Abstract

In the thesis the theoretical analysis of the superconducting phase has been conducted for the selected carbon-based materials (B_2C and CaC_6), for the hydrogen (atomic and molecular at the pressure of 414 GPa and 539 GPa, respectively), as well as for the hydrogen-rich B_2H_6 compound (at the pressure of 360 GPa). Due to the fact that, in the mentioned materials, the superconducting phase is induced by the electron-phonon pairing mechanism, and is characterised by the high value of the electron-phonon coupling constant, the numerical calculations has been conducted within the Eliashberg equations formalism. On the basis of the character of the electron pairing coupling and depairing correlations, the properties of a given systems have been described in the framework of the isotropic or anisotropic approach.

In particular, it has been shown that the low-dimensional B_2C compound is characterized by the critical temperature $T_C \in \langle 13,20.4 \rangle$ K, for the Coulomb pseudopotential values $\mu^\star \in \langle 0.1,0.2 \rangle$. By considering the specific form of the Eliashberg function as well as the possibility of the appearance of the van Hove singularity close or at the Fermi level, it has been stated that the value of T_C can be further raised. Moreover, it has been predicted that the dimensionless thermodynamic ratios are equal to: $R_\Delta \in \langle 3.87,3.79 \rangle$, $R_H \in \langle 0.155,0.157 \rangle$, and $R_C \in \langle 1.67,1.62 \rangle$, and do not deviate much from the BCS predictions. In the assumed notation, the R_Δ is the ratio of the value of the low-temperature order parameter to the critical temperature, R_H corresponds to the low-temperature value of the critical field, and the R_C ratio is directly related to the specific heat of the superconducting state.

In the case of the second carbon-based material, namely the CaC_6 compound, the numerical calculations have been conducted within the one- and three-band Eliashberg formalism (bands denoted respectively as a, b, and c). It has been shown that the anisotropy of the interactions strongly influences the value of the order parameter. In particular, for the isotropic case the low-temperature order parameter value equals 1.855 meV, whereas in the anisotropic case it amounts: 1.180 meV, 2.364 meV, and 1.864 meV. In the case of the order parameter, the calculated dimensionless thermodynamic ratios for the one-band case are: $R_\Delta = 3.77$, and for the three-band case: $R_\Delta^a = 2.40$, $R_\Delta^b = 4.83$, and $R_\Delta^c = 3.80$. Qualitatively, similar effect has been observed for the value of the electron effective mass ($m_e^\star$), *i.e.*

in the anisotropic case: $m_e^\star = 1.831 m_e$, and for the anisotropic case: $(m_e^\star)^a = 1.682\,(m_e)^a$, $(m_e^\star)^b = 2.258\,(m_e)^b$, and $(m_e^\star)^c = 1.930\,(m_e)^c$, where m_e denotes electron band mass. It has been also proved that the anisotropy of the interactions leads to the notable decrease of the value of the low-temperature thermodynamic critical field, but does not affects the value of the jump of the specific heat at the critical temperature.

The multi-band calculations have been also conducted for the metallic molecular hydrogen at $p = 414$ GPa. Within the three-band model, it has been stated that $T_C = 84$ K. The values of the dimensionless ratio R_Δ respectively equals: 5.55, 3.96, and 3.53. I should be noted that the first of the listed values strongly deviates from the BCS predictions. Obtained results confirmed also that the discussed anisotropy notably influences values of the normalized total electronic density of states, the thermodynamic critical field, the difference of the free energy, as well as the difference of the specific heat between the superconducting and normal state. At the same time, it has been observed that the isotropic results which can be found in the literature are underestimated. Finally, the maximum values of the electron effective mass in the given band equals: $(m_e^\star)^a = 2.99\,(m_e)^a$, $(m_e^\star)^b = 2.10\,(m_e)^b$, and $(m_e^\star)^c = 1.94\,(m_e)^c$.

Due to the lack of the electron-phonon and electron-electron interactions anisotropy, the thermodynamic properties of the supercondcuting phase in the atomic hydrogen ($p = 539$ GPa), have been analysed within the one-band Eliashberg formalism. It has been shown that the superconducting condensate is characterized by the very high value of the critical temperature ($T_C = 356$ K), which is much higher then the one predicted for the $p = 414$ GPa case. Furthermore, the values of the corresponding thermodynamic ratios amount: $R_\Delta = 4.95$, $R_H = 0.126$, and $R_C = 2.78$, and deviates from the BCS predictions.

In the last step, the thermodynamic properties of the superconducting state have been discussed for the B_2H_6 hydrogen-rich compound at the pressure value of 360 GPa. The numerical calculations have been conducted in the framework of the one-band Eliashberg equations. It has been observed that regardless of the value of the Coulomb pseudopotential, the critical temperature is high and equals: $T_C \in \langle 147{,}87 \rangle$ K, for $\mu^\star \in \langle 0.1, 0.3 \rangle$. It has been also shown, that the dimensionless thermodynamic properties present strong discrepancies when compared to the BCS predictions. This effect is especially visible for the low values of the Coulomb pseudopotential: $R_\Delta \in \langle 4.24{,}3.98 \rangle$, $R_C \in \langle 2.33{,}2.17 \rangle$, and $R_H \in \langle 144{,}0.168 \rangle$.

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