Abstract of the doctoral thesis

The doctoral dissertation concerns the issue of superconducting state induction in metallic hydrogen and other selected hydrogen-containing systems (H_2S, H_5S_2, H_4S_3, LaH_{10}, C-S-H). The dissertation consists of seven chapters.

The first chapter contains an overview of the literature on the subject. It is mainly based on publications including characterization of the superconducting state in hydrogen and selected hydrogen-rich compounds.

The second chapter presents a quantum description of the physical properties of the hydrogen molecule. The discussed results are an introduction to a full understanding of how to describe the superconducting properties of metallic hydrogen.

In the next chapter, the properties of the superconducting state potentially induced in hydrogen are analyzed. Due to the enormous mathematical complexity of the issue, *ab initio* calculations were carried out for the model of two compressed hydrogen planes. All physically relevant electron correlation channels have been considered (U and K). Additionally, there were considered the non-conventional electron-phonon coupling functions (g_U and g_K), related directly to the on-site and the inter-site Hubbard interactions.

The thermodynamic properties of the superconducting state were determined within the Eliashberg formalism. Based on *ab initio* calculations, the form of the isotropic Eliashberg function was determined, and then the input parameters to the Allen-Dynes formula. In this chapter, it is shown that a superconducting state can be induced in the studied system: in the harmonic approximation with a maximum critical temperature value of about 200 K, or in the more exact anharmonic approach 84 K ($F = 3$ Ry/a_0). It has been proved that the effective value of the depairing electronic correlations in the metallic hydrogen is relatively low ($\mu^\star_H \sim \mu^\star_M \sim 0.17$) and is only weakly dependent on the compressive force F. Based on the performed calculations, it was found that a correctly selected value of $\mu^\star$ significantly reduces the value of the critical temperature in relation to that obtained for $\mu^\star = 0.1$. It is worth noting that the calculated values of the critical temperature correlate well with the literature values and with the maximum critical temperatures measured experimentally for H_3S and LaH_{10}.

The determined thermodynamic parameters of the superconducting state in hydrogen, despite the high T_C, assume values for which the dimensionless thermodynamic ratios R_Δ,

R_C, R_H and R_{H2} differ only slightly from the values predicted by the mean-field BCS theory.

Critical analysis of the issue led to the conclusion that the induction of a superconducting state in metallic hydrogen with a T_C value comparable to room temperature is not possible.

The fourth chapter presents the classical electron-phonon Eliashberg formalism, based on the analysis of the superconducting phase inducing in the YB_6 system. This system was chosen as an example only to illustrate how to perform the analysis. The superconducting state in YB_6 compound is characterized by a relatively low value of the critical temperature. Nevertheless, its thermodynamic properties clearly differ from the predictions of the BCS model. This fact is associated with significant strong-coupling effects and retardation effects occurring in yttrium hexaboride ($k_B T_C/\omega_{\ln} \sim 0.1$).

The presented classical Eliashberg formalism was used to describe high-temperature superconducting states in subsequent chapters of the dissertation.

In the fifth chapter of the doctoral dissertation, the thermodynamic properties of the superconducting phase of the H_5S_2 system within the classical Eliashberg formalism were determined. Very high values of the Coulomb pseudopotential ($\mu^\star$) were obtained. Then the classical Eliashberg analysis was extended, the vertex corrections for the electron-phonon interaction were taken into account. Moreover, the parameters of the superconducting state induced in the H_4S_3 and H_2S systems were analyzed. It is worth noting that in addition to the experimental results for H_3S in the $T_C - p$ chart, there are also experimental points corresponding to much lower values of T_C, that may come from another compound. Potential candidates are H_2S, H_5S_2 and H_4S_3. The performed calculations showed that H_2S is responsible for the experimentally observed superconductivity in the sulfur-hydrogen system for samples prepared at low temperature.

The next chapter contains some interesting results and insights. Due to the fact that in the system with LaH_{10} stoichiometry the induction of the superconducting state with the critical temperature values close to room temperature was experimentally confirmed, the thermodynamic parameters of this superconductor were determined in the dissertation. It has been shown that the superconducting state is characterized by a strong electron-phonon coupling and is not of the BCS type.

The chapter also presents criteria that may help in the future to find a material with the desired high-temperature superconducting properties. Selected compounds of the $La_\delta X_{1-\delta}H_{10}$-type (LaXH-type) were investigated for selection of a system with an even higher critical temperature value. It has been proved that an appropriate doping the system can lead to the induction of the superconducting state at room temperature (LaScH and LaYH are potential candidates).

Due to the experimental confirmation of room temperature superconductivity in the C-S-H system, the dissertation was expanded to include a seventh chapter. This chapter

contains an analysis of possible scenarios responsible for the induction of superconductivity in the C-S-H system. It has been shown that the superconducting state in C-S-H can be induced by a strong electron-phonon interaction, as for the LaH_{10}, H_3S and YH_6 superconductors. The anomalously high value of $\omega_{\ln}/k_B = 7150$ K, excludes the realization of the intermediate (or weak) electron-phonon coupling scenario in the tested superconductor. Eliashberg formalism suggests a low value of the Ginzburg-Landau parameter: $[\kappa]_{\text{C-S-H}} = 1.73$, as for other high-temperature superconductors containing hydrogen: $[\kappa]_{LaH_{10}} = 1.60$, $[\kappa]_{H_3S} = 1.53$, $[\kappa]_{YH_6} = 1.34$. The chapter presents results showing that the conclusions of Hirsch and Marsiglio, based on the fact that the calculations were performed using weak electron-phonon coupling formulas, are incorrect.

The dissertation ends with a summary of the results, a scientific literature list, and a list of figures.

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