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Thermoelectric Properties and Surface States in the Layers of Bi_2Te_3 Topological Insulators

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Abstract—The thermoelectric properties and Shubnikov–de Haas (SdH) oscillations of monocrystalline layers of a topological insulator (TI) of *n*-type bismuth telluride were investigated. The monocrystalline Bi_2Te_3 layers were fabricated by the mechanical exfoliations of layers from a monocrystalline ingot of the appropriate composition. The cyclotron effective masses, the Dingle temperature, and the quantum mobilities of charge carriers were calculated from the experimental data by SdH oscillations both in longitudinal ($H \parallel I$) and in perpendicular ($H \perp I$) magnetic fields at temperatures in the range of 2.1–4.2 K. It was found that the phase shift of the Landau levels index is 0.5 both for the parallel and for the perpendicular magnetic fields associated with the Berry phase of surface states. The power factor in the temperature range of 2–300 K was calculated from the temperature dependences of resistance and thermal e.m.f. It was stated that the power factor $\alpha^2\sigma$ has a maximum value in the temperature range of 100–250 K, which corresponds to the maximum values for perfect monocrystals described in the literature. Taking into account that the heat conductivity in the thin layers is essentially lower than in the bulk samples, it is reasonable to expect a considerable increase in the thermoelectric efficiency over a wide temperature range, which is of great importance for the development of new highly effective thermoelectric materials based on thinner Bi_2Te_3 TI layers for practical applications in thermogenerators and coolers.

Keywords: topological insulators, bismuth telluride, single-crystal layers, SdH oscillations, thermoelectricity
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INTRODUCTION

Bismuth Telluride Bi_2Te_3 is known as one of the best thermoelectric materials of both *n*- and *p*-conductivity, in which the thermoelectric efficiency is $ZT \approx 1$ when $T = 300$ K [1–5].

The thermoelectric efficiency Z is defined by the expression $Z = \alpha^2\sigma/\chi$, ($\chi = \chi_e + \chi_L$, χ_e is the electron heat conductivity, χ_L is the lattice heat conductivity), where α is the Seebeck coefficient; σ is the specific conductivity, and χ is the heat conductivity. Numerous studies on the influence of different factors including doping, structure, crystallographic orientation, temperature, sizes, which were aimed at the quality of variables α, σ, χ, factors in Z, were conducted for a long time [6–10]. The charge carrier mobility, which depends on the scattering mechanisms, is one of the important parameters. To control the scattering mechanisms one can using doping, temperature, perfection of structure, sample size, deformation, etc. The longstanding attempts to increase ZT did not yet lead to a fundamental breakthrough. The search for new materials and ways to improve the thermoelectric parameters associated with new phenomena is currently paid much attention. Such fields include topological insulators (TI) [11–15] and dimensionally limited structures.

A new class of materials, topological insulators based on semiconductors with an inverted spectrum of charge carriers, has been widely studied recently both theoretically and experimentally [11–15] because, on one hand, TIs have unique properties related to electron spin and nontrivial physics, and on the other hand, it is assumed that their thermoelectric efficiency will increase [11, 15]. Tellurides Bi_2Te_3 and selenides Bi_2Se_3 of bismuth, as well as semiconductor alloys $Bi_{1-x}Sb_x$ are related to the TIs. It was shown that a strong spin-orbit interaction in the TIs leads to inversion of energy spectrum and generation of spin–split topological surface states with the dispersion of Dirac type [15], that is, a linear dependence of energy on

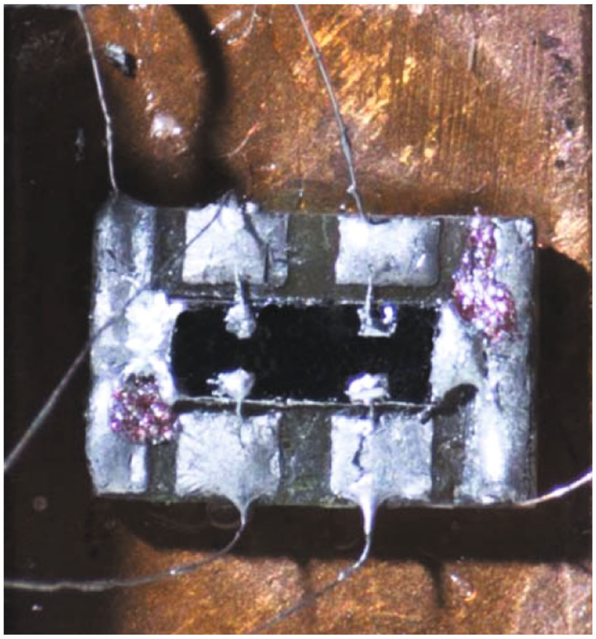

Fig. 1. Monocrystalline Bi_2Te_3 layer with four soldered measuring contacts.

impulse $E = hkv_F$, where v_F is the Fermi electron velocity, $v_F = \frac{hkF}{m}$. Because of this, the electrons are not sensitive to scattering at defects, which does not violate the symmetry of time reversal, i.e., the electrons in these states can move along the surface of the bulk material without energy loss. So, the surface states in the TIs are more stable and provide high surface conductivity, whereas the material in the bulk has a bandgap and is nearly a dielectric.

The theoretical assumptions and experimental results show that in low-dimensional thermoelectric materials the thermoelectric efficiency can increase both at the expense of increasing the power factor $\alpha^2\sigma$ due to the manifestation of a quantum dimensional effect and due to a reduction in the heat conductivity because of scattering of phonons at the boundary [16–20].

Decreasing the heat conductivity in Bi_2Te_3 nanolayers as compared with bulky crystals by 2.5–3.5 times was revealed experimentally [21]. The temperature dependence limited by the scattering of phonons at the boundary was detected, which should lead to an increase in the thermoelectric efficiency (ZT), particularly in the low temperature region. The objective of the present work is a comprehensive analysis of the thermoelectric properties of Shubnikov–de Haas (SdH) oscillations of monocrystalline Bi_2Te_3 layers fabricated by the mechanical exfoliation method, the study of the features of surface states, the definition and analysis of mobilities of charge carriers, and the evaluation of thermoelectric efficiency in Bi_2Te_3 layers of n-type TI in the temperature range of 2.1–300 K.

SAMPLES AND EXPERIMENTAL TECHNIQUE

The monocrystalline layers of Bi_2Te_3 n-type alloys with 10–30 μm thickness were fabricated by the mechanical exfoliation method of the layers from a bulk monocrystalline ingot of similar composition, using a scotch tape like the manufacturing technique for graphene layers with the sequential separation of layers from ordinary crystalline graphite [22]. The mechanical cleavage of the layers made it possible to fabricate the high-quality thin layers. X-ray diffraction studies revealed that the layers had a monocrystalline structure and the cleavage plane of the layer was perpendicular to the trigonal axis C_3. The layer was placed on a specially manufactured substrate of copper-foil-coated glass fiber laminate. A four-contact method was used for electrical measurements (Fig. 1) within the temperature range of 1.5–300 K.

The contacts were fastened by indium cold soldering or quick solder (Wood alloy). The resistance of the contacts was tested by recording the current–voltage characteristics. The transverse magnetoresistance ($H \perp I$) and the longitudinal magnetoresistance ($H \parallel I$) were studied in magnetic fields up to 14 T in the field of a Bitter magnet, as well as a superconducting solenoid at temperatures of 2.1–4.2 K.

The thermal e.m.f. was measured by the double-contact method. In this case, the contacts in the end of layer were implemented with InGa-eutectic, which moistened the ends of the layer under study. The layer was fastened to the copper-foil-coated glass fiber laminate between two bulk copper blocks with a built-in and calibrated differential Cu-Fe based thermocouple. The temperature gradient in the low temperature region did not exceed 0.5–1 K, in the region $T > 50$ K, $\Delta T \approx 2$–3 K.

When measuring the Shubnikov–de Haas oscillations a modulation technique was used, which made it possible in automatic mode to record the field dependences of resistance $R(H)$ and their derivatives $\partial R/\partial H(H)$ [23]. The measuring accuracy of the thermal e.m.f. was 3–5%.

The measurements in the strong magnetic fields up to 14 T were conducted in the International Laboratory of High Magnetic Fields and Low Temperatures (Wrocław, Poland).

RESULTS AND DISCUSSION

The magnetoresistance in transverse ($H \perp I$) and longitudinal ($H \parallel I$) magnetic fields with magnitudes up to 14 T was studied in monocrystalline layers of Bi_2Te_3