Peculiarities of the electronic transport in topological materials of Bi$_2$Se$_3$ and Mo$_x$W$_{1-x}$Te$_2$ ($x = 0; 0.5; 1$)

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Abstract. The electrical resistivity of thin films of a topological insulator of Bi$_2$Se$_3$ with a thickness of 10 nm to 75 nm, single crystal of Bi$_2$Se$_3$ with thickness of 0.65 mm and single crystals of topological Weyl semimetals Mo$_x$W$_{1-x}$Te$_2$ ($x = 0; 0.5; 1$) in the temperature range from 4.2 to 300 K was measured. A size effect in the electrical conductivity of Bi$_2$Se$_3$ films was observed, i.e. linear dependence of the conductivity of the film on its reciprocal thickness. It is suggested the existence of two different conduction channels in the Mo$_{0.5}$W$_{0.5}$Te$_2$ compound.

1. Introduction

In recent years new quantum materials with a topologically nontrivial band structure resulting from strong spin-orbit interaction have been predicted theoretically and discovered experimentally. First of all, these are topological insulators (TI) [1]. In these compounds there is an energy gap in the bulk of the material, characteristic of an insulator, and protected gapless conducting states on its surface. Such materials include Bi$_2$Se$_3$, Bi$_2$Te$_3$, Sb$_2$Te$_3$ and etc. The rigid coupling between the directions of the pulse and the electron spin leads to the appearance of spin polarization of charge carriers and the possibility of spin-polarized current flowing near the surface of the TI with virtually no losses [1]. In addition, the presence of such unique surface states in topological insulators [2, 3] makes them promising materials for the creation of electronic devices with high speed and low power consumption. Other promising materials are the recently discovered topological Weyl semimetals (TWS) with nontrivial charge transfer, both in the volume and on the surface of such materials [4, 5]. A characteristic feature of Weyl's semimetals is the presence of exotic gapless surface states — Fermi arcs. The quasiparticles in the bulk of Weyl semimetals are “massless” Weyl fermions [2], with a ”zero” effective mass, which are also protected topologically. This means that such quasiparticles can be controlled much faster than conventional charge carriers, and the probability of their scattering is sufficiently small. Later it was found that the properties of Weyl semimetals occur in other compounds, such as semimetallic dichalcogenides of transition metals MoTe$_2$, WTe$_2$ and ternary compounds Mo$_x$W$_{1-x}$Te$_2$ [4-6]. It is known [7-9] that the WTe$_2$ compound usually exhibits semimetallic properties and has a “metallic” type of temperature dependence of the electroresistivity $\rho(T)$, whereas the MoTe$_2$ has a “semiconductor” dependence $\rho(T)$.

Apparently, the above mentioned peculiarities of topological insulators and Weyl semimetals, i.e., a significant difference between bulk and surface as well as the different nature and type of conductivity, should manifest themselves in the electronic transport of such materials, in particular, in...
the electroresistivity. The aim of this report is to study the features of the electronic transport in a topological insulator of Bi$_2$Se$_3$ and Weyl semimetals of Mo$_x$W$_{1-x}$Te$_2$ (x = 0; 0.5; 1).

2. Experimental

Thin films of Bi$_2$Se$_3$ were grown by the molecular beam epitaxy method on Al$_2$O$_3$ substrates [10, 11] with thickness from 10 to 75 nm. Single crystal (SC) of Bi$_2$Se$_3$ with thickness 0.65 mm was cleaved from a boule grown by melting stoichiometric mixtures of high-purity elemental Bi and Se. Mo$_x$W$_{1-x}$Te$_2$ single crystals (x = 0; 0.5; 1) were grown by the method of chemical vapor transport using Br$_2$ as a transport agent. The XRD data and the atomic content of elements analysis showed the synthesized samples of TI have Bi$_2$Se$_3$ composition (see Refs. [10, 11]), and samples of TWS have Mo$_x$W$_{1-x}$Te$_2$ (x = 0, 0.5, 1) composition (see Refs. [12]). The atomic content of elements was measured by a scanning electron microscope equipped with an EDAX X-ray microanalysis attachment. Our examination showed that the deviations from a stoichiometric composition were insignificant in all samples. The measurements of the electroresistivity were carried out by the conventional 4-points method at dc-current in the temperature range from 4.2 to 80 K and in magnetic fields of up to 10 T. The results are presented in units of conductivities $\sigma_0 \approx 1/\rho_0$ and $\sigma_{xx} \approx 1/\rho_{xx}$, since $\rho_{xx} \gg \rho_{xy}$ (see also Refs. [7-9]).

3. Results

Figure 1a shows the temperature dependence of the electroconductivity for Bi$_2$Se$_3$ samples. One can see the conductivity value depends on a sample dimension. Since the conductivities of TIs in a bulk and near the surface differ significantly, TI can be represented as a system of two parallel-connected conductors: a “metal” surface and a “semiconductor” bulk (see [13, 14] and references therein). As was shown in [13], the conductivity $\sigma$ of such a system can be represented as:

$$\sigma \approx \sigma_{surf} \cdot \frac{\delta}{d} + \sigma_{bulk} \quad (1)$$

Where $\sigma_{surf}$ is a surface conductivity of the subsurface layer with a thickness of $\delta$, $\sigma_{bulk}$ is a bulk conductivity. Thus, the dependence of conductivity $\sigma$ on the inverse film thickness $d^{-1}$ should be observed, i.e. $\sigma = f(d^{-1})$.

As a result of the experiments performed, a size effect was discovered, i.e. the dependence of the conductivity on the inverse film thickness. Figure 1b shows the dependence of the conductivity at $T = 4.2$ K on the inverse thickness of the samples of TI Bi$_2$Se$_3$.

![Figure 1(a, b). (a) Temperature dependence of conductivity of TI Bi$_2$Se$_3$ films and SC; (b) Size effect in TI Bi$_2$Se$_3$ without a magnetic field at T = 4.2 K.](image)
By plotting the graphs presented in fig. 1b for the temperature range, it is possible to calculate the temperature dependences for the bulk and surface contributions to the total conductivity. As shown in [13], the “surface” of Bi$_2$Se$_3$ thin films has a metallic conductivity, while the “bulk” is a semiconductor one. However, if we consider a situation where, in addition to thin films, we have a “thick sample,” the situation changes drastically. In this case, the “bulk” of sample also acquires a metallic conductivity type.

In topological materials there are exotic features in electronic transport, for example, in electrical conductivity. In topological insulators, these are significant differences in surface and bulk conductivity. Weyl semimetals of Mo$_x$W$_{1-x}$Te$_2$ composition also have interesting features in conductivity. The WTe$_2$ compound has orthorhombic symmetry, however, the MoTe$_2$ compound can crystallize, depending on the cooling rate, with both orthorhombic symmetry and hexagonal. In the case of orthorhombic symmetry, the compound has a metallic conductivity type, and in the case of hexagonal symmetry, it is semiconductor. Figure 2 shows the temperature dependence of conductivity for WTe$_2$ (a) and MoTe$_2$ (b) compounds.

![Figure 2(a, b). (a) Temperature dependence of conductivity TWS WTe$_2$; (b) Temperature dependence of conductivity TWS MoTe$_2$.](image)

In the case of the Mo$_{0.5}$W$_{0.5}$Te$_2$ ternary compound, it can be assumed that there are two different conduction channels in this compound: the “metallic” conductivity from WTe$_2$ and the “semiconductor” conductivity from MoTe$_2$. Figure 3 shows the experimental temperature dependence of the conductivity of the Mo$_{0.5}$W$_{0.5}$Te$_2$ compound in comparison with the calculated curve obtained by summing the conductivities of WTe$_2$ and MoTe$_2$ with the corresponding weighting factors.

As seen from Fig. 3, the experimental and calculated curves have quite similar behaviour and the conductivity values are in a good agreement too. Apparently, the proposed assumption about the presence of two conduction channels due to the presence of charge carriers of a “semiconductor” and “metallic” type can occur in the Weyl semimetal Mo$_{0.5}$W$_{0.5}$Te$_2$. However, this requires further experimental and theoretical studies.
Figure 3. Temperature dependence of conductivity TWS $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$ ($x = 0; 0.5; 1$) in comparison with the calculated curve (y-axis on the right).

4. Conclusions
The peculiarities of the electroconductivity in the TI Bi$_2$Se$_3$ and TWS $\text{Mo}_{0.5}\text{W}_{0.5}\text{Te}_2$ were observed and studied. It was shown that it possible to experimentally “separate” the bulk and surface contributions into the conductivity of the TI Bi$_2$Se$_3$. It was found that the value of the surface contribution by almost an order of magnitude exceeds the value of the bulk. The obtained results can be used for “separation” and evaluation of the values of surface and bulk conductivity also in other TIs and systems with non-uniform distribution of direct current over the cross section of the sample. It is suggested the existence of two different conduction channels in the $\text{Mo}_{0.5}\text{W}_{0.5}\text{Te}_2$ compound. Comparison of calculations with experiment shows a fairly good consistency.

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References
[1] Zhang H, Liu C X, Qi X L, Dai X, Fang Z, Zhang S C 2009 Nat. Phys. 5 438
[2] Xu S Y, Belopolski I, Alidoust N, Neupane M, Bian G, Zhang C, Sankar R, Chang G, Yuan Z, Lee C, Huang S, Zheng H, Ma J, Sanchez D S, Wang B, Bansil A, Chou F, Shibayev P P, Lin H, Jia S, Hasan M Z 2015 Science 349 6248
[3] Liu Z K, Yang L X, Sun Y, Zhang T, Peng H, Yang H F, Chen C, Zhang Y, Guo Y F, Prabhakaran D, Schmidt M, Hussain Z, Mo S K, Felser C, Yan B, Chen Y L 2016 Nat. Mat. 15 27
[4] Huang L, McCormick T M, Ochi M, Zhao Z, Suzuki M T, Arita R, Wu Y, Mou D, Cao H, Yan J, Trivedi N, Kaminski A 2016 Nat. Mat. 15 1155
[5] Li P, Wen Y, He X, Zhang Q, Xia C, Yu Z M, Yang S A, Zhu Z, Alshareef H N, Zhang X X 2017 Nat. Commun. 8 2150
[6] Belopolski I, Sanchez D S, Ishida Y, Pan X, Yu P, Xu S Y, Chang G, Chang T R, Zheng H, Alidoust N, Bian G, Neupane M, Huang S M, Lee C C, Song Y, Bu H, Wang G, Li S, Eda G, Jeng H T, Kondo T, Lin H, Liu Z, Song F, Shin S, Hasan M Z 2016 Nat. Commun. 7 13643
[7] Volkenshtein N V, Glinski M, Marchenkov V V, Startsev V E, Cherepanov A N 1989 Sov. Phys. JETP 68 1216
[8] Marchenkov V V, Cherepanov A N, Startsev V E, Czurda C, Weber H W 1995 J. Low Temp. Phys. 98 425
[9] Marchenkov V V, Weber H W, Cherepanov A N, Startsev V E 1996 J. Low Temp. Phys. 102 133
[10] Liu Y H, Chong C W, Jheng J L, Huang S Y, Huang J C A, Li Z, Qiu H, Huang S M, Marchenkov V V 2015 Appl. Phys. Lett. 107 012106
[11] Liu Y, Chong C, Chen W, Huang J C A, Cheng C, Tsuei K, Li Z, Qiu H, Marchenkov V V 2017 Jpn. J. Appl. Phys. 56 070311
[12] Marchenkov V V, Domozhirova A N, Makhnev A A, Shreder E I, Naumov S V, Chistyakov V V, Huang J C A, Eisterer M 2019 Low temperature physics 45 241
[13] Marchenkov V V, Chistyakov V V, Huang J C A, Perevozchikova Y A, Domozhirova A N, Eisterer M 2018 EPJ Web of Conferences 185 01002
[14] Marchenkov V V, Weber H W 2003 J. Low Temp. Phys. 132 135