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Magnetoresistance and quantum oscillations in the WTe_2 semimetal

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The discovery of extreme magnetoresistance (XMR) in non-magnetic materials attracted attention to the WTe_2 semimetal. We have carried out studies of magnetoresistance in a tungsten ditelluride single crystal in the magnetic field range up to 14 T. Magnetoresistance increased with increasing field following a near quadratic law without saturation. The Shubnikov–de Haas oscillations were observed. Four fundamental frequencies were found in the oscillations spectrum, which correspond to two electron and two hole pockets caused by strong spin-orbit coupling.

Keywords: WTe_2 semimetal, magnetoresistance, Shubnikov–de Haas oscillations, oscillations spectrum.

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1. Introduction

Layered crystals of tungsten ditelluride WTe_2 are semimetals with Td structure (rhombic space group $Pmn2_1$) [1], that remains stable at temperature change [2,3]. Recently, the extreme increase of resistance at constant magnetic field was revealed in WTe_2, as in some other compounds with metal conductivity [4–7]. Value of magnetoresistance (MR), defined as ratio of resistance change to the value of resistance in zero field, was approximately proportional to the squared magnetic field induction. The feature of MR in WTe_2 is a lack of saturation up to the fields of 60 T [4]. The Shubnikov–de Haas oscillations were also observed in the field dependence of magnetoresistance [8–11]. Oscillation spectrum presented the direct information on Fermi energy of electron and hole pockets in WTe_2. These data are of special interest since tungsten ditelluride was considered as possible Weyl semimetal based on theoretical predictions and experimental results, obtained using various methods (see, for instance, [12–14] and references in these works). Measurements of MR and Shubnikov–de Haas oscillations at various temperatures allow studying temperature evolution of electron and hole pockets, that is important at analysis of electron bands topology transformation [15]. Published data on quantum oscillations frequencies, their temperature dependencies and value of MR do not always correspond to each other, that may be caused by difference of electron properties of crystals, grown under various conditions and using various methods. In this work we present the results of a study of MR and Shubnikov–de Haas oscillations in WTe_2 single crystal, grown in the Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, Yekaterinburg.

2. Samples and experiment

WTe_2 tungsten ditelluride monocrystal was grown by the chemical vapor transport method. Bromine was used as a transport agent. Crystal was growing in vacuum-sealed quartz ampule for three weeks. Sample for the study was cut out from the grown crystal in a form of a thin plate with thickness of about 0.2 mm, oriented perpendicular to c axis. Crystal structure, single crystallinity and directions of crystallographic axes were controlled through X-ray diffraction. Triple layers of Te–W–Te atoms (W–Te bond is covalent) form the planes, perpendicular to c axis and coupled with a weak van der Waals interaction. Tungsten atoms form the chains, oriented along crystallographic a axis, inside the layers.

Measurement of the sample resistance in the direction of the crystal axis a was performed with PPMS-16 system manufactured by Quantum Design the built-in four-probe technique. Temperature dependence of resistance in zero magnetic field was obtained in a range from 2 to 300 K. Resistance dependence on magnetic field of up to 14 T was measured at temperatures of 2 and 5 K. Magnetic field was directed along the crystal axis c. According to [9], MR in this geometry has the highest value.

3. Results and discussion

Measurement of resistance with temperature in zero magnetic field is shown in Fig. 1. Increase of resistance with increasing temperature has a metal nature. In a range from 90 to 200 K the sample resistance demonstrates the linear dependence on temperature. Despite the strong rise of resistance increasing temperature, ratio RRR of resistance values at 300 K and at 2 K is 31, that is significantly less, than was obtained in other works [4,8–10]. This is, probably, due to higher amount of defects in our examined sample.

The MR curves, measured at temperatures of 2 and 5 K, are presented in Fig. 2. Magnetoresistance in percents was calculated as per formula $\mathrm{MR} = [R(B) - R(0)]/R(0) \times 100$, where $R(B)$, and $R(0)$ are the sample resistance in field B and in zero field respectively. At 14 T magnetoresistance reaches the value of $3.45 \cdot 10^3\%$ for temperature of 2 K and $3.31 \cdot 10^3\%$ for temperature of 5 K. The obtained values of MR are less, than in the works [4,8–10], that correlates with the lower RRR ratio. As in the previous studies of magnetoresistance in semimetal WTe_2, there is no saturation at dependence of MR on the field. For both temperatures in the whole range of the fields the monotonous MR rise at increasing magnetic field without oscillations considering is described with power function, close to quadratic, $\mathrm{MR} \propto B^{1.78}$. Quadratic dependence is theoretically predicted for metals, semimetals and semiconductors in a region of weak magnetic fields. It is also observed for compensated conductors with closed Fermi surface in a region of strong effective magnetic fields [16]. Lack of magnetoresistance saturation indicates the compensation of electrons and holes [4,17]. Within a two-band model [18], in which one electron and one hole bands are examined, the longitudinal resistivity in magnetic field is described with the following relation:

$$\rho = \frac{1}{e}\,\frac{(n_e\mu_e + n_h\mu_h) + (n_e\mu_e\mu_h^2 + n_h\mu_h\mu_e^2)B^2}{(n_e\mu_e + n_h\mu_h)^2 + (n_h - n_e)^2\mu_e^2\mu_h^2B^2}, \tag{1}$$

where n_e and n_h are the electron and hole concentrations, respectively, and μ_e and μ_h are the corresponding mobilities. At compensation condition $n_e = n_h$, by introducing the average mobility $\overline{\mu}$, we obtain the following for MR

$$\mathrm{MR} = (\overline{\mu}B)^2. \tag{2}$$

Two-band model was used for explanation of the high MR in bismuth and graphite, in which, however, the saturation was observed in the field of about several T, indicating the undercompensation of electrons and holes [19,20].

According to data, obtained in this work, the average mobility $\overline{\mu}$ can be defined. At 2 K the average mobility is $4.2 \cdot 10^3\,\mathrm{cm^2V^{-1}s^{-1}}$. It is close to mobility, obtained in [21]. Thus, within the two-band model, the high mobility of electrons and holes under condition of their concentration equality is responsible for the high value of magnetoresistance.

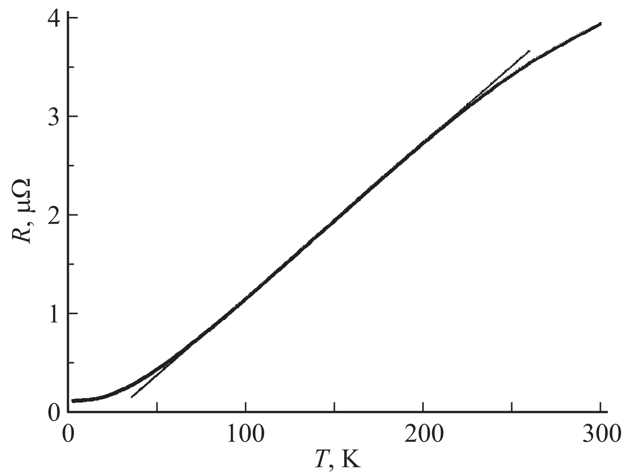

Figure 1. Temperature dependence of resistance in zero external magnetic field. Straight line indicates the linear dependence.

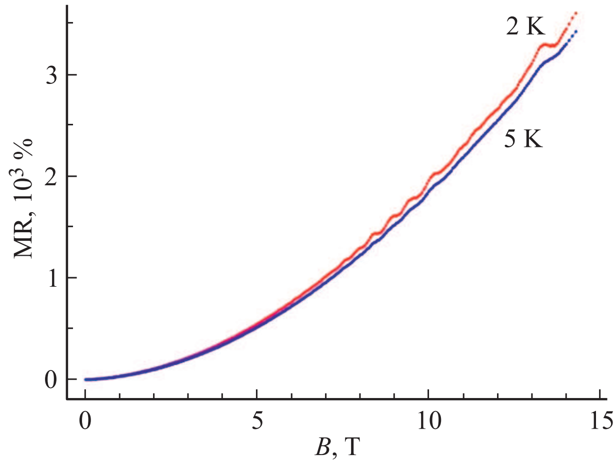

Figure 2. Magnetoresistance dependence on external magnetic field at temperatures of 2 and 5 K.

It should be noted, that for interpretation of extreme MR the models were used, that consider the peculiarity of electron bands topology in topological materials, resulting in limitation of charge carrier back-scattering [6,22–25]. However, for WTe_2 as a candidate for Weyl semimetals the additional studies support the correctness of electrons and holes compensation [26].

Shubnikov–de Haas (ShdH) quantum oscillations are observed on MR curves, obtained at 2 and 5 K (Fig. 2). As expected, ShdH oscillations attenuate with increasing temperature. Analysis of quantum oscillations of MR was performed using discrete Fourier transformation. For oscillations differentiation against dependencies of MR on magnetic field at both temperatures the monotonous MR rise was approximated with fourth degree polynomial and

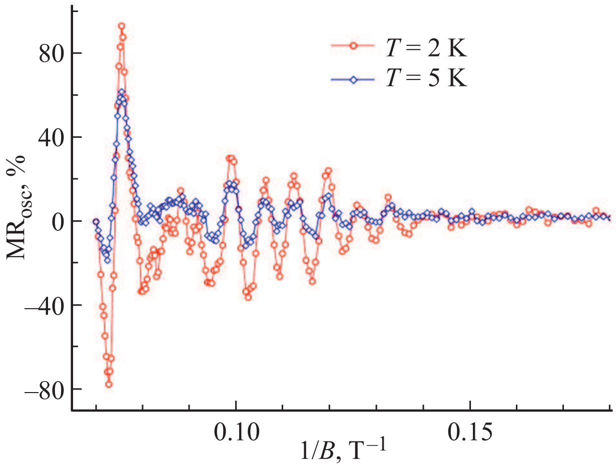

Figure 3. Shubnikov–de Haas oscillations depending on reciprocal field at temperatures of 2 and 5 K.

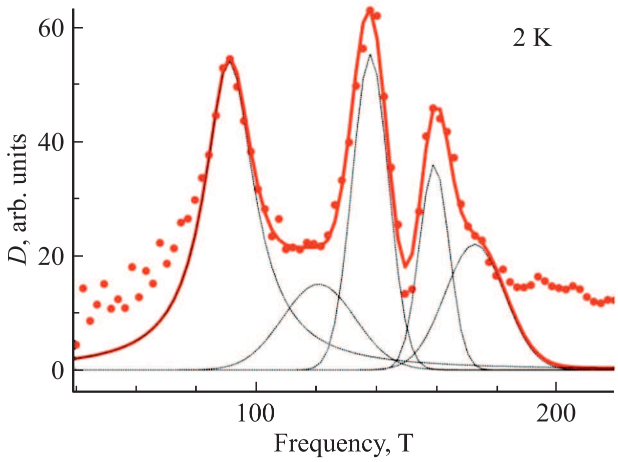

Figure 4. Oscillations spectrum at temperature of 2 K. Dots — result of Fourier transforms, thin solid lines — calculated individual spectral components, heavy solid line — total contribution of spectral components.

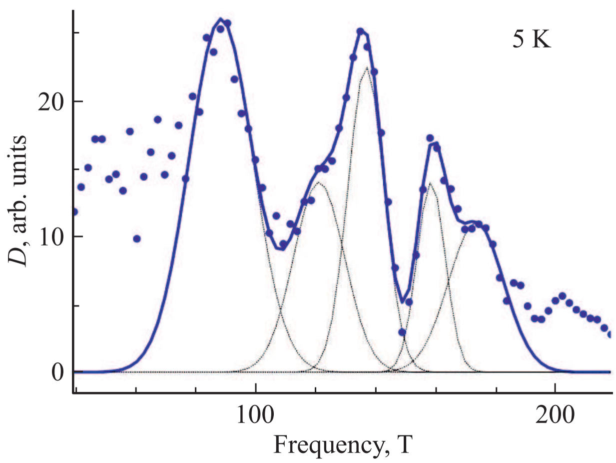

Figure 5. Oscillations spectrum at temperature of 5 K. Dots — result of Fourier transform, thin solid lines — calculated individual spectral components, heavy solid line — total contribution of spectral components.

Frequencies of spectrum components F, their relative intensity I_{rel} and area A of cross sections of Fermi surface of electron and hole pockets, calculated for 2 and 5 K

	2 K			5 K		
	$F(T)$	I_{rel}	$A\,(\mathrm{nm}^{-2})$	$F(T)$	I_{rel}	$A\,(\mathrm{nm}^{-2})$
h_1	90.5	1	0.86	88.5	0.41	0.85
e_1	120.2	0.27	1.15	121.2	0.18	1.16
e_2	137.3	0.49	1.31	136.8	0.20	1.30
h_2	158.5	0.26	1.51	158.5	0.10	1.51
*	172	0.32		173.5	0.15	

substracted from experimental curves. Figure 3 shows ShdH oscillations depending on reciprocal magnetic field. Figures 4 and 5 demonstrate Fourier transforms, obtained at temperatures of 2 and 5 K, respectively. The contributions of individual spectral components and their sum are shown along with the calculation. Five frequencies F, corresponding to individual components, and intensities of the components are presented in the table. According to [9,10] the first four obtained frequencies should be connected to electron and hole pockets, split due to spin-orbital interaction. These frequencies in ShdH oscillations spectrum correspond to indices h_1, e_1, e_2 and h_2 in the table, where h and e indicate the hole and electron pockets. Numbers 1 and 2 correspond to two possible spin orientations. The fifth frequency, indicated with * symbol, is probably the second harmonic of the lowest frequency. Onsager relation

$$F = (\Phi_0/2\pi^2)A, \tag{3}$$

allows us to evaluate the size A of maximum cross section of Fermi surface of electron and hole pockets, perpendicular to magnetic field direction, using the calculated frequencies of quantum oscillations. In (3) Φ_0 is the magnetic flux quantum. Cross section areas are also presented in the table. Sum of cross sections for electron pockets differs from sum of cross sections for hole pockets only by 3%, that corresponds to close concentration of electrons and holes in the examined crystal.

Frequencies of ShdH oscillations, obtained in this work, can be compared with frequencies of quantum oscillations, presented in the published studies of WTe_2 crystal [8–10,21,27,28]. Four fundamental frequencies of quantum oscillations, which spread of values overlaps the difference with the frequencies obtained by us (table), were observed in most of the works, except for [21]. Thus, the presence of defects in the examined crystal, which result in reduction of RRR, does not significantly impact the value of cross section of Fermi surface of electron and hole pockets.

ShdH oscillations can be interpreted based on Lifshitz–Kosevich theory [10]. According to this theory, the temperature dependence of oscillations intensity allows evaluating the effective electrons mass m^*. However, in our case with measurements at two temperatures, evaluations for effective mass have low accuracy.

4. Conclusion

The single-crystal sample of WTe_2 semimetal, studied by us, is characterized by ratio $RRR = 31$, indicating the presence of significant amount of defects. Magnetoresistance at temperatures of 2 and 4 K reaches the values, exceeding $3 \cdot 10^3\%$. Shubnikov–de Haas oscillations spectrum contains for fundamental frequencies, consistent with the results of the published studies of magnetoresistance in tungsten ditelluride. Thus, crystal structure defects, resulting in magnetoresistance reduction, do not significantly impact the electron bands topology in WTe_2.

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Conflict of interest

The authors declare that they have no conflict of interest.

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