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High-pressure superconductivity in yttrium: The strong-coupling approach

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ABSTRACT

In the framework of the Eliashberg formalism, the properties of the superconducting state inducing in yttrium for the pressure at $p_1 \equiv 26$ GPa and $p_2 \equiv 31$ GPa ($[T_C]_{p_1} = 7.9$ K and $[T_C]_{p_2} = 9.27$ K) have been determined. It has been proven that the value of the Coulomb pseudopotential is high and increases with the increasing pressure: $[\mu^\star]_{p_1} = 0.181$ and $[\mu^\star]_{p_2} = 0.251$. Next, the order parameter ($\Delta(T)$), the thermodynamic critical field ($H_C(T)$), the specific heat in the superconducting state ($C^S(T)$), and the specific heat in the normal state ($C^N(T)$) have been calculated. It has been proven that the values of the dimensionless parameters $R_\Delta \equiv \frac{2\Delta(0)}{k_B T_C}, R_C \equiv \frac{C^S(T_C)-C^N(T_C)}{C^N(T_C)}$, and $R_H \equiv \frac{T_C C^N(T_C)}{H_C^2(0)}$ significantly deviate from the predictions of the classical BCS theory: $R_\Delta \in \{3.97, 4.13\}, R_C \in \{2.16, 2.41\}$, and $R_H \in \{0.153, 0.152\}$. The electron effective mass is high for both pressures $[m_e^\star]_{p_1}^{T=T_C} = 2.16 m_e$ and $[m_e^\star]_{p_2}^{T=T_C} = 2.64 m_e$, where the symbol m_e denotes the electron band mass.

1. Introduction

The superconducting state induced by the electron–phonon interaction is usually characterized by a relatively low value of the critical temperature (T_C) [1–3].

One of the few exceptions is the compound MgB_2 with the critical temperature equal to 39 K [4]. However, this is the system with a very unusual form of the electron–phonon interaction, which is characterized by high anisotropy [5,6].

In addition to the superconductors with the electron–phonon pairing mechanism, a special attention should be paid to the systems discovered in 1986 (the so-called cuprates) [7]. It turns out that these compounds may go into the superconducting state at the surprisingly high temperature. For example, for $HgBa_2Ca_2Cu_3O_{8+y}$ it was obtained: $T_C = 164$ K, wherein the value of the external pressure (p) was equal to 31 GPa [8]. Unfortunately, despite very serious efforts made so far, all trials to raise the critical temperature in this group of materials have failed.

Note that in the case of cuprates there is no generally acceptable theory to explain the mechanism responsible for the formation of the superconducting condensate. Most researchers emphasize the importance of the strong electron correlations [9]. However, some of them pay attention to the role of the electron–phonon interaction [10–15].

The problems associated with the increase in the value of T_C in cuprates have led to a renewed interest in the electron–phonon superconductors. In particular, it has been noticed that the electron–phonon interaction can be a very efficient pairing mechanism for the systems, which are exposed to the influence of high pressure.

Performed theoretical calculations show that the highest value of T_C (comparable to the room temperature) in the group of the high-temperature superconductors can be obtained for the superconducting state inducing in metallic hydrogen [16–20].

In 2004, it was further suggested [21] that the high-temperature superconducting state will also be present in the compounds rich in hydrogen [22–26].

Recently, the latest experimental data have confirmed the results of the long lasting theoretical research. In December 2014, the discovery of the superconducting condensate with the extremely high critical values of the critical temperature in H_2S and H_3S was announced [27]. In particular, for the compound H_2S (in the range of the pressures from 115 GPa to 200 GPa) the critical temperature increases from 31 K to 150 K. In the case of H_3S, the critical temperature can be even higher: $T_C = 190$ K for $p > 150$ GPa.

Very interesting results have also been obtained for the superconducting state inducing in the pure elements exposed to the influence of high pressure. It turned out that the value of the coupling constant for the electron–phonon interaction can significantly increase with the increasing p, which entails a significant increase in T_C. In particular, the highest values of the critical temperature have been obtained for calcium ($T_C = 29$ K,

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$p=216$ GPa [28,29]), yttrium ($T_C=19.5$ K, $p=115$ GPa [30,31]), sulfur ($T_C=17.3$ K, $p=160$ GPa [32,33]), and lithium ($T_C=14$ K, $p=30$ GPa [34,35]).

In the presented study, we have analyzed the high-pressure superconducting state inducing in yttrium.

It is worth noting that yttrium exposed to the ambient pressure does not go into the superconducting state ($T>6$ mK) [36], because it has not got a sufficient number of d electrons in the conduction band. The more d electrons a given conduction band has the higher density of states and the more likely it is to support the superconductivity. The application of pressure increases the number of d electrons in a band by $s\rightarrow d$ transfer [37]. The condensate of the Cooper pairs can be achieved only above the pressure at 11 GPa ($T_C\sim 1.3$ K) [38]. The critical temperature increases with the increasing pressure ($dT_C/dp\sim 0.35$ K/GPa), reaching the value of $\sim$ 9 K at $\sim$ 30 GPa. The studies conducted in the works [30,31] prove that the increase of the pressure to 115 GPa causes a further increase in T_C to the value of 19.5 K.

The value of the coupling constant of the electron–phonon interaction in yttrium in the pressure range from 5 GPa to 31 GPa (the structure $Fm\overline{3}m$ (no. 225)) has been analyzed in the work [39]. It has been shown that the interaction of the electron gas with the vibrations of the crystal lattice is relatively poor for the lower p. Note that from the theoretical point of view, the obtained result has displayed a possibility of the BCS theory to describe the thermodynamic properties of the superconducting state [40,41].

The situation is quite different for the higher pressures analyzed in the presented study ($p_1=26$ GPa and $p_2=31$ GPa), where the strong-coupling effects are significant. In the cases under consideration, the advanced Eliashberg formalism should be used [3].

2. The model

The Eliashberg equations on the imaginary axis ($i\equiv\sqrt{-1}$) take the following form [42]:

$$\phi_n=\frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\lambda(i\omega_n-i\omega_m)-\mu^{\star}\theta(\omega_c-|\omega_m|)}{\sqrt{\omega_m^2Z_m^2+\phi_m^2}}\phi_m, \tag{1}$$

$$Z_n=1+\frac{1}{\omega_n}\frac{\pi}{\beta}\sum_{m=-M}^{M}\frac{\lambda(i\omega_n-i\omega_m)}{\sqrt{\omega_m^2Z_m^2+\phi_m^2}}\omega_mZ_m, \tag{2}$$

where the symbols $\phi_n\equiv\phi(i\omega_n)$ and $Z_n\equiv Z(i\omega_n)$ denote the order parameter function and the wave function renormalization factor, respectively. The symbol $\omega_n\equiv(\pi/\beta)(2n-1)$ represents the n-th Matsubara frequency and $\beta\equiv(k_BT)^{-1}$ (k_B is the Boltzmann constant). The order parameter is defined in the following way: $\Delta_n\equiv\phi_n/Z_n$.

The electron–phonon pairing kernel is given by

$$\lambda(z)\equiv 2\int_0^{\Omega_{\max}}d\Omega\frac{\Omega}{\Omega^2-z^2}\alpha^2F(\Omega), \tag{3}$$

where $\alpha^2F(\Omega)$ is the Eliashberg function, which models the electron–phonon interaction. In the case of yttrium, the Eliashberg functions for the pressures p_1 and p_2 have been determined in the work [39]. The *ab initio* calculations have been conducted with the help of the QUANTUM-ESPRESSO package [43]. The maximum phonon frequencies are respectively $[\Omega_{\max}]_{p_1}=26.42$ meV and $[\Omega_{\max}]_{p_2}=27.86$ meV.

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

The Eliashberg equations have been solved for 2201 Matsubara frequencies ($M=1100$). The methods presented in the works [44–47] have been used in the present calculations.

The solutions of the Eliashberg equations are stable for $T_0\geq 1$ K.

3. Results

The physical values of the Coulomb pseudopotential have been determined in the first step: $[\mu^{\star}]_{p_1}=0.181$ and $[\mu^{\star}]_{p_2}=0.251$, whereas the following condition has been used: $[\Delta_{m=1}(\mu^{\star})]_{T=T_C=0}$ (see also Fig. 1). The calculations have assumed the experimental values of the critical temperature of respectively $[T_C]_{p_1}=7.9$ K and $[T_C]_{p_2}=9.27$ K [36].

The obtained results show that the values of the parameter $\mu^{\star}$ are relatively high and continue to rise with the increasing pressure. From the physical standpoint, this means that the depairing electron correlations cannot be ignored in the quantitative analysis of the thermodynamic properties of the superconducting state inducing in yttrium.

Fig. 2(A)–(B) 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. 2 (C)).

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

$$\Delta_{m=1}(T)=\Delta_{m=1}(T_0)\sqrt{1-\left(\frac{T}{T_C}\right)^{\kappa}}, \tag{4}$$

where $[\Delta_{m=1}(T_0)]_{p_1}=1.34$ meV, $[\Delta_{m=1}(T_0)]_{p_2}=1.64$ meV, and $\kappa=3.85$.

Note that the values of the function $\Delta_{m=1}(T)$ cannot be properly set within the framework of the BCS theory, as $[\kappa]_{\mathrm{BCS}}=3$ [48].

The form of the wave function renormalization factor on the imaginary axis is shown in Fig. 3(A) and (B). 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. 3(C). However, throughout the analyzed temperature range, the wave function renormalization factor assumes high values. Suffice it to note that the BCS theory predicts $Z_m=1$.

From the physical side, the high values of the function $Z_{m=1}(T)$ are related to the significant strong-coupling effects appearing in yttrium. These effects can be modeled by the electron–phonon coupling constant, which for the analyzed pressure is adequately equal to $[\lambda]_{p_1}=1.08$ and $[\lambda]_{p_2}=1.64$. Note that the quantity λ should be calculated using the formula: $\lambda\equiv 2\int_0^{+\infty}d\Omega\frac{\alpha^2(\Omega)F(\Omega)}{\Omega}$.

In the last step, it can be noted that the numerical results obtained for the wave function renormalization factor can be

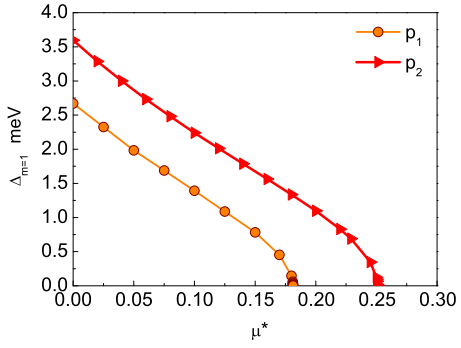

Fig. 1. (Color online) The dependence of the maximum value of the order parameter on the Coulomb pseudopotential.