ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF TOPOLOGICAL INSULATORS Bi_2Te_3 AND Bi_2Se_3

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Bismuth chalcogenides Bi_2Te_3 and Bi_2Se_3 are typical representatives from the family of topological insulators. With the help of external influence (magnetic field, temperature, pressure, etc.), their electronic structure can be changed and, consequently, their physical properties can be modified. This, in turn, can be used in various devices. Due to their special surface states, Bi_2Te_3 and Bi_2Se_3 have great potential applications in spintronic and thermoelectric devices, biological and chemical sensors, as well as in photonic and optoelectronic applications. Therefore, obtaining new knowledge about the features of electronic structure and electronic transport in such topological materials is of great interest, and such studies are relevant both from a fundamental and applied point of view.

Theoretical calculations of the electronic structure of Bi_2Te_3 and Bi_2Se_3 compounds were carried out within the framework of the density functional theory, taking into account spin-orbit coupling [1]. A band gap was obtained in the band structure of the compounds, in Bi_2Te_3 its width was 0.48 eV, and in Bi_2Se_3 – 0.41 eV, which are consistent with previous calculations. To account for the various temperature values at which experimental studies were conducted, the crystal structure parameters at the corresponding temperature values [2] and temperature smearing were used, which led to a small electron density at the Fermi energy E_F. The density of electronic states at the Fermi level $N(E_F)$ is one of the most important characteristics and is closely related to many electronic properties, in particular, to the concentration of current carriers n. Also in this work, the temperature dependences of electrical resistance and Hall resistance of single crystals of topological insulators Bi_2Te_3 and Bi_2Se_3 were measured in the temperature range from 4.2 to 300 K and in magnetic fields up to 10 T [1]. It was found that the concentration of current carriers n depends on temperature in different ways [3,4]: in the case of Bi_2Te_3, n increases with temperature, however, it is almost temperature independent for Bi_2Se_3. One of the possible reasons for the different behavior of the $n(T)$ dependencies may be the different behavior of the density of states at the Fermi level with a change in temperature. As a result of the analysis of our theoretical and experimental data of the conducted studies, a correlation was found between the density of electronic states at the Fermi level and the concentration of current carriers. In the case of Bi_2Te_3, the density of states at the Fermi level and the concentration of current carriers increases with increasing temperature. On the contrary, the opposite trend is observed for Bi_2Se_3 – both characteristics decrease with increasing temperature.

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