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Properties of the Superconducting State in Hexagonal $BaSn_5$

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The thermodynamic properties of the superconducting state in hexagonal $BaSn_5$ superconductor have been investigated. It has been shown that: (i) the critical value of the Coulomb pseudopotential is equal to 0.152; (ii) the dimensionless ratios: $2\Delta(0)/k_BT_C$, $\Delta C(T_C)/C^N(T_C)$ and $T_CC^N(T_C)/H_C^2(0)$ are equal to: 3.88, 1.78, and 0.151, respectively; (iii) the ratio of the effective to bare electron mass reaches maximum of 1.96 for $T = T_C$.

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1. Introduction

Although there are confirmed reports about superconductivity in sulfur hydrides near 200 K [1] the necessity to maintain very high pressure excludes the possibility of practical use of this superconductor at the moment. Use of cuprates is also complicated due to their mechanical properties, especially brittleness [2]. Thus, intermetallic superconductors are commonly used for technological applications. In superconducting magnets and wires most popular are Nb_3Sn and Nb_3Ge compounds with A15 structure [3]. A few years ago it has been shown that $BaSn_5$ has similar electronic properties to the A15 superconductors [4].

In the presented paper thermodynamic properties of superconducting state induced in hexagonal $BaSn_5$ (T_C = 4.4 K) were determined. The numerical analysis was based on the Eliashberg equations on the imaginary axis [5–7].

Let us pay attention that the Eliashberg approach extends the original idea of Bardeen, Cooper, and Schrieffer [8], taking exactly into consideration the electron–phonon interaction. In the framework of the Eliashberg formalism, the strong coupling corrections to the BCS results are dependent on the value of the parameter $k_BT_C/\omega_{\ln}$. The symbol $\omega_{\ln}$ is called the logarithmic phonon frequency

$$\omega_{\ln} \equiv \exp\left(\frac{2}{\lambda}\int_0^{\Omega_{\max}} \mathrm{d}\Omega \frac{\alpha^2F(\Omega)}{\Omega}\ln(\Omega)\right) \tag{1}$$

and in our case it is equal to 72.92 meV. For $BaSn_5$ superconductor, the Eliashberg function ($\alpha^2F(\Omega)$) has been calculated by employing an *ab initio* pseudopotential method and a linear response scheme in the paper [9]. The maximum phonon frequency ($\Omega_{\max}$) and the electron–phonon coupling constant (λ) are equal to 16.52 meV and 0.96, respectively. In the case of the BCS limit, the Eliashberg function is non-zero only for very high frequency, so that $k_BT_C/\omega_{\ln} \to 0$. In $BaSn_5$, value of the ratio $k_BT_C/\omega_{\ln}$ is equal to 0.0052. In this case the thermodynamic parameters cannot be calculated exactly in the framework of the BCS model.

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2. The Eliashberg equations

The Eliashberg equations on the imaginary axis for half-filled electron band can be written in the following form [5]:

$$\Delta_nZ_n = \frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{K(n,m)-\mu^*\theta(\omega_c-|\omega_m|)}{\sqrt{\omega_m^2+\Delta_m^2}}\Delta_m \tag{2}$$

and

$$Z_n = 1+\frac{\pi}{\beta\omega_n}\sum_{m=-M}^{M}\frac{K(n,m)}{\sqrt{\omega_m^2+\Delta_m^2}}\omega_m, \tag{3}$$

where the symbol $\Delta_n \equiv \Delta(\mathrm{i}\omega_n)$ denotes the order parameter and $Z_n \equiv Z(\mathrm{i}\omega_n)$ is the wave function renormalization factor; n-th Matsubara frequency is defined as: $\omega_n \equiv \frac{\pi}{\beta}(2n-1)$, where $\beta \equiv 1/k_BT$. The electron–phonon pairing kernel $K(n,m)$ is given by

$$K(n,m) \equiv 2\int_0^{\Omega_{\max}}\mathrm{d}\Omega\frac{\Omega}{(\omega_n-\omega_m)^2+\Omega^2}\alpha^2F(\Omega). \tag{4}$$

In Fig. 1 we have presented the form of $K(n,m)$ for the positive Matsubara frequencies and the temperature 0.6 K. It is easy to notice that the pairing kernel is always positive and it achieves the strong maximum for $\omega_n = \omega_m$. The above result means that Eqs. (2) and (3) can have the superconducting solution ($\Delta_n \neq 0$)).

The depairing electron correlations are parameterized by the Coulomb pseudopotential (μ^*). The symbol θ denotes the Heaviside unit function, ω_c is the cut-off energy and $\omega_c = 5\Omega_{\max}$.

The physical values of the Coulomb pseudopotential have been determined in the first step: μ^* = 0.152, whereas the following condition has been used:

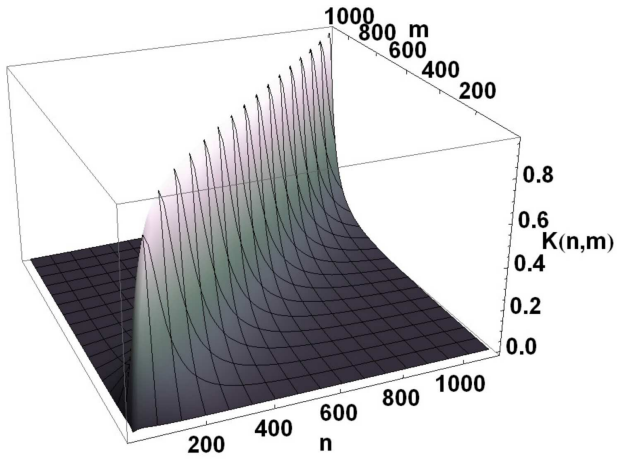

Fig. 1. The pairing kernel $K(n,m)$ as a function of the numbers n and m.

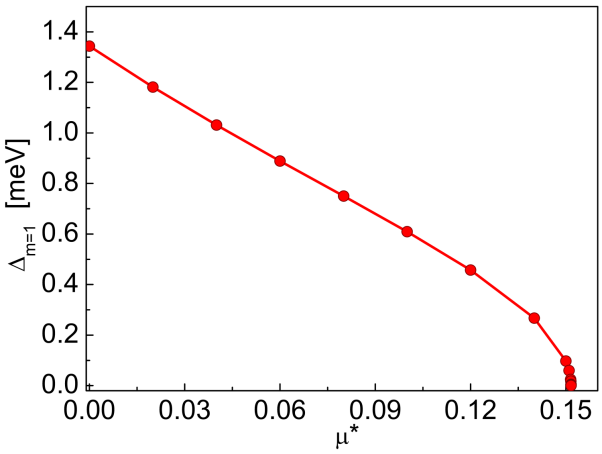

Fig. 2. The dependence of the maximum value of the order parameter on the Coulomb pseudopotential.

$[\Delta_{m=1}(\mu^*)]_{T=T_C} = 0$. The calculations have assumed the experimental values of the critical temperature of $T_C = 4.4$ K [4]. The dependence of the maximum value of the order parameter on the Coulomb pseudopotential has been shown in Fig. 2.

The Eliashberg equations have been solved for 2201 Matsubara frequencies ($M = 1100$) by using the method presented in [10] and [11] and recently tested in [12]. In the considered case, the obtained Eliashberg solutions are stable for $T \geq 0.6$ K.

3. The numerical results

Figure 3a presents the form of the order parameter on the imaginary axis for the selected values of temperature. It can be seen that the maximum value of the function Δ_m is taken for $m = 1$.

The temperature dependence of the order parameter is convenient to be traced by plotting the curve $\Delta_{m=1}(T)$ (Fig. 3b).

In the case of $BaSn_5$, the obtained numerical data can be reproduced by the formula

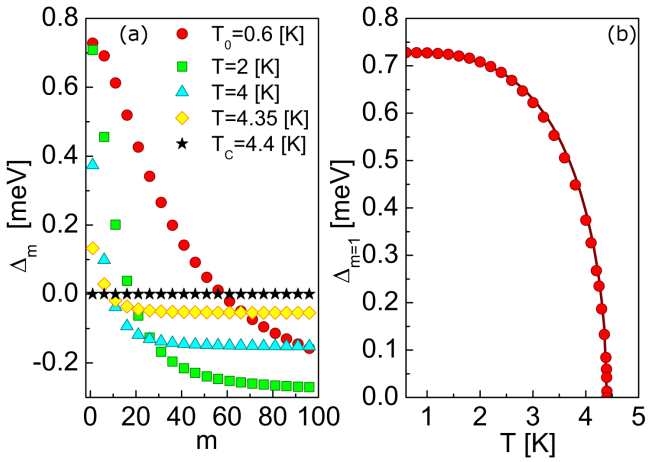

Fig. 3. (a) The order parameter on the imaginary axis for the selected values of temperature. The first 100 values of the function Δ_m are plotted. (b) The influence of temperature on the maximum value of the order parameter. The symbols represent the numerical results. The line was obtained by using Eq. (5).

$$\Delta_{m=1}(T) = \Delta_{m=1}(T_0)\sqrt{1-\left(\frac{T}{T_C}\right)^{\kappa}}, \tag{5}$$

where $\Delta_{m=1}(T_0) \approx \Delta_{m=1}(T = 0.6\text{ K}) = 0.73$ meV, and $\kappa = 3.6$.

Let us note that the values of the function $\Delta_{m=1}(T)$ cannot be properly set within the framework of the BCS theory, as $[\kappa]_{BCS} = 3$ [13].

The physical value of the order parameter should be calculated analytically continuing the Eliashberg equations solutions on the real axis ($\Delta_m \to \Delta(\omega)$). For this purpose, the following formula can be used:

$$\Delta(\omega) = \frac{p_1 + p_2\omega + \ldots + p_r\omega^{r-1}}{q_1 + q_2\omega + \ldots + q_r\omega^{r-1} + \omega^r}. \tag{6}$$

The values of the parameters p_j and q_j have been determined according to the method presented in the publication [14]. Additionally, it has been assumed: $r = 50$.

The results for the order parameter have been shown in Fig. 4. It can be seen that the real part of the function $\Delta(\omega)$ takes the non-zero values only for the low frequencies. From the physical point of view, this means the lack of damping effects. For the higher values of the frequency both $\mathrm{Re}(\Delta(\omega))$ and $\mathrm{Im}(\Delta(\omega))$ are characterized by the complicated courses.

In the next step we have to calculate the physical value of the order parameter by using the following equation:

$$\Delta(T) = \mathrm{Re}(\Delta(\omega = \Delta(T), T)). \tag{7}$$

For $T_0 = 0.6$ K the following result has been obtained: $\Delta(0) = 0.74$ meV, while $\Delta(0) \equiv \Delta(T_0)$.

The form of the wave function renormalization factor on the imaginary axis is shown in Fig. 5a. Just as it was in the case of the order parameter, the function Z_m takes the highest value for $m = 1$.

On the other hand, the effect of temperature on $Z_{m=1}$ is rather negligible, which was presented in Fig. 5b.

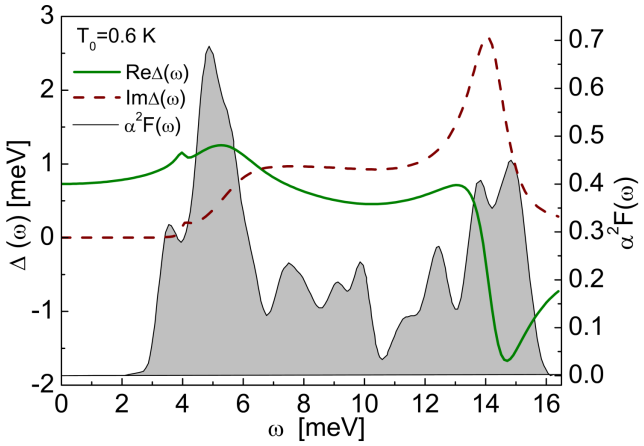

Fig. 4. Real and imaginary part of the order parameter on the real axis for $T = 0.6$ K. The Eliashberg function [9] is present in the background — the correlation between the course of the order parameter and the spectral function is clearly visible.

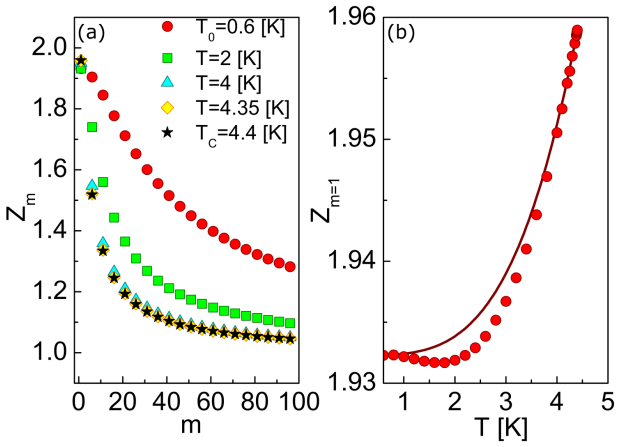

Fig. 5. (a) The wave function renormalization factor on the imaginary axis for the selected values of temperature. The first 100 values of the function Z_m are plotted. (b) The influence of temperature on the maximum value of the renormalization factor. The symbols represent the numerical results. The line was obtained by using Eq. (8).

However, throughout the analyzed temperature range, the wave function renormalization factor assumes high values. Suffice it to note that the BCS theory predicts $Z_m = 1$.

The high values of the function $Z_{m=1}(T)$ are related to the significant strong-coupling effects appearing in $BaSn_5$.

It can be noted that the numerical results obtained for the wave function renormalization factor can be reproduced using the following formula:

$$Z_{m=1}(T) = Z_{m=1}(T_0) + [Z_{m=1}(T_C) - Z_{m=1}(T_0)] \left(\frac{T}{T_C}\right)^{\kappa}, \quad (8)$$

where $Z_{m=1}(T_0) = 1.93$, and $Z_{m=1}(T_C) = 1 + \lambda$.

The free energy difference between the superconducting and normal state (ΔF) for an interacting electron–phonon systems should be determined by using the expression [15]:

$$\frac{\Delta F}{\rho(0)} = -\frac{2\pi}{\beta} \sum_{n=1}^{M} \left(\sqrt{\omega_n^2 + \Delta_n^2} - |\omega_n|\right) \times (Z_n^S - Z_n^N \frac{|\omega_n|}{\sqrt{\omega_n^2 + \Delta_n^2}}), \quad (9)$$

where Z_n^S and Z_n^N denote the wave function renormalization factors for the superconducting (S) and normal (N) state, respectively. In Fig. 6 (lower part) we have plotted the dependence of ΔF on the temperature. From the physical point of view, the negative values of ΔF prove that the superconducting state is stable below the critical temperature.

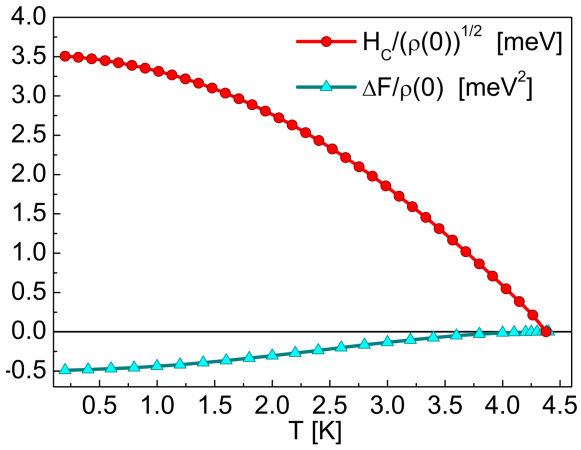

Fig. 6. (lower part) The free energy difference between the superconducting state and the normal state as a function of temperature. (upper part) The thermodynamic critical field as a function of temperature.

In the next step we have calculated the values of the thermodynamic critical field (cgs units)

$$\frac{H_C}{\sqrt{\rho(0)}} = \sqrt{-8\pi\,[\Delta F/\rho(0)]}. \quad (10)$$

The temperature dependence of $H_C/\sqrt{\rho(0)}$ has been shown in Fig. 6 (upper part).

Next, the specific heat in the normal state can be obtained with the help of formula

$$\frac{C^N(T)}{k_B \rho(0)} = \frac{\gamma}{\beta}, \quad (11)$$

where the Sommerfeld constant is given by $\gamma \equiv \frac{2}{3}\pi^2(1+\lambda)$. The dependence of the specific heat for the superconducting and the normal state on temperature is presented in Fig. 7. The characteristic jump occurs at the critical temperature and is marked with the vertical dashed line.

The thermodynamic functions designated in this work allow us to calculate the value of the dimensionless ratios:

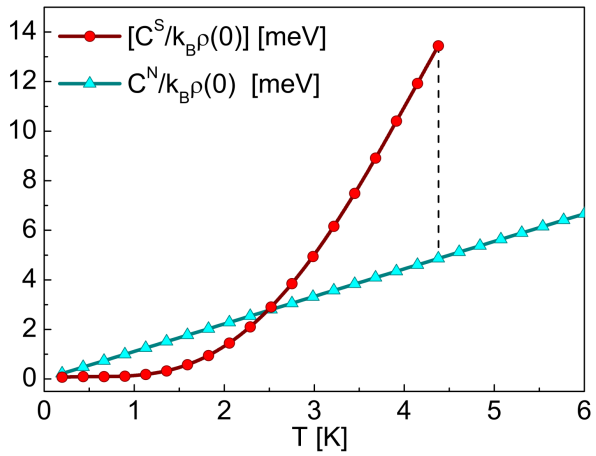

Fig. 7. The dependence of the specific heat in the superconducting and normal state on the temperature.

$$R_\Delta \equiv \frac{2\Delta(0)}{k_B T_C} = 3.88, \tag{12}$$

$$R_C \equiv \frac{\Delta C(T_C)}{C^N(T_C)} = 1.78, \tag{13}$$

$$R_H \equiv \frac{T_C C^N(T_C)}{H_C^2(0)} = 0.151. \tag{14}$$

It should be noted that the parameters R_Δ–R_H in the framework of the BCS theory take the universal values equal to 3.53, 1.43, and 0.168, respectively [8, 15].

4. Conclusions

The thermodynamic properties of superconducting state in hexagonal $BaSn_5$ has been analyzed in the framework of the Eliashberg approach. We have stated that the critical value of the Coulomb pseudopotential is equal to 0.152, which proves that the depairing correlations are not negligible in this superconductor. Additionally, we have shown that the dimensionless parameters R_Δ, R_C and R_H have the values: 3.88, 1.78, and 0.151, respectively, and this significantly differs from the predictions of BCS theory. Finally, the ratio of m_e^*/m_e reaches the maximum of 1.96 at the critical temperature. Above results show that the hexagonal $BaSn_5$ is superconductor with strong electron–phonon interaction and it cannot be properly described by using the classical BCS theory.

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