Electro- and magnetotransport properties of a WTe$_2$ single crystal

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Abstract. A single crystal of a topological Weyl semimetal WTe$_2$ was grown and its electrical resistivity and galvanomagnetic properties (magnetoresistivity and the Hall effect) were investigated in detail in the temperature range from 1.8 K to 300 K and in magnetic fields of up to 9 T.

1. Introduction

At present, searching for and studying new topological materials is the most important area of condensed matter physics, which is associated with great interest from the point of view of fundamental science, as well as with promising prospects for practical application. The nontrivial topology of the band structure of these materials leads to appearance of the unique electronic properties. In topological insulators [1, 2], the bulk electronic states are characterized by the presence of a gap, while the surface behaves like a topologically protected metal with a linear dispersion law. Topological Weyl semimetals [3-8] have unusual electronic states both on the surface and in the bulk. Bulk properties are determined by the presence of unique quasiparticles, massless Weyl fermions, that can be controlled much faster than ordinary charge carriers. The surface states in topological insulators and Weyl semimetals are spin-polarized, which makes such materials promising for creating spintronic devises, and massless charge carriers with high mobility in Weyl semimetals can be used in ultrafast micro- and nanoelectronics.

A necessary condition for the existence of a Weyl semimetal is known to be the breaking of inverse or time reversal symmetry; therefore, the attention of researchers is directed to the study of such materials. For the first time, the experimental evidence of a type I Weyl semimetal was obtained on TaAs single crystals [3] in 2015. Soon, other materials with similar properties were discovered, including WTe$_2$ [5], MoTe$_2$ [6] and their mixed compound Mo$_{1-x}$W$_x$Te$_2$ [7, 8], which can exhibit the properties of a type II Weyl semimetal.

Recently, much attention has been paid to the study of the electronic transport properties of WTe$_2$ and MoTe$_2$ single crystals. To date, a large magnetoresistive effect has been found in these compounds, which may be due to the almost ideal compensation of charge carriers at low temperatures, as well as their very high mobility [9-12]. However, such works are still quite rare, therefore it is of interest to study the electro- and magnetotransport properties of a WTe$_2$ single crystal.
2. **Experiment**

WTe$_2$ single crystals were grown by the chemical vapour transport method using Br$_2$ as a transport agent. Tungsten and tellurium powders in a stoichiometric ratio were sealed in a quartz ampoule with a bromine vapour density of approximately $5\,\text{mg/cm}^3$. Then, the ampoule was placed into a horizontal tube furnace with a linear temperature gradient, where the temperature of the hot zone was $850^\circ\text{C}$, and the temperature of the cold zone was $770^\circ\text{C}$. In this process, the initial components interact with the transport agent in the hot zone and are transferred to the cold zone, followed by crystallization. The growth procedure took place within 500 hours. X-ray diffraction analysis revealed that WTe$_2$ crystallizes in an orthorhombic structure with the lattice parameters $a = 3.435(8)\,\text{Å}$, $b = 6.312(7)\,\text{Å}$ and $c = 14.070(4)\,\text{Å}$. The chemical composition of the samples was confirmed by X-ray microanalysis using a FEI Inspect F scanning electron microscope equipped with an EDAX attachment.

The temperature dependences of the electrical resistivity $\rho(T)$ and galvanomagnetic properties (magnetoresistivity and the Hall effect) were measured by the standard method (see, e.g. [13, 14]) in the temperature range from 1.8 to 300 K in magnetic fields of up to 9 T. An electric current flowed in the (00$l$) plane of the sample, while the magnetic field was directed perpendicular to the (00$l$) plane. The measurements were carried out using a PPMS-9 system (Quantum Design) in the Collaborative Access Center "Testing Center of Nanotechnology and Advanced Materials" of IMP, UB of RAS.

3. **Results and discussion**

The temperature dependence of the electrical resistivity $\rho_0(T)$ of WTe$_2$ (figure 1(a)) is seen to have a “metallic” type and $\rho_0$ monotonically increases with temperature from 20 to $860\,\mu\text{Ohm}\cdot\text{cm}$ according to a law close to quadratic at low temperatures, reaches a linear dependence at $T > 60\,\text{K}$ with a tendency to saturation at temperatures above 240 K. The quadratic temperature dependence $\rho_0 \sim T^2$ up to 50 K was observed in metallic MoTe$_2$ in [15]. $T^2$– dependence of the electrical resistivity at low temperatures is known to be explained by several mechanisms, in particular, strong electron-electron scattering. In addition, it is shown in [16, 17] that electron-phonon-surface scattering can lead to $\rho_0 \sim T^2$ in pure metals. Since the WTe$_2$ single crystal has a layered structure, interface scattering of current carriers can occur, which can also lead to $\rho_0 \sim T^2$. At higher temperatures, $\rho_0 \sim T$, which can be explained by electron-phonon scattering at $T$ close to $\Theta_D/3$, where $\Theta_D = 133.8\,\text{K}$ is the Debye temperature of WTe$_2$ [18].

![Figure 1](image.png)

**Figure 1.** The temperature dependence of the electrical resistivity (a) and the field dependence of the magnetoresistivity at $T = 1.8\,\text{K}$ (b).

Figure 1(b) shows the field dependence of the magnetoresistivity $\rho_{xx}(B)$ of WTe$_2$ at $T = 1.8\,\text{K}$, which was calculated by the formula

$$\Delta\rho_{xx} / \rho_0 = (\rho_{xx} - \rho_0) / \rho_0 \cdot 100\%,$$

(1)
where $\rho_0$ is the electrical resistivity without a magnetic field, $\rho_{xx}$ is the resistivity in magnetic fields of up to 9 T. The magnetoresistivity is seen to reach 1700% at $T = 1.8$ K in a magnetic field of 9 T. The analysis of the dependence $\rho_{xx}(B)$ showed that the magnetoresistivity changes according to a law close to quadratic in fields of up to 9 T. This behaviour of the magnetoresistivity is inherent in compensated conductors with a closed Fermi surface (FS) in the region of high effective magnetic fields [19]. As shown in [20], volumes of the electron and hole FS sheets of WTe$_2$ are equal, i.e. this material is compensated. The data we obtained (figure 1(b)) confirm the above.

In compensated conductors with the closed FS, large values of the magnetoresistivity are observed in the region of high effective magnetic fields [19]. This is largely due to the fact that under these conditions the relation $l \gg r_H$ is fulfilled, where $l$ is the mean free path of current carriers and $r_H$ is the Larmor radius. Thus, in such materials, large values of the carrier mobility should be observed. In addition, Weyl semimetals are known to have high mobility of current carriers; therefore, the Hall effect was studied.

Figure 2 shows the temperature dependence of the Hall coefficient of WTe$_2$ in a field of 9 T as well as the concentration of charge carriers and their mobility. Analysing the data obtained, we can conclude that the majority charge carriers are electrons with a concentration $n \sim 10^{19}$ cm$^{-3}$ and mobility $\mu \approx 7500$ cm$^2$/V·s at $T = 1.8$ K. With increasing temperature, the concentration of current carriers increases, and the mobility decreases. These results are in good agreement with the data of [10], whose authors also studied the Hall effect in a semimetal WTe$_2$ with extremely high magnetoresistance.

4. Conclusions

The studies of the electrical resistivity and galvanomagnetic properties of the WTe$_2$ single crystal allow us to draw the following conclusions.

1. The temperature dependence of the electrical resistivity is shown to have a "metallic" type, increasing from 20 to 860 $\mu$Ohm·cm according to the quadratic law at low temperatures (up to 60 K) and linearly at higher temperatures with a tendency to saturation above 240 K. $T^2$–dependence of the electrical resistivity at low temperatures can be explained by several mechanisms, including strong electron-electron scattering as well as electron-phonon-surface scattering. However, to clarify the reasons for this behaviour of the electrical resistivity, further studies are required.

2. The results of the analysis of the field dependence of the magnetoresistivity suggest that the Fermi surface of the compound may contain closed sheets. The magnetoresistivity reaches 1700% at $T = 1.8$ K in a field of 9 T.
3. The Hall effect studies and the performed estimates showed that the main type of charge carriers are electrons with a concentration $n \sim 10^{19}$ cm$^{-3}$ and mobility $\mu \approx 7500$ cm$^2$/V·s at $T = 1.8$ K. With increasing temperature, the concentration of current carriers increases, and the mobility decreases.

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