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The Thermodynamic Critical Field of YNi_2B_2C Superconductor

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In the presented work the dependence of the thermodynamic critical field (H_{C}) on the temperature for the YNi_2B_2C superconductor was determined in the framework of the Eliashberg formalism. The numerical calculations were conducted with the use of the modified transport Eliashberg function. It has been stated that the normalized field function $H_{\mathrm{C}}(T)/H_{\mathrm{C}}(0)$ correctly reproduces the experimental data.

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1. Introduction

In the year of 1957, Bardeen, Cooper and Schrieffer introduced the first microscopic theory of the superconductivity (BCS) [1]. Unfortunately, in the framework of the BCS theory, the properties of the most low-temperature superconductors could be explained only in the qualitative way. The essential progress occurred in 1960 when Eliashberg presented the generalized BCS formalism, which enabled the detailed analysis of the thermodynamic and electrodynamic parameters of the superconductors with the electron–phonon pairing mechanism [2]. The results obtained by Eliashberg lead to the conclusion that the fundamental equation of the BCS theory should be replaced by the set of three non-linear equations (the so-called "Eliashberg set"). The Eliashberg equations set, determined on the imaginary axis, allows one to calculate three basic quantities: the order parameter function $\Delta_n \equiv \Delta(\mathrm{i}\omega_n)$, the wave function renormalization factor $Z_n \equiv Z(\mathrm{i}\omega_n)$ and the energy shift function $\chi_n \equiv \chi(\mathrm{i}\omega_n)$, where $\omega_n \equiv (\pi/\beta)(2n-1)$ is the n-th Matsubara frequency; the symbol β is given by the expression $\beta \equiv (k_{\mathrm{B}}T)^{-1}$ and k_{B} denotes the Boltzmann constant. Due to the very complicated structure of the Eliashberg equations, usually only the functions Δ_n and Z_n are used for the analysis of the superconducting properties of the particular material. The approximation above is identical with an assumption that the modeled system has the half-filled electron band.

In the presented paper we have determined the dependence of the thermodynamic critical field on the temperature for the YNi_2B_2C superconductor. From the physical point of view, the YNi_2B_2C compound is interesting due to its relatively high value of the critical temperature $T_{\mathrm{C}} \approx 15$ K [3, 4]. Additionally, it still remains unclear whether YNi_2B_2C is conventional or exotic superconductor. For example, let us recall here the experiments which indicate the multiband superconductivity or the nontrivial pairing symmetry [5, 6]. For this reason, the comparison between the theoretical and experimental $H_{\mathrm{C}}(T)/H_{\mathrm{C}}(0)$ function yields the information about the accuracy and scope of the predictions obtained in the framework of the one-band Eliashberg formalism.

2. Model

The thermodynamic critical field can be calculated by using the expression (CGS unit system) [2]:

$$\frac{H_{\mathrm{C}}}{\sqrt{\rho(0)}} = \sqrt{-8\pi\left[\Delta F/\rho(0)\right]}, \tag{1}$$

where $\rho(0)$ is the value of the electron density of states at the Fermi energy. In the framework of the Eliashberg formalism, the difference in the free energy between the normal and the superconducting state (ΔF) is being calculated on the basis of the following expression [7]:

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

where the symbol Z_n^{S} and Z_n^{N} denotes the wave function renormalization factor for the superconducting state and the normal state, respectively. In Eq. (2) M limits the number of the Matsubara frequency. In the case of

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YNi_2B_2C superconductor we have taken $M = 800$ in order to obtain the stability of the numerical results.

The Eliashberg equations for the half-filled electron band can be written in the form [2]:

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

$$Z_n = 1 + \frac{\pi}{\beta\omega_n} \sum_{m=-M}^{M} \frac{K(\omega_n - \omega_m)}{\sqrt{\omega_m^2 + \Delta_m^2}} \omega_m \,, \tag{4}$$

where the kernel $K(\omega_n - \omega_m)$ is defined by the expression:

$$K(\omega_n - \omega_m) \equiv 2 \int_0^{\Omega_{\max}} \mathrm{d}\Omega \frac{\alpha^2 F(\Omega)\Omega}{(\omega_n - \omega_m)^2 + \Omega^2} \,. \tag{5}$$

The symbol $\alpha^2 F(\Omega)$ denotes the ordinary Eliashberg function, with a use of which the electron–phonon interaction is being modeled; $\Omega_{\max}$ is the maximum phonon frequency. The quantity $\mu(\omega_m)$ that appears in Eq. (3) has the following form: $\mu(\omega_m) \equiv \mu^* \Theta(\omega_c - |\omega_m|)$, where μ^* is the Coulomb pseudopotential; Θ denotes the Heaviside unit function and ω_c is the phonon cut-off frequency. In the presented calculations $\mu^* = 0$ was assumed (in accordance with an analysis presented in [3]).

3. Results

The starting point for our deliberations is the transport Eliashberg function $[\alpha^2 F(\Omega)]_{\mathrm{tr}}$ (the A curve in the inset in Fig. 1) [3]. In most cases $[\alpha^2 F(\Omega)]_{\mathrm{tr}}$ does not differ too much from the ordinary Eliashberg function. According to the above, the ordinary Eliashberg function was obtained on the basis of the transport function by the timing it by W constant (the B curve). The fitting parameter $W = 1.283$ was chosen in the way to achieve the experimental value of the critical temperature ($k_B T_C = 1.335$ meV) when solving the Eliashberg equations. Finally, it has to be noticed that, for the considered Eliashberg function, the value of the maximum phonon frequency $\Omega_{\max}$ is equal to 67.51 meV.

The obtained Eliashberg function allows to estimate the value of the electron–phonon coupling constant: $\lambda \equiv 2\int_0^{\Omega_{\max}} \mathrm{d}\Omega \frac{\alpha^2 F(\Omega)}{\Omega}$. After the conductance of the numerical calculations it has been stated that $\lambda = 0.676$, which classifies YNi_2B_2C as the superconductor of the indirect value of the coupling constant. YNi_2B_2C is thus the compound whose properties cannot be quantitatively properly calculated in the framework of the classical BCS theory, that is right for the lower values of λ. Let us notice that the achieved result fairly well corresponds to the value $\lambda = 0.637$, which can be obtained on the basis of the results presented in [5].

Now, we determine the dependence of the normalized thermodynamic critical field on the temperature. The data obtained by using the complicated numerical analysis are plotted in Fig. 1. Additionally, the theoretical results were compared with the normalized values of the critical field, estimated on the basis of the experimental

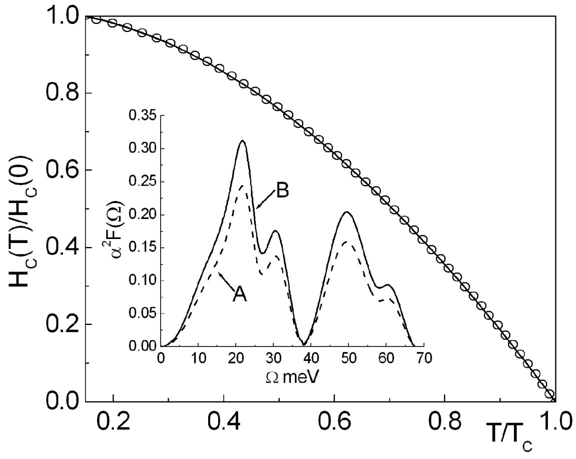

Fig. 1. The dependence of the normalized thermodynamic critical field on the ratio T/T_C. The maximum value of the field is equal to $H_C(0)/\sqrt{\rho(0)} = 11.11$ meV. The solid line corresponds to the theoretical results; the experimental data was marked by the empty circles [8]. In the inset the transport (A) and the ordinary (B) Eliashberg functions are plotted.

differences in entropy between the superconducting and normal state [8]. The high agreement of the theoretical predictions with the experimental results presented in Fig. 1 proves that the dependence of the thermodynamic critical field on the temperature for YNi_2B_2C superconductor can be very precisely reproduced with a use of the Eliashberg equations.

In the last part of the work we are turning the readers' attention towards the important issue. Some of the YNi_2B_2C superconductor's properties (e.g. the upper critical field temperature dependence $H_{C2}(T)$) should be analyzed in the framework of the highly advanced models. In the most probable way, the effective two-band Eliashberg model has to be applied, since this model successfully describes the value of $H_{C2}(0)$ and the positive curvature of $H_{C2}(T)$ at high and intermediate temperature [5, 9]. The raised issue is being intensively studied by us.

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