 4 of the experimental work [13], and also the experimental dependency (curve 2).

From Fig. 1 follows, that the superconducting transition temperature $T_c$ diminishes with the increasing of electron density ($\delta > 0$) and remains constant at the introduction of holes into $MgB_2$ ($\delta < 0$).

The decreasing of quantity $T_c$ with the increasing of $\delta$ is confirmed by experimental data for $MgB_{2-x}Ca$ and $Mg_{0.05}Cu_{0.05}B_{2-x}Ca$. For these compounds the parameter $\delta$ is determined by the relations $\delta = (x - 0.05)/8$, in accordance with the valence of the elements, which belong to the named compounds.

In the case of $Mg_{1-x}Li_xB_2$, $Mg_{1-x}Cu_xB_2$, $Mg_{0.8}Li_{0.2}B_{2-x}Ca$ for the quantities $\delta$ we have respectively $\delta = -x/8$, $-x/8$, $(-0.2 + x)/8$. This theory gives a constant value for critical temperature $T_c = 39.4K$ with the condition of variable and negative $\delta$ which takes place at any values of $x$ in the case of two first compounds and at $x < 0.2$ in the case of the last compound. Figure 1 demonstrates the qualitative agreement between our theory and the experiment. This agreement is based on the idea of two bands and energy bands filling factor. The theoretical curve lies above the experimental points. This difference is related with two factors: firstly, the theory parameters were determined on the basis of the value $T_c = 39.4K$ for the pure $MgB_2$, (in the experimental work [13] $T_c = 39K$); secondly, the interband scattering of electrons on impurity was not considered.

The theoretical dependencies of energy gaps $\Delta_1$ and $\Delta_2$ on $\delta$ parameter in the domain of values which are of interest to compare with experimental data are shown on Fig. 2. The values of these quantities for pure $MgB_2$ correspond to $\Delta_1 = 7.05meV$, $\Delta_2 = 2.68meV$, remain constant when the system is doped with holes, and decrease with the increasing of electrons number in the system. Thus, the behavior of these quantities as a function of parameter is analogous to the behavior of the quantity $T_c$.

On the Fig. 3 the dependencies of the ratios $\Delta_1/K_B T_c$ (curve 1) and $2\Delta_2/K_B T_c$ (curve 2) from relative change of charge density $\delta$ are presented. For pure $MgB_2(\delta = 0)$ we have $2\Delta_1/K_B T_c = 4.18$, $2\Delta_2/K_B T_c = 1.58$. These values remain constant at $\delta < 0$ and decrease at $\delta > 0$.

Fig. 4 The relative jump of electronic specific heat $(C_S - C_N)/C_N$ in the point $T = T_c$ as a function of parameter $\delta$ in $MgB_2$.

The relative jump of electronic specific heat in the point $T = T_c$ as a result of of $MgB_2$ doping is shown in Fig. 4. As it follows from this figure, at $\delta < 0$ the doping leads to a weak increasing of this quantity and to a much stronger increasing at $\delta > 0$. As was
expected, if the value of the jump \((C_S - C_N)/C_N = 1.43\) at \(T = T_c\), that corresponds to the presence of one energy band.

For certainty the dependency of chemical potential \(\mu\) from the parameter \(\delta\) in \(MgB_2\) is built on the basis of the second equation from (24) and is shown on the Fig. 5. This relation made possible to pass from the dependency of the given above thermodynamic quantities from chemical potential \(\mu\) to charge carrier density, and also to the relative value \(\delta = (\tilde{n} - \tilde{n}_0)/\tilde{n}_0\) Such transition allows comparing our two-band theory with experimental data concerning the substitution of \(Mg\) and \(B\) by other elements of the Mendeleev’s periodic table.

5. The scattering of electrons on impurity potential.

In the previous sections, on the basis of phonon mechanism, the theory of superconductivity in two-band systems with reduced charge carrier density and nonmagnetic impurity was built. In this case the impurity influence is determined by the change of chemical potential \(\mu\) (charge carrier density), which leads to the manifestation of the energy bands filling effect. The agreement with the experiment can be improved, if we will consider the processes of intra- and inter-band scattering of electrons on impurity potential. These processes affect not only the value of chemical potential \(\mu\), but also the thermodynamic characteristics of two-band system [9], [19], [21].

Further we will base on the results of the study [25] where the problem of the influence of nonmagnetic impurity on the superconducting transition in two-band systems with reduced charge carrier density is solved. With the precision of terms linear on impurity concentration we have:

\[
n_0 + \nu n_i = \sum_m N_m [\zeta_{cm} + x_m - \mu - (\zeta_m + x_m - \mu) - \left| \zeta_{cm} + x_m - \mu \right| + \left| \zeta_m + x_m - \mu \right| + \frac{2}{\pi} y_m \ln \frac{\left| \zeta_{cm} - \mu \right|}{\left| \mu - \zeta_m \right|}],
\]

(48)

where \(n_0\) is the charge carrier density of pure substance, \(\nu\) - the difference between the valence of introduced atoms and atoms of the main substance. The quantities \(x_m\) and \(y_m\) are determined with the precision of terms linear on impurity concentration by the following relations:

\[
x_m = -\frac{1}{2\pi} \sum_n \frac{1}{\tau_{mn}} \ln \left| \frac{\zeta_{cm} - \mu}{\mu - \zeta_m} \right|, \quad y_m = \sum_n \frac{1}{2\tau_{mn}}.
\]

(49)
As it follows from the expression (48) the chemical potential $\mu$ depends explicitly on impurity concentration and through the parameters of $\tau_{mn}$ which are determined by the relations $(m, n = 1, 2)$:

$$\frac{1}{2\tau_{mn}} = \tilde{n}_i \eta_{mn}$$  (50)

where $\tilde{n}_i = n_i/2N_1$, and $\eta_{mn}$ is determined by the inter- $(n \neq m)$ and intraband $(n = m)$ potentials of electrons scattering on impurity [25] which depend on Bloch functions and of unit cell volume.

For superconducting transition temperature we obtain

$$T_c = \bar{T}_{c0} - \alpha^{\pm} \frac{\pi}{8\pi_1} \left(1 + \frac{N_2}{N_1}\right)$$  (51)

where $T_{c0}$ is determined by the formulas (28) and (29) taken in the respective value intervals of chemical potential $\mu$ (intervals 2 and 3) related with $n_i$ through the relation (48), and $\alpha$ is determined by the expression [9], [19],[25]:

$$\alpha^{\pm} = \frac{1}{2} \left\{ 1 \pm \left[ \frac{N_1 - N_2}{N_1 + N_2} (\bar{\lambda}_{11} - \bar{\lambda}_{22}) + 2 \frac{N_1}{N_1 + N_2} \bar{\lambda}_{12} + 2 \frac{N_2}{N_1 + N_2} \bar{\lambda}_{21} \right] \times \left[ (\lambda_{11} - \lambda_{22})^2 - 4\lambda_{12}\lambda_{21} \right]^{-1/2} \right\}.$$  (52)

Here $\alpha^{\pm} < 1$ (the sign + or − is selected considering the maximal value of $T_c$, which ensures a steadier superconducting state in comparison with the normal one). The expression (51) is correct under the condition $(2\tau_{mn}\pi T_c)^{-1} \ll 1$, which takes place at low values of impurity concentration $n_i$ or at parameters $\eta_{nm}$.

In Fig. 6 the dependencies of critical temperature $T_c$ on the relative charge carrier density $\delta$ obtained on the basis of expressions (51) are shown. Curve 1 in this figure corresponds to the absence of electron scattering on impurity ($\eta_{nm} = 0, n; m = 1, 2$) and coincides with curve 1 in Fig. 1. Curve 2 corresponds to the values of $\eta_{11} = 0.65, \eta_{21} = 0.09$. The dashed curve is an experimental dependency [13]. As it follows from this figure, the assumption of filling mechanisms for two energy bands and the electron scattering on impurity potential leads to a good agreement between theory and experiment in the case of systems doped with electrons (compounds $Mg_{0.95}Cu_{0.05}B_{2x}C_x$ and $MgB_{2-x}C_x$). Substituting the atoms of $Mg$ by $Li$ and $Cu$ we do not consider the electron scattering on impurity, assuming that in layered compounds of $MgB_2$ the basic contribution to the superconductivity is given by the charges related to boron. The substitution of boron by $C$ atoms leads to the violation of lattice periodicity in this layer and to the appearance
of scattering processes on impurity. However, the substitution of Mg by the atoms of Cu or Li (compound of $Mg_{1-x}Li_xB_2$, $Mg_{1-x}Cu_xB_2$) only changes the effective valence of boron, which is responsible for superconducting state.

This idea is confirmed by the $\delta$ dependency of superconducting transition temperature $T_c$ on $\delta$ in the compounds $Mg_{0.8}Li_{0.2}B_{2-x}Cx$. In Fig. 6 this dependency is characterized by the curve 3, which passes near the experimental points for this compound. The decreasing of $T_c$ along with the decreasing of holes is obliged to charge scattering on impurity due to the substitution of boron by C atoms. The curve 3 in this figure is built on the basis of expression (51), in which the value of $T_c$ equal to 39, 4$K$ is undertaken and the parameters of $\eta_{11} = 0.5; \eta_{21} = 0.06$ are selected. The difference between these parameters and the parameters inherent for $MgB_2-C_x$, possibly, is caused by the difference between the unit cell volumes of these compounds [13].

Let’s note, that during the construction of this theory the influence of doping on electronic state density $N_1$ and $N_2$, and on characteristic phonon frequency $\omega_0$ wasn’t considered. The consideration of this influence probably can change the values of the parameters of $\eta_{nm}$.

6. Conclusions

The theory of thermodynamic properties of two-band superconductors with variable charge carrier density on the basis of phonon mechanism of superconductivity was presented in this work. This theory can describe the behavior of such values like $T_c$, $\Delta_1$, $\Delta_2$, $(C_S - C_N)/C_N$ at $T = T_c$ as functions of charge carrier density in $MgB_2$ when Mg and B are substituted by other elements from Mendeleev’s periodical table.

For this aim is necessary to do the following actions:

1. To proceed from the BCS-type equation for the two-band model [7] with electron-phonon interaction constants, renormalized due to strong electron-phonon interaction and Coulomb interaction of electrons.

2. To examine the interval where two-dimensional $\sigma$ and three dimensional $\pi$ bands overlap on the Fermi surface. To build the dependencies of the above-mentioned quantities from the chemical potential $\mu$, taking into account that the value $\mu = \mu_0 \approx 0.74eV$ in $MgB_2$ is near to the upper edge of $\sigma$ band, which is responsible for superconductivity [4].

3. To introduce the relative charge carrier density $\delta = (\mu - \mu_0)/\mu_0$, which coincides with corresponding value calculated on the basis of the valences of elements, belonging to the compounds $Mg_{1-x}Li_xB_2$, $Mg_{1-x}Cu_xB_2$, $Mg_{0.8}Li_{0.2}B_{2-x}Cx$, $Mg_{0.95}Cu_{0.05}B_{2-x}Cx$ and $MgB_{2-x}Cx$ at different values of $x$. The $\delta$ dependencies of $T_c$ which are built in such a
way allow to compare theoretical and experimental data (see Fig. 1). The theoretical results obtained in this work qualitatively agree with the experiments results [13]:

a) Namely, the introduction into MgB$_2$ of electrons ($\delta > 0$) decreases the critical temperature $T_c$(MgB$_{2-x}$C$_x$ and Mg$_{0.95}$Cu$_{0.05}$B$_{2-x}$C$_x$).

b) The doping with holes ($\delta < 0$) does not change the $T_c$ (Mg$_{1-x}$Li$_x$B$_2$, Mg$_{1-x}$Cu$_x$B$_2$) with the change of $\delta$.

c) The compound Mg$_{0.8}$Li$_{0.2}$B$_{2-x}$C$_x$ [13][13], in which $T_c$ reaches the value of 39.4K when $\delta = -0.02$ (that corresponds to MgB$_2$) and diminishes with hole density decreasing, can’t be framed in this scheme.

5. The obtained results demonstrate also the quantitative agreement of the theory proposed in this work with experimental data for superconducting transition temperature $T_c$ (see Fig. 6).

a) In this case together with energy bands filling factor (or change of chemical potential $\mu$) is necessary to consider the scattering of electron on impurity potential when the C atoms replace in the laminar structure the atoms of B, which is responsible for superconductivity.

Upon consideration of these two mechanisms we obtain a dependency (curve 2), well describing the experimental data (MgB$_{2-x}$C$_x$ and Mg$_{0.95}$Cu$_{0.05}$B$_{2-x}$C$_x$).

b) Doping with holes $\delta < 0$ (Mg$_{1-x}$Li$_x$B$_2$, Mg$_{1-x}$Cu$_x$B$_2$) does not change the value of $T_c$, since into the layer, responsible for superconductivity, impurity is not introduced, and the elements Li and Cu introduced instead of Mg only change the effective valence of B.

c) The decreasing of $T_c$ value (curve 3) in Mg$_{0.8}$Li$_{0.2}$B$_{2-x}$C$_x$ is related with electron scattering on impurity potential of C atoms.

References

[1] J. Nagamatsu, N. Nakagawa, T. Muranaka at al., Nature (London), 410, 63 (2001).

[2] F. Bouquet, I. Wang, I. Sheikin et al., Physica 385, 192 (2003), cond-mat. 0210706

[3] P.C. Confield, S. L. Bud’ko and D. K. Finemore, Physica C 385, 1 (2003).

[4] J. Kortus, I. I. Mazin, K. D. Belashchenko at al., Phys. Rev. Lett. 86, 4656 (2001).

[5] J. M. An and W. E. Pickett, Phys. Rev. Lett. 86, 4366 (2001).
[6] S. V. Shulga, S. L. Drechsler, H. Eschrig, at al., cond-mat/0103154.

[7] V. A. Moskalenko, Fiz. Met. Metalloved. 8, 503 (1959); Phys. Met. and Metallog. 8, 25 (1959).

[8] H. Suhl, B. T. Matthias and L. R. Walker, Phys. Rev. Lett. 3, 552 (1959).

[9] V. A. Moskalenko, M. E. Palistrant, V. M. Vakaliuk, Sov. Phys. Usp., 34, 717 (1991); cond-mat/03099671.

[10] M. E. Palistrant, cond.mat./0305496; Moldavian Journal of the Physical Sciences 3, 133 (2004).

[11] L. Z. Kon, cond.mat./0309707.

[12] M. E. Palistrant, International Journ. of Modern Physics 19, 929 - 970 (2005); cond.mat/0312302.

[13] S. Jemima Balaselvi, A. Bharathi, V. Sankara Sastry at al., cond-mat/0303022 (2003).

[14] Z. Hofanova, P. Szabo, P. Samuely at al., Phys. Rev. B 70, 064520 (2004).

[15] M. E. Palistrant and F. G. Kochorbe, Physica C 194, 351 (1992).

[16] F. G. Kochorbe, M. E. Palistrant, JETP 77, 442 (1993); Theoret. Mathem. Phys. 96, 1083 (1993).

[17] O. V. Dolgov, R. K. Kremer, J. Kortus at al. Phys. Rev. B 72, 024504 (2005).

[18] E. J. Nicol and J. P. Carbotte, Phys. Rev. B, 71, 054501 (2005).

[19] V. A. Moskalenko, M. E. Palistrant, Dokl. Acad. Nauk SSSR, 162, 539 (1965); JETP, 39, 770 (1965) (in Russian).

[20] A. A. Abrikosov, L. P. Gor’kov, I. E. Dzialoshinskii, Quantum Field Theoretical Methods in Statistical Physics, Moscow, Nauka (1962).

[21] V. A. Moskalenko, L. Z. Kon, M. E. Palistrant Low - Temperature Properties of Metals with Band - Spectrum Singularities [in Russian], Shtiintsa, Kishinev (1989).

[22] M. E. Palistrant, Theoret. and Mathem. Phys. 105, 1593 (1995).
[23] A. A. Golubov, J. Kortus, O. V. Dolgov at al., *J. Phys.: Condens Matter* **14**, 1353 (2002).

[24] A. Y. Liu, I. I. Mazin, J. Kortus at al., *Phys. Rev. Lett.* **87**, 087005 (2001).

[25] M. E. Palistrant, F. G. Kochorbe, *Low Temperat. Physics*, **26**, 799 (2000).
This figure "fig1.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0611275v1
This figure "fig2.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0611275v1
This figure "fig3.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0611275v1
This figure "fig4.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0611275v1
This figure "fig5.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0611275v1
This figure "fig6.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/0611275v1