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Electrical and optical properties of a PtSn₄ single crystal

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Abstract. A topological semimetal PtSn₄ single crystal was grown by method of crystallization from a solution in a melt. Then the electrical resistivity and galvanomagnetic properties (magnetoresistivity and the Hall effect) were studied in the temperature range from 4.2 to 80 K and in magnetic fields up to 100 kOe. The optical measurements were carried out at room temperature. The residual resistivity is shown to be low enough and amount to $\sim 0.5 \mu\text{Ohm}\cdot\text{cm}$. The temperature dependence of the electrical resistivity has a metallic type, increasing monotonically with temperature. A sufficiently large magnetoresistance of 750% is observed. The majority carriers are supposed to be holes with a concentration of $\sim 6.8 \cdot 10^{21} \text{ cm}^{-3}$ and mobility of $\sim 1950 \text{ cm}^2/\text{V}\cdot\text{s}$ at $T=4.2 \text{ K}$ as a result of the Hall effect studies. The optical properties of PtSn₄ have features characteristic of “bad” metals.

1. Introduction

The study of new topological materials is an extremely important direction in modern condensed matter physics. These materials have a wide potential for applications in electronics and spintronics, since they have unique electronic properties that arise due to their unusual band structure. Topological semimetals (TSM) are defined as systems where the conduction and valence bands cross each other either at discrete points (Dirac and Weyl semimetals) or along closed lines (topological nodal line semimetals) in the Brillouin zone which are protected topologically [1-3].

A new type of TSM, Dirac node arc semimetal, was recently proposed in PtSn₄ compound, where the Dirac node arc structure is extended along a short line in the momentum space [3, 4]. At present, there are known works devoted to theoretical and experimental investigations of a PtSn₄ single crystal [3-7]. In particular, the authors of paper [5] investigated the electrical, galvanomagnetic and magnetic properties of a PtSn₄ single crystal. At the same time, there is practically no information about its optical properties in modern scientific literature. Therefore, it is interesting to carry out a comprehensive study of the electronic properties of a PtSn₄ single crystal, including its electrical resistivity, galvanomagnetic, and optical characteristics.

2. Experiment

PtSn₄ single crystals were grown by method of crystallization from a solution in a melt and had a residual resistivity ratio (*RRR*) of about 100. As in [5], the melt was Sn-rich, and the ratio of the initial



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components corresponded to the formula $\text{Pt}_{0.04}\text{Sn}_{0.96}$. Single crystals were grown in an alumina crucible. The crucible with the initial components was placed in a quartz ampoule, which was pumped out, heated, and kept for several days. Then the system was cooled to room temperature. PtSn_4 single crystals were isolated from the solidified melt by dissolving an excess of Sn in hydrochloric acid. The crystals were resistant to this effect.

PtSn_4 compound crystallizes in an orthorhombic structure, which can be visualized as consisting of Sn-Pt-Sn layers (figure 1(a)) [5]. The arrangement of the Pt and Sn layers is perpendicular to the b axis. Figure 1(b) shows the X-ray diffraction taken from the crystal plane (010). The lattice parameter $b = 11.325 \text{ \AA}$.

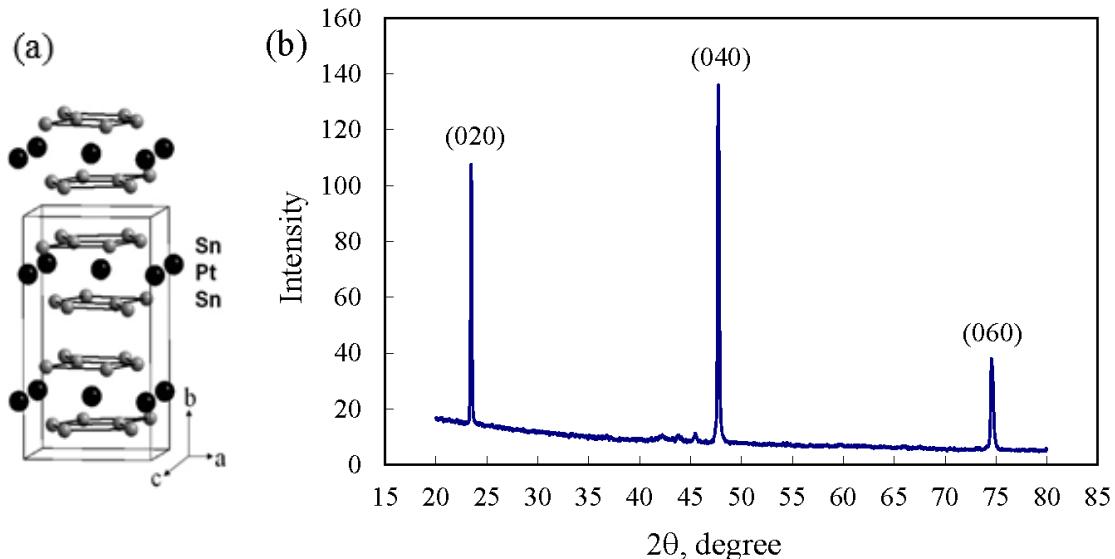


Figure 1. (a) Crystal structure of PtSn_4 [5]. (b) The X-ray diffraction pattern of PtSn_4 taken from the crystal plane (010).

The chemical composition of the sample was confirmed by X-ray microanalysis using an FEI Inspect F scanning electron microscope equipped with an EDAX X-ray microanalysis attachment. The microstructure of the surface was studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM). The research data confirmed the layered structure of the sample. The minimum detected layer thickness according to AFM was 20 nm. The electrical and galvanomagnetic properties were measured by the conventional 4-point method from 4.2 to 80 K and in magnetic fields of up to 100 kOe. The magnetic field vector was directed perpendicular to the crystal plane. The optical constants (refractive index n and absorption coefficient k) were measured by the Beatty method at room temperature with one reflection from the plane of the samples in the spectral range (0.2–5.0) eV. The experimental error of the optical constants n and k was 2–4% (in the middle infrared region (IR), it was ~6%). The values of n and k were used to calculate the real $\epsilon_1(\omega) = n^2 - k^2$ and imaginary $\epsilon_2(\omega) = 2n \cdot k$ parts of the complex permittivity, the real part of the complex optical conductivity $\sigma(\omega) = n \cdot k \cdot \omega / 2\pi$ (ω is the cyclic frequency of the light wave), and the reflectivity R , where R is determined by equation (1):

$$R(E) = \left[(n - 1)^2 + k^2 \right] / \left[(n + 1)^2 + k^2 \right]. \quad (1)$$

3. Results and discussion

Figure 2 presents the electrical and galvanomagnetic properties of a PtSn_4 single crystal. It can be seen from figure 2(a) that the temperature dependence of the electrical resistivity $\rho(T)$ has a metallic type,

and the residual resistivity is low ($\sim 0.5 \mu\text{Ohm}\cdot\text{cm}$). At the same time, there is a large positive magnetoresistivity

$$\Delta\rho_{xx}/\rho_0 = (\rho_{xx} - \rho_0)/\rho_0 \cdot 100\%, \quad (2)$$

where ρ_0 is the resistivity without a magnetic field and ρ_{xx} is the resistivity in a magnetic field. The value of $\Delta\rho_{xx}/\rho_0$ reaches 750% at $T=4.2$ K. Figure 2(b) shows the field dependences of the resistivity and magnetoresistivity at $T = 4.2$ K. The electrical resistivity and magnetoresistivity increase with increasing magnetic field H , which is associated with the effect of the Lorentz force on the movement of charge carriers. The analysis of the Hall effect data allowed us to establish that the majority carriers are holes (figure 2(c)), and to determine their concentration $n = 6.8 \cdot 10^{21} \text{ cm}^{-3}$ and mobility $\mu = 1950 \text{ cm}^2/\text{V}\cdot\text{s}$ at $T = 4.2$ K.

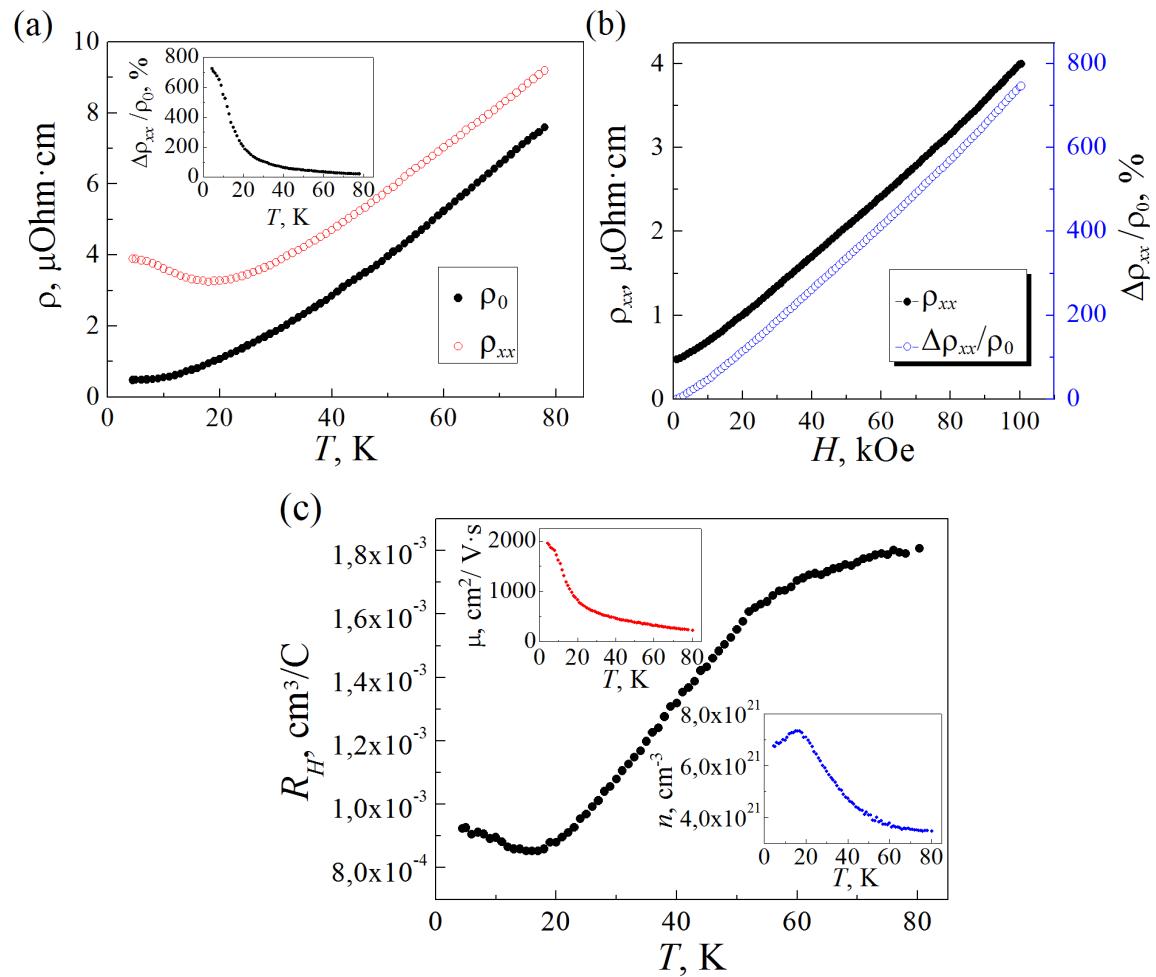


Figure 2. The electrical resistivity and galvanomagnetic properties of a PtSn₄ single crystal. (a) Temperature dependence of the resistivity without a magnetic field and in a magnetic field of 100 kOe. The inset shows the temperature dependence of the magnetoresistivity. (b) Field dependences of the electrical resistivity and magnetoresistivity. (c) Temperature dependence of the Hall coefficient. The inset shows the temperature dependence of the charge carrier concentration n and their mobility μ .

The Hall effect was studied in PtSn_4 single crystals in [5], where it was shown that the sign of the Hall coefficient changes and becomes positive at a temperature of about 30 K in a magnetic field of 50 kOe and, therefore, the majority carriers at $T > 30$ K are holes. This is in qualitative agreement with our results, given that the authors of [5] investigated very pure single crystals with the ratio $RRR = 1025$, which is much higher than $RRR = 100$ of our single crystal. This means that the conditions of stronger effective magnetic fields with higher $\omega_C\tau$ were implemented in [5] (ω_C is the Larmor frequency and τ is the relaxation time) [8].

The optical properties are presented in figure 3. The mechanism of intraband acceleration of electrons by the light wave field plays the main role in the formation of optical properties of metals and alloys in the IR spectral region [9]. Its contribution is determined by the parameters of conduction electrons, which are the plasma frequency Ω and the relaxation frequency γ , and decreases proportionally to the square of the incident light frequency ω . Negative values of the real part of the complex permittivity ϵ_1 in the IR spectral region are an optical criterion for the material conductivity of a metallic type. In the visible and ultraviolet (VUV) regions, the light absorption with the transfer of electrons from lower energy states to free upper ones dominates, which is called the interband absorption and gives information about the electron energy spectrum. The complex permittivity is the sum of the contributions from the intraband and interband absorption mechanisms that can coexist in a certain energy range. The graphs of the real $\epsilon_1(\omega)$ and imaginary $\epsilon_2(\omega)$ parts of the complex permittivity of a PtSn_4 single crystal (figure 3(a)) indicate that intraband optical transitions dominate in the IR region. In the longwave region of the spectrum, there are areas in which the dependence $1/\epsilon_1 = f(\omega^2)$ is described by a straight line. The slope of the straight line can be used to estimate the square of the plasma frequency of charge carriers ($\Omega^2 \sim 6 \cdot 10^{30} \text{ c}^{-2}$), and the cut-off segment on the ordinate axis (γ^2/Ω^2) gives the relaxation frequency ($\gamma \sim 2 \cdot 10^{14} \text{ c}^{-1}$). Negative ϵ_1 values in the VUV region indicate weak interband absorption. A similar effect was observed previously for other topological materials [10].

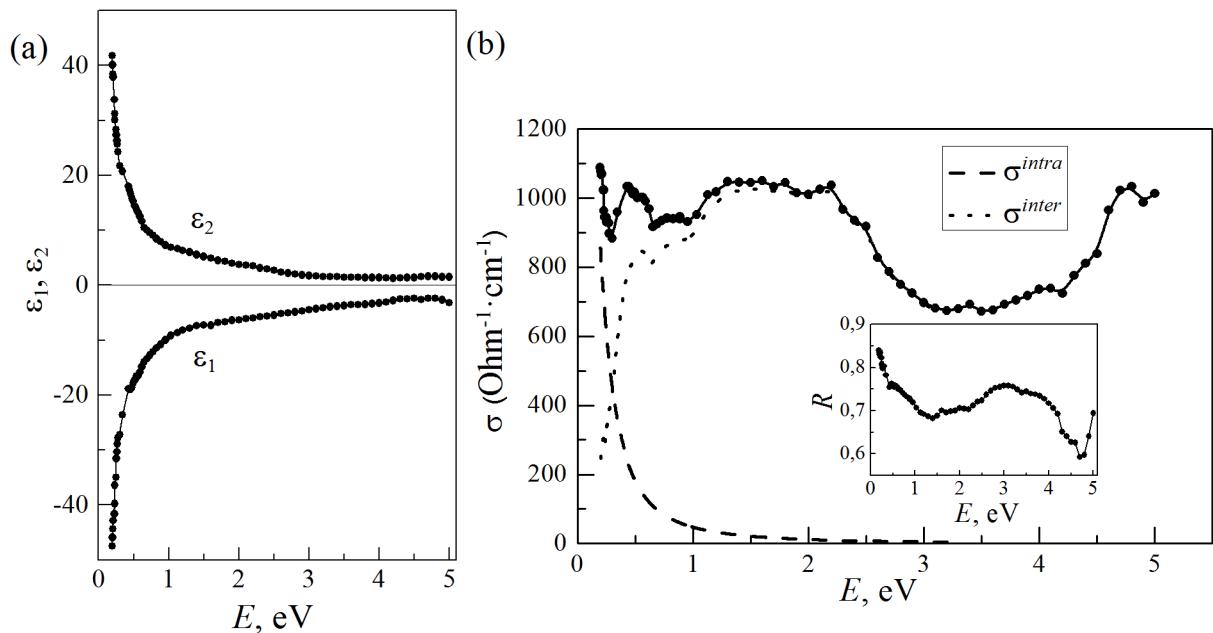


Figure 3. Dispersion of the real ϵ_1 and imaginary ϵ_2 parts of the complex permittivity (a) and optical conductivity $\sigma(\omega)$ (b) of PtSn_4 . The inset shows the dispersion of the reflectivity R .

Figure 3(b) shows the optical conductivity curve $\sigma(\omega)$ for a PtSn_4 single crystal. A rise in the optical conductivity is observed at energies of less than 0.3 eV, which can be associated with

intraband transitions (Drude rise). The estimated contribution of intraband absorption, shown by the dashed line, is calculated by the Drude formula (3) from the determined γ and Ω^2

$$\sigma_{intra} = \Omega^2 \cdot \gamma / (\omega^2 + \gamma^2) \cdot 4\pi. \quad (3)$$

This contribution decreases proportionally to the square of the incident light frequency ω and becomes negligible and disappears in the $E > 2$ eV range. After subtracting the intraband contribution from the experimental data, we obtain the contribution from interband transitions (dotted line). On the $\sigma(\omega)$ curve, peaks can be distinguished at energies of 0.44, 0.88 eV against the background of the Drude rise, indicating the presence of low-energy gaps in the band spectrum of the compound. In the VUV region, a wide band is formed in the 1-3 eV range. The minimum is in the 3-4 eV range and the subsequent growth of interband absorption is observed. As is known, the optical conductivity approaches the static σ_0 in the limit $\omega \rightarrow 0$. A significantly smaller value of static conductivity is obtained from estimates of γ and Ω^2 . This may be due to the fact that in an optical experiment it was not possible to reach the spectral region where only intraband absorption is present. The reflectivity dispersion of PtSn₄ (inset in figure 3(b)) in the IR region is characteristic of “bad” metals since its growth is observed in the intraband absorption region. In the VUV region, it has rather high values due to the low level of interband absorption. The features of the reflectivity curve correspond to the features of the $\sigma(\omega)$ curve: the maximum (minimum) of the reflectivity is observed in the region of the minimum (maximum) of the optical conductivity $\sigma(\omega)$.

4. Conclusion

Thus, the anomalies of the electrical and galvanomagnetic properties were observed, such as the low residual resistivity of ~ 0.5 $\mu\text{Ohm}\cdot\text{cm}$ with a relatively low concentration of charge carriers of $\sim 6.8 \cdot 10^{21} \text{ cm}^{-3}$, their high mobility of $\sim 1950 \text{ cm}^2/\text{V}\cdot\text{s}$ and large magnetoresistivity of $\sim 750\%$ at $T = 4.2$ K. The optical properties of PtSn₄ have features characteristic of “bad” metals. In the IR spectral region, interband absorption peaks are observed against the background of the Drude optical conductivity rise. This indicates the presence of low-energy gaps in the band spectrum of the compound. In the VUV regions of the spectrum, an absorption band is formed due to interband electron transitions.

Acknowledgments

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