Proceedings of the European Conference Physics of Magnetism, Poznań 2014

Characterization of Novel High-Pressure Close-Packed Superconducting Phase of Boron

D. Szczęśniak[a,*] and R. Szczęśniak[b]

[a]Institute of Physics, Jan Długosz University in Częstochowa, al. Armii Krajowej 13/15, 42-200 Częstochowa, Poland

[b]Institute of Physics, Częstochowa University of Technology, al. Armii Krajowej 19, 42-200 Częstochowa, Poland

We report study on the thermodynamic properties of the novel high-pressure superconducting phase of boron with hexagonal $P6_3/mcm$ structure. Our analysis is conducted at the pressure of $p = 400$ GPa, which is motivated by the highest value of the superconducting transition temperature ($T_{\rm C}$) observed previously under such conditions for the $P6_3/mcm$ boron. Our investigations of the thermodynamic properties are performed within the Eliashberg formalism, due to the strong-coupling character of the considered material. In particular, we calculate the thermodynamic properties of the superconducting state which allows us to determine the values of the characteristic dimensionless parameters; the zero-temperature energy gap to the critical temperature, the ratio of the specific heats, as well as the ratio connected with the zero-temperature thermodynamic critical field.

DOI: 10.12693/APhysPolA.127.254

PACS: 74.25.Bt, 74.62.Fj, 74.20.Fg

1. Introduction

Studies of superconductors under the condition of high pressure (p) are at present of great importance [1]. This interest steams from the fact that due to the externally applied pressure it is possible to induce the superconducting phase or enhance its properties in various materials.

One of the most interesting results, in this domain, concern the case of the simple metals [2–4]. For example, the elements like lithium or calcium have been experimentally proved to be characterized by the relatively high maximum superconducting transition temperatures ($T_{\rm C}$) of the order of ≈14 K (at $p = 30.2$ GPa) [5] and ≈29 K (at $p = 216$ GPa) [6], respectively. Moreover, on the basis of the theoretical calculations it has been shown that both of these materials are the strong-coupling superconductors [7, 8].

Following these results, one of the most recent related investigations consider the possibility of inducing superconducting phase in the metallic boron. Early theoretical research revealed that boron in the high-pressure α-Ga phase is expected to be a superconductor with a low electron–phonon coupling constant (λ) equal to 0.39 [9]. Although, recently Li et al. predicted novel B_{10} hexagonal $P6_3/mcm$ structure of boron, which is energetically more stable then the α-Ga phase within the pressure range from 375 to 500 GPa [10]. Moreover, on the basis of the *ab initio* calculations, Li et al. showed that the highest $T_{\rm C}$ value for the B_{10} can be obtained for $p = 400$ GPa. Under such conditions the B_{10} superconductor is characterized by the relatively high value of the electron–phonon coupling constant equal to 0.82.

In this work, we present study of the selected thermodynamic properties of this novel superconducting phase of boron at $p = 400$ GPa. Due to the mentioned value of the electron–phonon coupling constant, the B_{10} superconductor at $p = 400$ GPa should be analyzed within the strong-coupling limit ($\lambda > 0.3$ [11]). For this purpose we perform our analysis within the Eliashberg formalism [12], a strong-coupling generalization of the Bardeen–Cooper–Schrieffer theory [13, 14].

2. Theory

In particular, our numerical calculations are carried out using the set of the isotropic Eliashberg equations (for the computational details please see [15] and [16]), which are solved on the imaginary axis and in the mixed representation by adopting the electron–phonon Eliashberg spectral function presented in [10]. Furthermore, we assume that the Coulomb pseudopotential value is equal to 0.1, following value assumed in the paper [10]. Moreover, the Matsubara frequencies ($\omega_m \equiv \frac{\pi}{\beta}(2m-1)$, where parameter β is given by $\beta \equiv 1/k_{\rm B}T$, and $k_{\rm B}$ denotes the Boltzmann constant) are limited to $M = 1100$. Due to this fact the stability of our calculations is ensured for temperatures greater than $T_0 = 5$ K. Finally, the cut-off frequency is set to be $\omega_{\rm C} = 10\Omega_{\rm max}$, where $\Omega_{\rm max}$ is the maximum phonon frequency equal to 246.95 meV.

3. Results

In Fig. 1A, we present calculated maximum value of the order parameter ($\Delta_{m=1}$) as a function of temperature (T). The point where $\Delta_{m=1} = 0$ allows us to quantitatively determine the value of the superconducting transition temperature, which in our case is equal to 48.86 K. Supplementary results of the dependence of the order parameter (Δ_m) on m for selected values of temperature are presented in the inset of Fig. 1A.

*corresponding author; e-mail: d.szczesniak@ajd.czest.pl

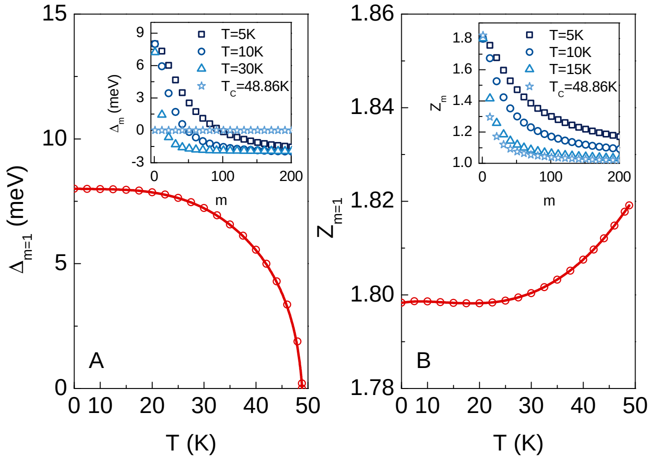

Fig. 1. The dependence of the maximum value of the order parameter (A) and the maximum value of the wave function renormalization factor (B) on temperature. Insets present the order parameter (A) and the wave function renormalization factor (B) as a function of m for selected values of temperature.

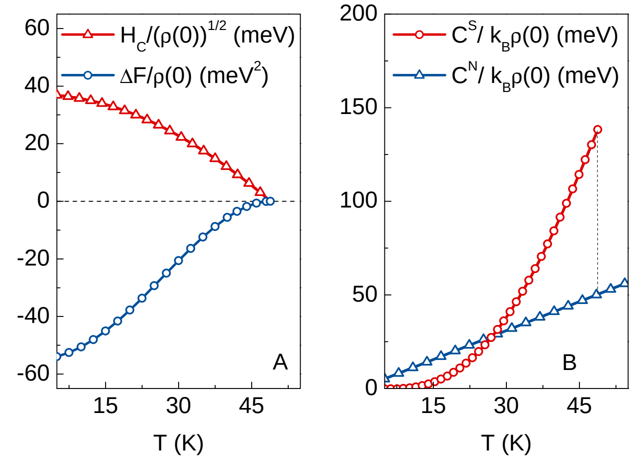

Fig. 2. The free energy difference between superconducting and normal state (A — lower panel) and the thermodynamic critical field (A — upper panel) as a function of temperature. The specific heat of the normal and superconducting state as a function of temperature (B).

On the other hand, Fig. 1B depicts maximum value of the wave function renormalization factor ($Z_{m=1}$) as a function of temperature. From the physical point of view, this dependence describes, with a good approximation, the functional behavior of the electron effective mass ($m^*_{\rm e}$) on temperature; $m^\star_{\rm e}(T) \simeq Z_{m=1}(T)m_{\rm e}$, where $m_{\rm e}$ denotes the band electron mass. In what follows, the obtained maximum value of the electron effective mass at $T = T_{\rm C}$ is equal to 1.82 $m_{\rm e}$. At this point we would like to underline that $m^\star_{\rm e}(T_{\rm C})$ can be also calculated on the basis of the following simple analytical formula:

$$m^\star_{\rm e}(T_{\rm C}) = (1+\lambda)m_{\rm e}. \quad (1)$$

By using this formula, one can easily note that the calculated value is in the perfect agreement with the value obtained previously on the basis of the Eliashberg equations. This fact ensures the accuracy of our numerical computations.

Similarly as in the case of the order parameter, results presented in Fig. 1B are supplemented by the functional dependance of the Z_m on m for selected values of temperature.

On the basis of the results presented in Fig. 1A and B we are next able to determine the temperature dependence of the free energy difference between the superconducting and normal state, the thermodynamic critical field as well as the specific heat of the superconducting state (for the computational details please see [15] and [16]).

The calculated free energy difference between the superconducting and normal state ($\Delta F/\rho(0)$, where $\rho(0)$ denotes the electronic density of states at the Fermi level) is plotted versus temperature in the lower part of Fig. 2A. The upper part of Fig. 2A presents the temperature dependence of thermodynamic critical field determined using the following expression:

$$H_{\rm C}/\sqrt{\rho(0)} = \sqrt{-8\pi[\Delta F/\rho(0)]}. \quad (2)$$

Obtained maximum value of the $H_{\rm C}/\sqrt{\rho(0)}$ equals 36.83 meV at $T = T_0$.

In Fig. 2B we present the specific heat of the normal and superconducting state calculated as a function of temperature. The specific heat of the superconducting state is determined by using the following relation:

$$C^{\rm S} = C^{\rm N} + \Delta C, \quad (3)$$

where $C^{\rm N}$ denotes the specific heat of normal state, and ΔC is the difference between the specific heat of superconducting and normal state. The maximum value of the $C^{\rm S}/k_{\rm B}\rho(0)$ at $T = T_{\rm C}$ equals 138.75 meV.

Moreover, in Fig. 2B, the characteristic jump of the specific heat of the superconducting state can be clearly observed at $T = T_{\rm C}$.

Obtained results for the thermodynamic critical field and the specific heat of the normal and superconducting state allows us next to determine the corresponding dimensionless ratios:

$$R_{\rm H} \equiv T_{\rm C}C^{\rm N}(T_{\rm C})/H^2_{\rm C}(0), \quad (4)$$

and

$$R_{\rm C} \equiv \Delta C(T_{\rm C})/C^{\rm N}(T_{\rm C}), \quad (5)$$

respectively. The calculated values are: $R_{\rm H} = 0.156$ and $R_{\rm C} = 1.75$.

In the final step, we calculate the physical value of the energy gap at the Fermi level ($2\Delta(0)$). For this purpose we solve the Eliashberg equations in the mixed representation (for more details please see papers [15] and [16]). Obtained results of the order parameter on the real axis ($\Delta(\omega)$) as a function of frequency (ω) for selected values of temperature are presented in Fig. 3.

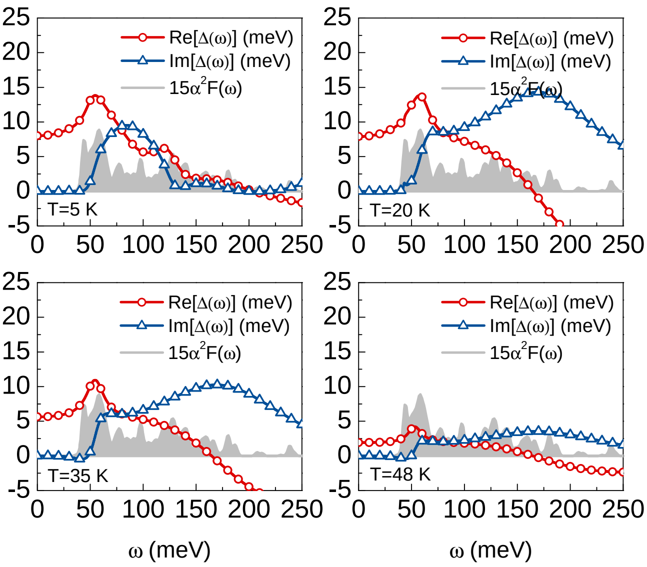

Fig. 3. The real and imaginary part of the order parameter as a function of frequency. The results are presented for selected values of temperature. The rescaled Eliashberg function for B_{10} superconductor at 400 GPa is also depicted.

On the basis of these results and by using the following expression:

$$\Delta(T) = \mathrm{Re}[\Delta(\omega = \Delta(T), T)], \tag{6}$$

where $\Delta(0)$ is assumed to be $\Delta(0) \simeq \Delta(T_0)$, the calculated $2\Delta(0)$ value equals 16.13 meV. Moreover, similarly as in the case of the previous calculations, we are able to determine the corresponding dimensionless ratio for the energy gap defined as:

$$R_{\Delta} \equiv 2\Delta(0)/k_{\mathrm{B}}T_{\mathrm{C}}. \tag{7}$$

In our case the calculated value amounts: $R_{\Delta} = 3.83$.

4. Summary

In the present paper we have determined the selected thermodynamic properties of the novel high-pressure B_{10} superconductor, by using the strong-coupling Eliashberg formalism.

In particular, for the chosen pressure value p = 400 GPa, the calculated value of the superconducting transition temperature is relatively high and equal to 48.86 K.

Moreover, we have analyzed the thermodynamic properties such as the thermodynamic critical field, the specific heat of the normal and superconducting state, and the energy gap at the Fermi level. Results obtained for these thermodynamic properties can be summarized by the calculated values of the corresponding dimensionless ratios: $R_{\mathrm{H}} = 0.156$, $R_{\mathrm{C}} = 1.75$, and $R_{\Delta} = 3.83$.

We note that within the Bardeen–Cooper–Schrieffer theory the characteristic dimensionless parameters take values: $R_{\mathrm{H}}^{\mathrm{BCS}} = 0.168$, $R_{\mathrm{C}}^{\mathrm{BCS}} = 1.43$, and $R_{\Delta}^{\mathrm{BCS}} = 3.53$. At this point we note that the differences between our results and the values predicted by the BCS theory arise due to the occurrence of the strong-coupling and retardation effects in the analyzed B_{10} superconductor. In what follows, our results point out that the B_{10} superconductor at $p = 400$ GPa cannot be properly described within the BCS theory.

Finally, the calculated electron effective mass is high and equal to 1.82 m_{e}.

References

[1] R. Szczęśniak, A.P. Durajski, *Solid State Sci.* **25**, 45 (2013).

[2] D.-W. Zhou, C.-Y. Pu, D. Szczęśniak, G.-F. Zhang, C. Lu, G.-Q. Li, J.-F. Song, *Chin. Phys. Lett.* **30** 027401 (2013).

[3] L. Shi, D.A. Papaconstantopoulos, *Phys. Rev. B* **73**, 184516 (2006).

[4] K. Shimizu, K. Amaya, N. Suzuki, *J. Phys. Soc. Jpn.* **74**, 1345 (2005).

[5] S. Deemyad, J.S. Schilling, *Phys. Rev. Lett.* **91**, 167001 (2003).

[6] M. Sakata, Y. Nakamoto, K. Shimizu, T. Matsuoka, Y. Ohishi, *Phys. Rev. B* **83**, 220512(R) (2011).

[7] R. Szczęśniak, D. Szczęśniak, *Phys. Status Solidi B* **249**, 2194 (2012).

[8] R. Szczęśniak, M.W. Jarosik, D. Szczęśniak, *Physica B* **405**, 4897 (2010).

[9] Y. Ma, J.S. Tse, D.D. Klug, R. Ahuja, *Phys. Rev. B* **70**, 214107 (2004).

[10] D. Li, K. Bao, F. Tian, X. Jin, D. Duan, Z. He, B. Liu, Tian Cui, *RSC Adv.* **4**, 203 (2014).

[11] M. Cyrot, D. Pavuna, *Introduction to Superconductivity and High-T_{C} Materials*, World Scientific, Singapore 1992.

[12] For the discussion of the Eliashberg formalism [originally formulated by G.M. Eliashberg *Sov. Phys. JETP* **11**, 696 (1960)] we refer to: J.P. Carbotte, *Rev. Mod. Phys.* **62**, 1027 (1990).

[13] J. Bardeen, L.N. Cooper, J.R. Schrieffer, *Phys. Rev.* **106**, 162 (1957).

[14] J. Bardeen, L.N. Cooper, J.R. Schrieffer, *Phys. Rev.* **108**, 1175 (1957).

[15] R. Szczęśniak, D. Szczęśniak, A.P. Durajski, *Solid State Commun.* **184**, 6 (2014).

[16] R. Szczęśniak, D. Szczęśniak, K.M. Huras, *Phys. Status Solidi B* **251**, 178 (2014).