Abstract

The mainstream of superconductivity research is the search for materials with the highest possible critical temperature, which is related to their potential use for industrial purposes. In this context, Ashcroft's thesis indicating hydrogen as a high-temperature superconductor and suggesting its combination with heavier elements to induce chemical precompression and reduce the external pressure necessary to obtain the superconducting phase proved to be groundbreaking. As it turns out, most superconductors with high transition temperatures to the superconducting state are characterised by a high value of the electron-phonon coupling constant, therefore the standard BCS model cannot be used in their theoretical analysis. In the framework of the dissertation, the results of studies on superconducting systems within the framework of the classical and multiband Eliashberg formalism are presented, and then an attempt is made to generalise the model to cases where another non-trivial interaction is additionally present.

In the first part of the dissertation, the classical Eliashberg formalism is presented as a theory which can be applied in the analysis of superconductors with significant strong coupling and retardation effects. Using the above-mentioned model, the properties of the superconducting state induced in selenium and tellurium under high pressure conditions were analysed. The obtained results, in comparison with literature data, allowed concluding that in the discussed elements a structural transformation occurs above pressures of 248 GPa and 67 GPa, respectively. Moreover, the temperature of the transition into the superconducting state is higher than previously predicted: 8.13 K for selenium and 5.96 K for tellurium.

In the next step, the multiband Eliashberg formalism is presented, which is a generalisation of the classical model that allows correct determination of the properties of the superconducting state in systems exhibiting anisotropy of electron-phonon interaction. Calcium intercalated graphite, in which the Fermi surface can be divided into six effective bands, was chosen for the analysis. In particular, areas between the carbon layers can be distinguished where the electron-phonon coupling is much smaller than within the individual planes. An in-depth analysis showed that, in the case of CaC_6 compound, the number of bands included in the calculation has a significant effect on the results obtained for low temperatures, while near the critical temperature the six-band approach

gives very similar results to the one- and three-band approaches.

The third chapter is devoted to the analysis of the superconducting state in hydrogen-rich compounds. Two high-pressure systems - hydrogen and thorium and hydrogen and lanthanum - are discussed in detail. It is shown what stable structures will be formed at pressures in the range 0-300 GPa with varying content of individual atoms and then their superconducting properties are investigated. The choice of the analysed systems was dictated by Ashcroft's thesis suggesting the existence of high critical temperature values at relatively low pressures in compounds combining hydrogen with heavier elements. In turn, high-temperature superconductors are usually characterised by non-standard properties (including a high electron-phonon coupling constant), so the formalism of Eliashberg equations was used for the analysis.

Analysing the Th-H system, eight structures not previously reported in the literature were found, two of which are high-temperature superconductors ($P2_1/c - ThH_7$, $Fm\bar{3}m - ThH_{10}$), characterised by high electron-phonon coupling constants (0.84 and 2.5, respectively). Particularly promising was the $Fm\bar{3}m - ThH_{10}$, in which hydrogen atoms form cubic cages around thorium atoms giving a contribution to the phonon density of states over a wide frequency range. An in-depth analysis using the formalism of Eliashberg equations showed that ThH_{10} transitions to a superconducting state at $T_C = 241.2$ K. Furthermore, this compound is characterised by a high energy gap ($\Delta_g = 104$ meV) and electron effective mass ($m_e^* = 3.63\ m_e$). It should be noted that this superconductor achieves a high critical temperature at relatively low pressure (100 GPa) - for comparison, H_3S and $C - S - H$ achieve similar critical temperatures ($[T_C]_{H_3S} = 204$ K, $[T_C]_{C-S-H} = 288$ K) at pressures of 200 and 267 GPa, respectively.

During the analysis of the La-H system, the main focus was on explaining the discrepancies obtained during experimental studies. For this purpose, the critical temperatures of all the structures that become stable under pressure were theoretically determined. It was found that the experimentally observed transition to the superconducting state at 112 K can be explained by the formation of systems with stoichiometry LaH_5, LaH_8 or LaH_9. The subsequent metal-superconductor phase transition, observed at 215 K, can be explained by LaH_4, LaH_6, LaH_7 and LaH_{10} (occurring in the space group $R\bar{3}m$), while the disappearance of electrical resistance at the record high critical temperature of 260 K explains LaH_{10} in another structural arrangement - $Fm\bar{3}m$. In addition, during the study a previously unknown stable system $P6mmm - LaH_{16}$ was discovered, which is also a high-temperature superconductor. Depending on the pressure (200-300 GPa), its critical temperature varies in the range 118-156 K.

In the last part of the dissertation, the influence of spin-orbit coupling on the phonon-induced superconducting state which is created on model two-dimensional lattices (square and triangular) was analysed. In the first step Eliashberg functions, phonon and electron densities of states and electron-phonon coupling constants were analytically determined

for different values of γ_0 parameter modelling spin-orbit interaction. The obtained results allowed finding the critical values of γ_0, for which the superconducting state is characterized by the highest critical temperature (resulting from high electron density of states and strong interaction of electrons with crystal lattice vibrations). The analytically determined maximum critical temperatures for square and triangular lattices are 133.5 K and 20.4 K, respectively. It should be clearly emphasised that the Allen-Dynes formula is based on strong approximations, therefore, in the next step the Eliashberg equations taking into account the chemical potential and the full form of the electron density of states were applied to determine the parameters of the superconducting state. The results obtained showed that the critical temperature for a square lattice would be much lower than predicted (38.4 K) while on a triangular lattice the superconducting phase would not be induced (as indicated by the zero value of the order parameter).

Special attention should be paid to the fact that the Eliashberg formalism, despite being the most accurate model for the analysis of systems with strong electron-phonon coupling, is not adapted directly to the study of the consequences of the existence of additional interactions in the system. For this reason, an attempt has been made within the framework of the dissertation to generalise the classical formalism in such a way as to take into account the existence of spin-orbit coupling. For this purpose, the Nambu spinors used to derive the equations were extended to four-component operators and the Rashba-type spin-orbit coupling components were added to the Hamiltonian. The obtained model, in spite of its very complicated form, can be used in the future not only for accurate analysis of real systems with significant spin-orbit interactions but also as a first step to create other generalized models for the analysis of phonon-induced superconducting state taking into account additional non-trivial interactions (such as correlated electron clusters or magnetic admixtures).

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