Role of bulk and surface current carriers in resistivity of thin films of the topological insulator Bi₂Se₃

Alexandra N. Perevalova^a, Bogdan M. Fominykh, Vasiliy V. Chistyakov, Vyacheslav V. Marchenkov^b

M.N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, 620108 Ekaterinburg, Russia

^adomozhirova@imp.uran.ru, ^bmarch@imp.uran.ru

Corresponding author: Alexandra N. Perevalova, domozhirova@imp.uran.ru

PACS 73.50.-h, 73.63.-b

ABSTRACT The temperature dependences of the electrical resistivity of topological insulator Bi_2Se_3 thin films with thicknesses of 20 and 40 nm were measured in the temperature range from 4.2 to 80 K. Their resistivity was shown to depend on thickness. A method was proposed for "separation" of the bulk and surface resistivity of films, with the help of which corresponding estimates were made. It was demonstrated that the surface resistivity is more than two orders of magnitude less than the bulk resistivity at T = 4.2 K.

KEYWORDS thin films, Bi₂Se₃, topological insulator, electrical resistivity, bulk and surface resistivities

ACKNOWLEDGEMENTS The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (theme "Spin" No. 122021000036-3). The authors thank J. C. A. Huang for providing thin films and E. B. Marchenkova for assistance in their characterization.

FOR CITATION Perevalova A.N., Fominykh B.M., Chistyakov V.V., Marchenkov V.V. Role of bulk and surface current carriers in resistivity of thin films of the topological insulator Bi₂Se₃. *Nanosystems: Phys. Chem. Math.*, 2024, **15** (4), 465–468.

1. Introduction

Topological insulators attract the attention of a large number of researchers due to their unusual electronic band structure and the possibility of application in spintronics and other fields [1, 2]. Topological insulators are materials that have an energy gap in the bulk and gapless states with a linear dispersion law, called the Dirac cone, on the surface. Surface states arise due to band inversion in the bulk in the presence of strong spin-orbit interactions and are protected by time-reversal symmetry. Their existence can be explained by the fact that when a topological insulator is in contact with an ordinary insulator (including vacuum) having the opposite band order, the gap closes at the boundary as the topology changes from nontrivial to trivial. Therefore, "metallic" states always exist on the surface of a topological insulator [3–5]. The current carriers in the near-surface "metallic" layer are massless Dirac fermions, the spin of which is locked to the momentum. Such carriers are protected from scattering by defects and non-magnetic impurities. Typical representatives of three-dimensional topological insulators are bismuth selenide and bismuth telluride [6, 7]. These compounds have relatively large band gap values of ~0.2 – 0.3 eV, which is important for practical applications.

Bismuth chalcogenides, including Bi_2Se_3 and Bi_2Te_3 , are layered compounds with a rhombohedral lattice (space group $R\bar{3}m$). The crystal structure can be represented as a set of quintuple layers (QL) perpendicular to the c axis. Each QL consists of five atomic layers alternating in the sequence Se(Te)1-Bi-Se(Te)2-Bi-Se(Te)1. Within a QL, atoms have strong ionic or covalent bonds, but QLs are bound together by weak van der Waals forces. The height of a QL is ~1 nm. Using angle-resolved photoemission spectroscopy (ARPES), it was shown that Bi_2Se_3 films exhibit a Dirac dispersion law on the surface, i.e. they manifest the properties of a topological insulator, at a thickness of 5 nanometers or more, which corresponds to 5 or more QLs [4].

Currently, there is a large number of works devoted to the study of the electronic structure and transport properties of topological insulators (see, for example, [6-12]). One of the main methods for studying Dirac surface states is ARPES, which allows one to directly observe the presence of Dirac cones on the surface of a topological insulator [7,10]. However, this method places fairly high demands on the quality of samples. Another effective way is to analyze the quantum oscillations in magnetoresistivity and Hall resistivity [11, 12]. This method allows one to estimate the Berry phase and determine which current carriers, surface or bulk, dominate in magnetotransport, as well as estimate their parameters, such as concentration, mobility and effective mass. Determination of the contribution of surface and bulk current carriers to the transport properties of topological insulators could be useful for practical applications. It was experimentally demonstrated in [13] that the conductance of Bi₂Se₃ nanodevices is determined by parallel surface and bulk contributions. Therefore,

the question arises about the possibility of "separation" of the contributions to conductivity (resistivity) from the bulk and surface in such materials.

In this work, a relatively simple method is proposed for "separation" of the bulk and surface resistivities of topological insulator films, with the help of which corresponding estimates are made for Bi_2Se_3 thin films.

2. Experiment

Thin films of the topological insulator Bi_2Se_3 with thicknesses of 20 and 40 nm were synthesized by molecular beam epitaxy on Al_2O_3 substrates.

Determination of the chemical composition of the films and measurements of the temperature dependences of the electrical resistivity $\rho(T)$ were carried out at the Collaborative Access Center "Testing Center of Nanotechnology and Advanced Materials" of M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences. The chemical composition of the thin films was confirmed by energy dispersive X-ray microanalysis (EDXMA) using a Quanta 200 scanning microscope with an EDXMA attachment (Table 1). It can be seen that the composition is close to nominal.

TABLE 1.	Results of	f the ana	vsis o	of the	chemical	composition	of the	Bi ₂ Se ₂	films
TUDDD I.	reound o	i une unu	, , , , , , , , , , , , , , , , , , , ,	1 1110	onounoun	composition	or the	D1/000	111110

Film thickness nm	Content of chemical element, at.%				
	Bi	Se			
20	40.05	59.95			
40	39.62	60.38			

Electrical resistivity ρ was measured at direct current using the four-point method with switching the direction of the current through the sample (see, for example, [14]) at temperatures from 4.2 to 80 K.

3. Results and discussion

Figure 1 shows the temperature dependences of the resistivity ρ for two films of Bi₂Se₃ with thicknesses of 20 and 40 nm. It can be seen that the resistivity values of the films differ significantly and depend on their thickness. Thus, for the 20 nm-thick film, the electrical resistivity increases from 215 to 282 $\mu\Omega$ ·cm, and for the 40 nm-thick film, it increases from 420 to 523 $\mu\Omega$ ·cm in the temperature range from 4.2 to 80 K. It can be assumed that the difference in resistivity values is due to the difference in the "surface/bulk" ratio for the two films, that is, a significant difference in the values of bulk and surface conductivities. Similar effects were observed in [15, 16] for thin films of Bi₂Se₃ and Bi₂Te₃.



FIG. 1. Temperature dependences of the electrical resistivity of the thin films of the topological insulator Bi_2Se_3 with thicknesses of 20 nm (a) and 40 nm (b)

One can try to estimate the contributions of surface and bulk resistivity (conductivity) to the total resistivity (conductivity) of the Bi_2Se_3 films under study. Fig. 2 schematically shows the cross sections of the two films. Since surface and bulk conductivities in topological insulators can differ significantly, the total conductivity can be represented as a parallel connection of conductors. In this case, the resistances R_1 and R_2 of topological insulator thin films can be expressed as follows:

$$\frac{1}{R_1} = \frac{1}{\rho_1} \cdot \frac{a \cdot d_1}{L} \approx \frac{1}{\rho_{\text{bulk}}} \cdot \frac{a \cdot d_1}{L} + \frac{1}{\rho_{\text{surf}}} \cdot \frac{2\delta \cdot a}{L},\tag{1}$$

Role of bulk and surface current carriers in resistivity of thin films of the topological insulator Bi₂Se₃

 $\rho_{\mathfrak{t}}$

$$\frac{1}{R_2} = \frac{1}{\rho_2} \cdot \frac{b \cdot d_2}{L} \approx \frac{1}{\rho_{\text{bulk}}} \cdot \frac{b \cdot d_2}{L} + \frac{1}{\rho_{\text{surf}}} \cdot \frac{2\delta \cdot b}{L}.$$
(2)

Here ρ_1 and ρ_2 are resistivities of the first and second films (Fig. 2); d_1 and d_2 are their thicknesses; a and b are widths of the films; δ is a thickness of the near-surface "metallic" layer, which is much less than the thickness of the films; L is a distance between potential contacts; ρ_{surf} and ρ_{bulk} are surface and bulk resistivities, respectively. It is easy to show that ρ_{surf} and ρ_{bulk} can be represented as:

$$\rho_{\text{surf}} \approx \frac{2\delta \left(\frac{1}{d_1} - \frac{1}{d_2}\right)}{\rho_1^{-1} - \rho_2^{-1}},\tag{3}$$

$$_{\text{nulk}} \approx \frac{d_2 - d_1}{\frac{d_2}{\rho_2} - \frac{d_1}{\rho_1}}.$$
(4)

467



FIG. 2. Schematic representation of the cross-section of two films of a topological insulator: d_1 and d_2 are thicknesses of the first and second films, respectively; a and b are widths of the films; δ is the thickness of the near-surface "metallic" layer; an electric current j is directed perpendicular to the plane of the figure

The thickness of the near-surface layer δ was set equal to 1 nm, which corresponds to the thickness of one QL in the Bi₂Se₃ crystal structure [4]. This value does not exceed the thickness of the two-dimensional conduction channel of 1.7 nm, estimated for Bi₂Se₃ in [17]. Note also that in this model representation there is a sharp boundary between surface and bulk, which does not entirely correspond to reality.

Using the above expressions and assumptions, estimations of surface and bulk resistivities were performed. Fig. 3 shows the temperature dependences of the contributions to the resistivity from surface, ρ_{surf} , and bulk, ρ_{bulk} , current carriers in the Bi₂Se₃ films. It can be seen that the dependence $\rho_{surf}(T)$ exhibits metallic behaviour, i.e. the electrical resistivity grows with increasing temperature according to a power law, and the dependence $\rho_{bulk}(T)$ exhibits semiconductor behaviour, i.e. ρ_{bulk} decreases with increasing temperature. In general, this is consistent with the presence of metallic states on the surface of a topological insulator and an energy gap in its bulk. At T = 4.2 K, the surface resistivity ρ_{surf} depends on temperature according to a quadratic law, and a linear dependence $\rho_{surf}(T)$ is observed at higher temperatures. The quadratic temperature dependence of the electrical resistivity can be explained by electron-electron scattering, as well as by an "electron-phonon-surface" interference scattering mechanism described in [18, 19]. However, further research is required to understand the reason for such dependence.



FIG. 3. Temperature dependences of the contributions of surface ρ_{surf} (a) and bulk ρ_{bulk} (b) current carriers to the resistivity of the Bi₂Se₃ thin films

4. Conclusion

It was found that the temperature dependences of the resistivity of the topological insulator Bi_2Se_3 films demonstrate metallic behavior, and the resistivity value depends on the thickness of the film.

The relatively simple method for "separating" the bulk and surface resistivities of topological insulator films was proposed, with the help of which corresponding estimates were made for thin films of Bi_2Se_3 with thicknesses of 20 and 40 nm.

The performed estimates showed that the contribution of surface carriers to the electrical resistivity of Bi_2Se_3 grows with increasing temperature, whereas the contribution of bulk carriers decreases. The value of the surface resistivity is more than two orders of magnitude less than the bulk resistivity at low temperatures. In general, this is consistent with existing concepts about the presence of "metallic" states on the surface of a topological insulator and an energy gap in its bulk.

References

- [1] Gilbert M.J. Topological electronics. Commun. Phys., 2021, 4, 70.
- [2] He M., Sun H., He Q.L. Topological insulator: Spintronics and quantum computations. Front. Phys., 2019, 14, 43401.
- [3] Hasan M.Z., Kane C.L. Colloquium: Topological insulators. Rev. Mod. Phys., 2010, 82, 3045.
- [4] Qi X.-L., Zhang S.-C. Topological insulators and superconductors. Rev. Mod. Phys., 2011, 83, P. 1057–1110.
- [5] Xiao J., Yan B. First-principles calculations for topological quantum materials. Nat. Rev. Phys., 2021, 3, P. 283–297.
- [6] Zhang H., Liu C.-X., Qi X.-L., Dai X., Fang Z., Zhang S.-C. Topological insulators in Bi₂Se₃, Bi₂Te₃ and Sb₂Te₃ with a single Dirac cone on the surface. *Nature Phys.*, 2009, 5, P. 438–442.
- [7] Xia Y., Qian D., Hsieh D., Wray L., Pal A., Lin H., Bansil A., Grauer D., Hor Y.S., Cava R.J., Hasan M.Z. Observation of a large-gap topologicalinsulator class with a single Dirac cone on the surface. *Nature Phys.*, 2009, 5, P. 398–402.
- [8] Stepina N.P., Golyashov V.A., Nenashev A.V., Tereshchenko O.E., Kokh K.A., Kirienko V.V., Koptev E.S., Goldyreva E.S., Rybin M.G., Obraztsova E.D., Antonova I.V. Weak antilocalization to weak localization transition in Bi₂Se₃ films on graphene. *Physica E*, 2022, **135**, 114969.
- Wang W.J., Gao K.H., Li Z.Q. Thickness-dependent transport channels in topological insulator Bi₂Se₃ thin films grown by magnetron sputtering. Sci. Rep., 2016, 6, 25291.
- [10] Pan Z.-H., Vescovo E., Fedorov A.V., Gardner D., Lee Y.S., Chu S., Gu G.D., Valla T. Electronic structure of the topological insulator Bi₂Se₃ using angle-resolved photoemission spectroscopy: Evidence for a nearly full surface spin polarization. *Phys. Rev. Lett.*, 2011, **106**, 257004.
- [11] Cao H., Tian J., Miotkowski I., Shen T., Hu J., Qiao S., Chen Y.P. Quantized Hall effect and Shubnikov-de Haas oscillations in highly doped Bi₂Se₃: evidence for layered transport of bulk carriers. *Phys. Rev. Lett.*, 2012, **108**, 216803.
- [12] Vedeneev S.I. Quantum oscillations in three-dimensional topological insulators. Phys.-Usp., 2017, 60, 385.
- [13] Steinberg H., Gardner D.R., Lee Y.S., Jarillo-Herrero P. Surface state transport and ambipolar electric field effect in Bi₂Se₃ nanodevices. *Nano Lett.*, 2010, 10, P. 5032–5036.
- [14] Marchenkov V.V., Weber H.W., Cherepanov A.N., Startsev V.E. Experimental verification and quantitative analysis of the temperature (phonon) breakdown phenomenon in the high-field magnetoresistivity of compensated metals. J. Low Temp. Phys., 1996, 102, P. 133–155.
- [15] He H.-T., Wang G., Zhang T., Sou I.-K., Wong G.K.L., Wang J.-N. Impurity effect on weak antilocalization in the topological insulator Bi₂Te₃. *Phys. Rev. Lett.*, 2011, **106**, 166805.
- [16] Le P.H., Wu K.H., Luo C.W., Leu J. Growth and characterization of topological insulator Bi₂Se₃ thin films on SrTiO₃ using pulsed laser deposition. *Thin Solid Films*, 2013, **534**, P. 659–665.
- [17] Cao H., Tian J., Miotkowski I., Shen T., Hu J., Qiao S., Chen Y.P. Quantized Hall effect and Shubnikov-de Haas oscillations in highly doped Bi₂Se₃: Evidence for layered transport of bulk carriers. *Phys. Rev. Lett.*, 2012, **108**, 216803.
- [18] Startsev V.E., D'yakina V.P., Cherepanov V.I., Volkenshtein N.V., Nasyrov R.Sh., Manakov V.G. Quadratic temperature dependence of the resistivity of tungsten single crystals. Role of surface scattering of electrons. *Sov. Phys. JETP*, 1980, **52** (4), P. 675–679.
- [19] Marchenkov V.V. Quadratic temperature dependence of magnetoresistivity of pure tungsten single crystals under static skin effect. Low Temp. Phys., 2011, 37, P. 852–855.

Submitted 8 May 2024; revised 14 August 2024; accepted 15 August 2024

Information about the authors:

Alexandra N. Perevalova – M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, 620108 Ekaterinburg, Russia; ORCID 0000-0002-8540-8720; domozhirova@imp.uran.ru

Bogdan M. Fominykh – M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, 620108 Ekaterinburg, Russia; ORCID 0000-0002-4755-3839; bogdan.fominyh@mail.ru

Vasiliy V. Chistyakov – M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, 620108 Ekaterinburg, Russia; ORCID 0000-0002-2684-256X; saddax@yandex.ru

Vyacheslav V. Marchenkov – M. N. Mikheev Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, 620108 Ekaterinburg, Russia; ORCID 0000-0003-2044-1789; march@imp.uran.ru

Conflict of interest: the authors declare no conflict of interest.