UPPER CRITICAL FIELD IN MgB$_2$ SYSTEM ON BASE OF TWO-BAND MODEL

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The discovery of the high temperature of transition in superconducting state $T_c \sim 40$K in the simple intermetallic compound MgB$_2$ [1] has stimulated researches of this material properties both in the experimental and theoretical plans. The significant result of these researches is the discovery of two energetic gaps in the spectrum of the elementary excitations [2] and the possibility of theoretical describing of this compound on the base of the two-band model [3].

This two-band model and its generalization for the anisotropic value of the energetic gaps $\Delta_1$ and $\Delta_2$ case, [4, 5] confirm the experimental results for the thermal capacity $C_s$ dependence on temperature, the penetration depth of the magnetic field and other characteristics in the MgB$_2$ compound.

As it is known, the superconductive metals undergo the transition from the superconductive phase into normal in the magnetic field at its certain value. This transition which is relevant to the full penetration of the magnetic field into the superconductor, occurs in the moment when the field achieves the value of the upper critical field $H_{c2}$.

The main purpose of the work is researching of pure two-band superconductor of the secondary type for arbitrary temperatures close to the upper critical field and the definition of temperature dependence of the $H_{c2}$ value. The calculations are based on the fundamental equations of the electrodynamics of two-band superconductors [6], which are valid both for pure and doped superconductors.

If the exterior magnetic field is great enough the order parameter $s_m$ ($m = 1, 2$) of two-band superconductor are small, and we can use equations ref. [6] for pure two-band superconductor:

$$\Delta^*_m(\vec{x}) = \frac{1}{\beta} \sum_{\omega} \sum_{n,m} V_{nm} \int d\vec{y} g_{n\nu}^{*}(\vec{y},\vec{x}/\omega) \Delta^*_\nu(\vec{y}) g_{\nu n}^{*}(\vec{y},\vec{x}/-\omega). \tag{1}$$

We restricted here by linear terms on $n$ quantities in comparison with reduced in [6] because in the $H=H_{c2}$ point solutions with the infinitely small values $\Delta_m$ occur. Green function is defined by equation at presence of the magnetic field [7]:

$$g_{mr}^{*}(r,r'/\omega) = e^{i\varphi(r,r')} g_{n\nu}^{*}(r,r'/\omega), \quad \varphi(r,r') = e \int_{r'}^{r} A(\vec{l}) d\vec{l}. \tag{2}$$

where $g_{n\nu}^{*}$ is Green function of an electron in normal metal without magnetic field. The presence of the magnetic field is taken into account by the phase multiplier.

We decompose in equation (1) the normal metal function $g_{n\nu}^{*}$ into the bloch row by the Bloch functions $\Psi_{n\vec{k}}(\vec{x}) = e^{i(\vec{k}\cdot\vec{x})} U_{n\vec{k}}(\vec{x})/\sqrt{N}$ ($U_{n\vec{k}}$ is the Bloch amplitude):

$$g_{n\nu}^{*}(\vec{y},\vec{x}/\omega) = \sum_{\vec{k},\vec{k}'} g_{n\nu}^{*}(\vec{k}',\vec{k}/\omega) \Psi_{n\vec{k}'}(\vec{y}) \Psi_{n\vec{k}}^{*}(\vec{x}) \tag{3}$$
and use approaching of the diagonal Green functions. Magnetic field is guided along the z axis. Besides we choose the vector potential as \( A_x = A_y = 0; \quad A_z = H_0 \cdot x \).

On the base of (1) - (3) after calculating the integral by impul \( \tilde{k} \), averaging by elementary cells, applying Maki and Tsuzuki metodic [7] and assuming \( \Delta_m(x) = \Delta_m \exp \left\{ -H_0 \cdot x^2 \right\} \), we obtain:

\[
\Delta_m^* = \sum_n V_{nm} N_n \rho_n^{-1/2} \Delta_n^* \int_0^\infty \frac{du}{\delta_n^*} \int_0^\infty \frac{d\zeta}{\sinh \left[ u \zeta \rho_n^{-1/2} \right]} \left[ -\frac{\zeta^2}{4} (u^2 + 1) \right] I_0 \left[ \frac{\zeta^2}{4} \left( u^2 - 1 \right) \right], \quad (4)
\]

where \( \nu_n \) and \( N_n \) are accordingly electron speed and electron density of state on \( n \)-th cavity of the Fermi surface,

\[
\delta_n^* = (eH_0)^{1/2} \frac{v_n}{2\gamma e_0 \omega_D^{(n)}}, \quad \rho_n = \frac{v_n^2 eH_0}{(2\pi T)^2}. \quad (5)
\]

\( \gamma \) is the Euler constant, \( \omega_D^{(n)} \) is the cutoff frequency.

Basing on (5) it is easy to obtain the equation for the upper critical field definition in the following form:

\[
\Delta_m^* + \sum_n V_{nm} N_n \Delta_n^* \ln \frac{2\gamma \omega_D^{(n)}}{\pi T_c} - \sum_n V_{nm} N_n \Delta_n^* \left[ \ln \frac{T}{T_c} f(\rho_n) \right] = 0, \quad (6)
\]

where

\[
f(\rho_n) = \rho_n^{-1/2} \int_0^\infty \frac{d\zeta}{\sinh \left[ u \zeta \rho_n^{-1/2} \right]} \times \left\{ 1 - \exp \left[ -\frac{\zeta^2}{4} (u^2 + 1) \right] I_0 \left[ \frac{\zeta^2}{4} \left( u^2 - 1 \right) \right] \right\}. \quad (7)
\]

Equality to zero of the system (6) determinant corresponds to the presence of non-zero solutions, that is the connected pairs forming. The field, in the presence of which such solutions can appear, is the upper critical field \( H_{c2} \). So the \( H_{c2} \) value is determined from the condition of the system (6) solvability:

\[
a f(\rho_1) f(\rho_2) + B_1 f(\rho_1) + B_2 f(\rho_2) + C = 0, \quad (8)
\]

where

\[
B_n = N_n V_{nn} - \alpha \xi_c^{(n)}; \quad (n = 1, 2)
\]

\[
C = 1 - N_1 V_{11} \xi_T^{(1)} - N_2 V_{22} \xi_T^{(2)} + \alpha \left[ \xi_T^{(1)} + \xi_T^{(2)} \right]; \quad a = N_1 N_2 \left( V_{11} V_{22} - V_{12} V_{21} \right);
\]

\[
\xi_T^{(n)} = \ln \frac{2\gamma \omega_D^{(n)}}{\pi T}; \quad \xi_c^{(n)} = \ln \frac{2\gamma \omega_D^{(n)}}{\pi T_c}.
\]

The analytic solutions to equation (8) could be computed for two limit cases as follows:

\( a. \ \rho_n << 1 \quad (T_c - T << T_c); \quad b. \ \rho_n >> 1 \quad (T << T_c), \)

for which functions \( f(\rho_n) \) are defined in works [7]:

\[
f(\rho_n) = \frac{7}{6} \zeta(3) \rho_n - \frac{31}{10} \zeta(5) \rho_n^2 + \frac{381}{28} \zeta(7) \rho_n^3, \quad \rho_n << 1 \quad (9)
\]
\[ f(\rho_n) = \ln \frac{2(2\gamma \rho_n)^{1/2}}{e_0} - \frac{1}{\pi^2 \rho_n} \left[ \frac{\xi'(2)}{2} + \frac{\xi(2)}{2} \ln \frac{2}{\pi^2 \gamma \rho_n} \right], \quad \rho_n \gg 1. \] (10)

In the case of \((T_c - T \ll T_c)\) applying the formulas in (10) and (11) we obtain the following expression for the \(H_{c2}\) value

\[ H_{c2}(T) = \frac{4\pi^2 T^2}{e} \left[ \eta_1 \eta_2 + \eta_1^2 \eta_2 \right]^{1/2} \frac{6}{7\xi(3)} \Theta. \]

\[ \Theta = 1 + \Theta \left\{ \frac{v_1^2}{v_2^2} \eta_1^2 + \eta_2^2 \frac{31}{10} \xi(5) \left( \frac{6}{7\xi(3)} \right)^2 \right\}, \] (11)

\[ \eta = \frac{N_1 V_1 - N_2 V_2}{\sqrt{(N_1 V_1 - N_2 V_2)^2 + 4N_1 N_2 V_1 V_2}}. \] (12)

In the \(b\) case (\(T\) close to zero) we obtain:

\[ \frac{H_{c2}(T)}{H_{c2}(0)} = \left[ 1 + \frac{16\gamma}{e_0 \pi^2} \left( \frac{T^2}{T_c} \right)^2 \exp \left( \frac{\lambda \gamma^+ + 1}{\lambda \gamma^-} \right) \right] + \left[ \xi(2) \ln \frac{4T}{e_0 \pi T_c} \right] + \frac{S}{2} \nu(\lambda) - \frac{\nu(1)}{2} \left( \lambda \gamma^+ - \frac{1}{\lambda} \gamma^- \right) \ln \lambda, \] (13)

where

\[ \nu(\lambda) = \sqrt{(\ln \lambda - \eta)^2 + \frac{4N_1 N_2 V_1 V_2}{a^2}}, \quad S = \pm 1 \]

\[ \gamma^\pm = \frac{1}{2} \left[ \pm \frac{\eta^- - \ln \lambda}{S \nu(\lambda)} \right]. \]

We obtained equation (8), on the base of which the value of the upper critical field in the two-band model can be calculated on the whole temperature interval \(0 \leq T \leq T_c\). The analytic solutions of this equation were obtained for \(T \rightarrow T_c\) (11) and \(T \rightarrow 0\) (13). It is easy to notice that \(H_{c2}\) depends on the correlations of the speeds \(v_1\) and \(v_2\) of the electrons on the Fermi surface, and on the constants of the electronic-phonon interaction \(\lambda_{\text{int}}\).

If \(H_{c2}^0(0)\) and \(T_{c0}\) are introduced (upper critical field and critical temperature of the one-band low-temperature superconductor), on the base of (14) we obtain:

\[ \frac{H_{c2}(0)}{H_{c2}^0(0)} = \left( \frac{T_c}{T_{c0}} \right)^{1/2} \frac{v_1}{v_2} \exp \left( \nu(1) - \nu(\lambda) \right). \] (15)

The numerical estimations let us make the conclusion, that the upper critical field of two-band superconductors for \(T=0\) can exceed the value of \(H_{c2}^0(0)\) for usual superconductors by two-three orders. These big values \(H_{c2}(0)\) are provided by high \(T_c\) and by ratio \(v_1/v_2 > 1\) or \(v_1/v_2 > 1\).

We put the goal to research the dependence from the temperature of the value \(H_{c2}\) for the connection \(\text{MgB}_2\) in the whole temperature interval \(0 < T < T_c\). For this it is necessary to
estimate the parameters of the two band theory \( \lambda_{nm} \), using the experimental data obtained by researching this substance [8], [9]:

\[
\Delta_1(0)=6.8 \text{meV}; \quad Z(0)=\frac{\Delta_1(0)}{\Delta_2(0)}=3.8, \quad \frac{N_1}{N_2}=0.8, \quad \frac{C_S-C_N}{C_N} = 0.78. \quad (16)
\]

In corresponding with the two band theory of superconductors we have [10]

\[
\Delta_1(0)=2 \hbar \omega_0 e^{-\xi(0)}; \quad \Delta_2(0)=\Delta_1(0)/Z(0), \quad (17)
\]

where

\[
\xi(0)=\frac{a N_2 V_{22}-N_2 V_{12}/Z(0)}{Z(0)}.
\]

the heat capacity jump at \( T = T_c \) is determining by the relation [10]

\[
Z_c = \frac{\Delta_1(T \rightarrow T_c)}{\Delta_2(T \rightarrow T_c)} = \frac{1-N_2 V_{22}}{N_1 V_{12}} \xi_c. \quad (19)
\]

The estimate of the ratio \( Z_c \) on the base of experimental data (16) and equations (19) we get: for \( \omega_D^{(1)} = 700 \text{ K}, N_1 V_{11} = 0.3, N_2 V_{12} = 0.12 \); for \( \omega_D^{(2)} = 500 \text{ K}, N_1 V_{11} = 0.33, N_2 V_{12} = 0.13 \) for \( \omega_D = 300 \text{ K}, N_1 V_{11} = 0.42, N_2 V_{12} = 0.16 \).

The interrupted curve is corresponding to the experimental dependence [11]. Fig.1 presents the dependence of the upper critic field \( H_{c2} \) from the temperature, which is obtained by numerical method of solving equation (8) and using its analytic solutions when \( T << T_c \) (13) and \( T \sim T_c \) (11).

The used parameters are

\( N_1 V_{11} = 0.3, N_2 V_{12} = 0.12, N_1/N_2 = 0.8 \).

The case \( \frac{v_1}{v_2} = 1 \) (curve 1); \( \frac{v_1}{v_2} = 2 \) (curve 2); \( \frac{v_1}{v_2} = 3 \) (curve 3).

The interrupted curve is corresponding to the experimental dependence [11].

Using other parameters of theory obtained for \( \omega_D^{(1)} = \omega_D^{(2)} = 500 \text{ K} \) and \( 300 \text{ K} \) we do not get an essential new result. A more important role belongs to the values of ratios \( v_1/v_2 \).

It is easy to see that with growth of \( v_1/v_2 \), the curvature in this dependence changes.
The obtained above results let us make the conclusion about qualitative describing of the experimental data by the behavior of the ratio $H_{c2}(T)/H_{c2}(0)$ as a function of temperature [11] in the intermetallic compound $\text{MgB}_2$, and also about big values of $H_{c2}(0)$ in this compound in comparison with one-band system case.

References