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Electronic properties of the topological insulator Sb_2Te_2Se

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The structural and electronic properties of thin layers of single crystals of the topological insulator Sb_2Te_2Se were studied by X-ray diffraction and magneto-optical spectroscopy. A sharp edge of the absorption band as well as Fabry-Perot oscillations were revealed in the transmission spectra measured at 4.2 K which made it possible to estimate the band gap $E_g \approx 374$ meV and the refractive index $n \approx 8.5$. The application of magnetic fields up to 11 T led to a significant decrease in the amplitude of the oscillations attributed to the Faraday effect. The Verdet constant was estimated to be of $V \approx 10^3$ degrees/cm $\cdot$ T.

Keywords: topological insulator, Sb_2Te_2Se, magneto-optics, transmission spectrum.

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1. Introduction

Topological insulators are a new class of quantum materials that have been actively studied in recent years. These materials are insulators in the bulk, but have topologically protected spin-polarized conducting surface states [1] with dispersion ratios in the form of a Dirac cone, which opens up great prospects for such materials to be used in spintronics [2] and quantum electronics [3].

The majority of recent studies of topological insulators are related to their non-trivial properties. However, their volumetric electronic properties may also be very unusual [4,5]. The interest in the volumetric properties of these materials is also attributable to their high performance characteristics in thermoelectric devices.

The structural and electronic properties of single crystals of a topological insulator Sb_2Te_2Se grown by the vertical Bridgman method were studied in this paper by X-ray diffraction and magnetooptical spectroscopy.

2. Objects and methods of the experiment

Single crystal samples Sb_2Te_2Se were grown by the vertical Bridgman method [6]. The phase purity and crystal structure of the grown material were studied by X-ray diffraction (XRD) at room temperature using Shimadzu XRD-7000 Maxima diffractometer (CuK_α-radiation, graphite monochromator, range of 2θ from 5 to 95° in increments of 0.02° and the count time of 12 s per step).

Transmission spectra in the energy range from 0.2 to 0.5 eV at 4.2 K were obtained using Bruker IFS 66v/S FTIR spectrometer with a globar as a light source and a silicon bolometer as a detector at the Laboratoire National des Champs Magnetiques Intenses (LNCMI, Grenoble, France). Films with a thickness of $\sim 10\,\mu$m were peeled off from a single crystal sample perpendicular to the c axis and then placed on a copper foil with holes of about 1×1 mm cut in the center. The magnetic transmission spectra were measured on a superconducting magnet up to 11 T in the Faraday configuration with light propagating along the axis c.

3. Experimental findings and discussion

3.1. X-ray diffraction

The GSAS-II [7] software package was used for crystal structure refinement by the Rietveld method. The powder diffractograms provided in Figure 1 showed that the material does not contain secondary phases, the crystal structure corresponds to the known data [8]: space group $R\bar{3}m$, lattice cell parameters $a = 4.1848(3)$ Å, $c = 29.9094(8)$ Å, coordinates of atoms: Sb $(3m, 0\,0\,0.3931)$, Te $(3m, 0\,0\,0.7860)$, Se $(\bar{3}m, 0\,0\,0)$. The high non-monotonic background in Figure 1 is attributable to the glass substrate and the small amount of sample. These reasons also lead to a relatively high divergence factor $\omega R_p = 3.34\%$, the degree of matching $\chi^2 = 2.13$.

4. Magnetooptical measurements

Figure 2 shows the transmission spectra in the absence of a magnetic field and in a magnetic field of 11 T. A sharp edge of the absorption band is observed, which makes it possible to estimate the width of the band gap of $E_g \approx 374$ meV. Significant Fabry-Perot oscillations are also observed, indicating a small sample thickness and a high degree of parallelism between its upper and lower surfaces. It can be seen that the use of a magnetic field has a significant effect on Fabry-Perot oscillations.

We define the oscillating part for quantification of the changes caused by the magnetic field by subtracting the monotone component I_{sm} and normalizing it: $I_{\mathrm{FP}} = (I - I_{sm})/I_{sm}$. Figure 3 shows the resulting spectrum of oscillations of I_{FP} in the range from 310 to 364 meV at different values of the magnetic field.

It can be seen that the magnetic field significantly weakens the intensity of Fabry-Perot oscillations. The attenuation becomes greater near the edge of the absorption band. We associate this attenuation with the Faraday rotation of the polarization plane of the light propagating through the sample. Despite the fact that unpolarized light was used in the experiment, Faraday rotation affects the transmission intensity due to self-interference: the transmitted waves add up with their reflections from the upper and lower boundaries of the sample. Reflected waves differ from directly transmitted waves in phases, as well as in the rotation angles of the polarization vectors.

A wave propagating through a sample with a thickness of d is described as $\Phi = e^{ikd}$, where its complex wave vector $k = k' + ik'' = n\omega/c$ is determined by the complex refraction index n, the frequency of light ω and the speed of light in a vacuum c. The real part k' describes a change of the phase of the wave, the imaginary part k'' describes a change of the amplitude of the wave. After passing through a sample with a thickness of d, the light transmission coefficient $T_\pm$ with right $(+)$ and left $(-)$ circular polarization can be described as

$$T_\pm = \frac{(1 - R^2)e^{i(k\pm b)d}}{1 - R^2 e^{i2(k\pm b)d}}, \tag{1}$$

where $R = |R|e^{i\varphi}$ — coefficient of reflection from the boundaries of surfaces, φ — phase shift of the reflected wave relative to the incident wave, b — rotation angle of the

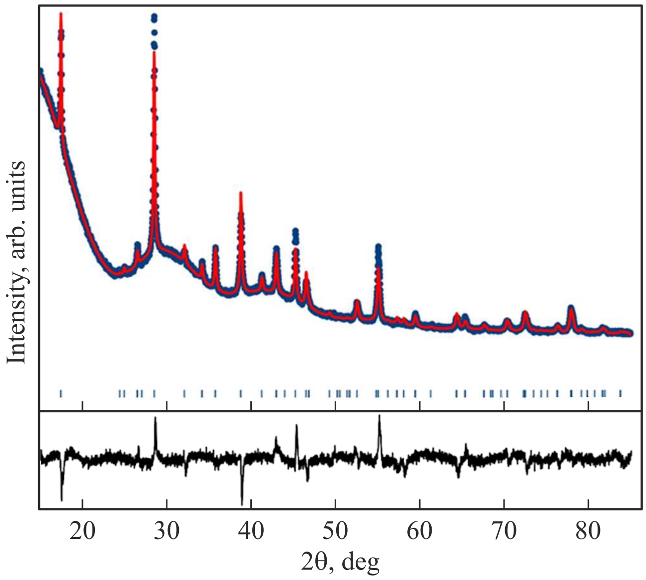

Figure 1. Experimental (circles) and calculated (red line) diffractograms, as well as the difference between them (black line at the bottom). The Bragg maxima are shown by vertical strokes. (The colored version of the figure is available on-line).

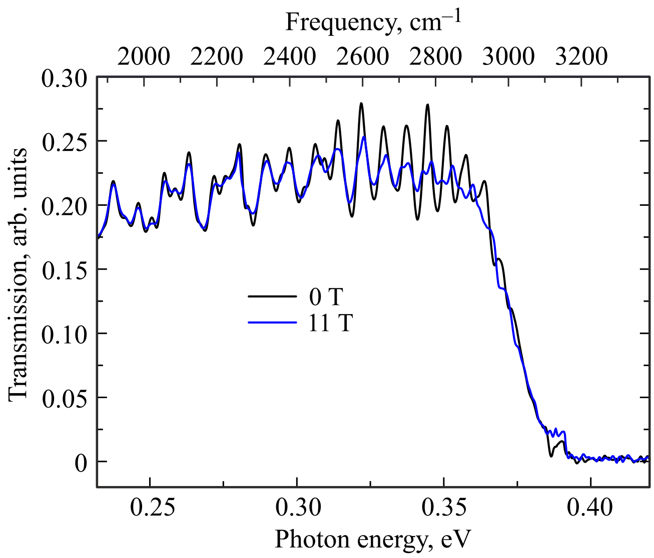

Figure 2. Transmission spectra measured in the magnetic field 0 and 11 T.

polarization vector per unit of sample thickness. The angle of rotation of the polarization vector ψ after passing through a sample with a thickness of d obeys Faraday's law [9] and is proportional to the magnetic field B: $\psi = bd = VBd$, where V is the Verde constant. The denominator is obtained as the sum of a direct wave (the amplitude of which is taken as one) and a wave after double reflection from two boundaries.

The intensity of transmission of linearly polarized light can be calculated as half the sum of the squares of the modules of the transmission coefficients for light with right and left circular polarization:

$$I = \frac{|T_+|^2 + |T_-|^2}{2}$$

$$= \frac{1}{2} \sum_{\sigma=\pm 1} \frac{|(1-R^2)|^2 e^{-2k''d}}{1+|R^2 e^{-2k''d}|^2 - 2|R^2 e^{-2k''d}| \cos[2((k'+\sigma b)d+\varphi)]}, \tag{2}$$

where $\sigma = \pm 1$ is for the light with right $(+)$ and left $(-)$ circular polarization.

The transmission intensity in the first approximation can be written as

$$I \approx (1 - 2\mathrm{Re}(R^2))e^{-2k''d} \times \left(1 + 2|R^2 e^{-2k''d}| \cos(2bd) \cos[2(k'd + \varphi)]\right). \tag{3}$$

Let $e^{-2k''d}$ be a constant η, then the monotone and oscillating parts in a limited range k can be written as

$$\langle I \rangle \approx (1 - 2\mathrm{Re}(R^2))\eta, \tag{4}$$

$$I_{FP} \approx \frac{I - \langle I \rangle}{\langle I \rangle} = 2|R|^2 \eta \cos(2bd) \cos[2(k'd + \varphi)]. \tag{5}$$

It can be seen from the formula (5) that the amplitude of the oscillations should decrease according to the following law in case of application of a magnetic field:

$$A_B = A_0 \cos(2VBd), \tag{6}$$

where A_0 and A_B — the amplitude of the oscillations at a zero magnetic field and in a field with a value of B, respectively.

Figure 4 shows the Fourier transform of the Fabry-Perot oscillations shown in Figure 3. The Fourier spectrum at 0 T is dominated by a harmonic with a Fourier frequency of 0.017cm, which, according to equation (5), corresponds to an optical thickness of $nd = 85\,\mu$m. The Fourier spectrum also contains other harmonics due to the inhomogeneity of the sample in thickness d. With a sample thickness of 10 mm, we obtain an estimate of the refraction index of $n \approx 8.5$. The resulting value is close to $n \approx 6$ for Bi_2Se_3 [5].

The inset to Figure 4 shows the dependence of the amplitude of the dominant harmonic on the magnetic field and its approximation by the function (6). The approximation allows estimating the Verde constant of $V \approx 10^3$ deg/cm · T, the value of which is consistent with the value obtained for Bi_2Se_3 [5].

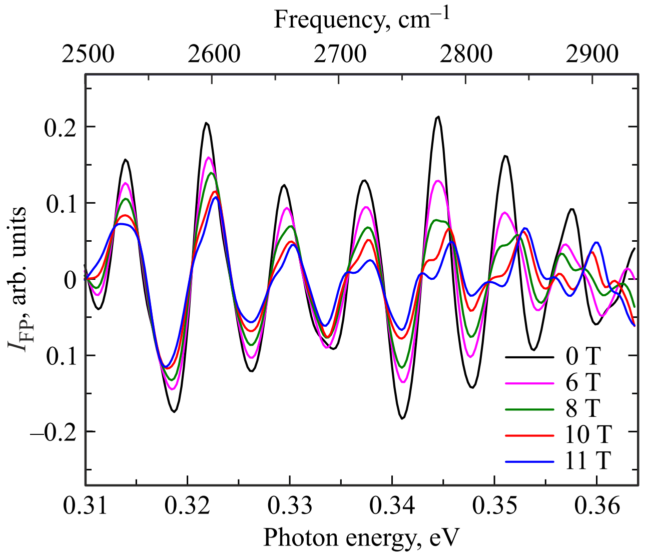

Figure 3. The spectrum of Fabry-Perot oscillations at different magnetic fields.

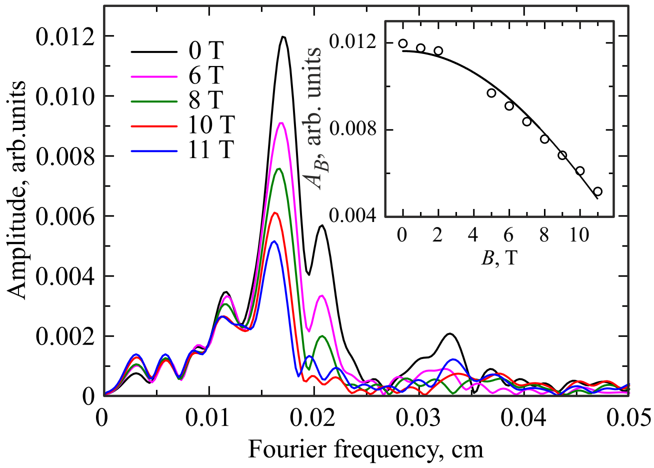

Figure 4. Fourier transform of Fabry-Perot oscillations with different magnetic fields. The inset shows the dependence of the amplitude of the dominant harmonic on the magnetic field (circles) and its approximation by the function (6) (split line).

5. Conclusion

The structural and electronic properties of thin layers of single crystals of a topological insulator Sb_2Te_2Se were studied using X-ray diffraction analysis and magnetooptical transmission.

The high structural quality of the lattice with the space group of $R\bar{3}m$ and the unit cell parameters $a = 4.1848(3)$ Å, $c = 29.9094(8)$ Å is confirmed by X-ray diffraction method.

The edge of the absorption band is visible in the infrared transmission spectra at 4.2 K, which allows estimating the band of $E_g \approx 374$ meV, as well as Fabry-Perot oscillations used to estimate the refraction index of $n \approx 8.5$.

The application of magnetic fields weakens the amplitude of Fabry-Perot oscillations. It is assumed that this is attributable to the Faraday rotation of the light polarization plane during the passage of the sample in a magnetic field. The average value of the Verde constant of $V \approx 10^3$ deg/cm $\cdot$ T was estimated in the range from 310 to 364 meV.

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Conflict of interest

The authors declare that they have no conflict of interest.

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