EXPERIMENTAL AND THEORETICAL FIELD DEPENDENCES OF THE THERMOPOWER OF $Pb_{1-x}Sn_xTe$

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Abstract

Experimental studies of transport phenomena in $Pb_{1-x}Sn_xTe$ provide the most complete information on the kinetics and energy spectrum of charge carriers over a wide range of charge carrier concentration, impurities, and temperature.

Experimental field dependences of the thermopower of $Pb_{1-x}Sn_xTe$ with different carrier concentrations were determined at a temperature of 77 K in magnetic fields of up to 3 T; theoretical field dependences were calculated. The dependence of the thermopower on magnetic field exhibited a peak. The nonmonotonic dependence of the thermopower can be attributed to the anisotropy of the electron spectrum, the anisotropy of the electron relaxation time, and the multivalley pattern.

The differential thermopower was calculated using the formula given in the paper of V. D. Kagan, N. A. Red'ko, N. A. Rodionov, and V. I. Pol'shin. Satisfactory agreement between theory and experiment was obtained.

1. Introduction

Significant interest in studying the properties of narrow-gap semiconductors, particularly lead telluride–tin telluride single crystals, is attributed to wide possibilities of the practical use of these materials as detectors and radiation sources in the infrared spectrum, thermocouples, strain gauges, etc. At the same time, scientific interest in these materials is primarily associated with their unusual galvanomagnetic, thermomagnetic, and magneto-optical properties.

Calculation of kinetic coefficients in semimetals and narrow-gap semiconductors in general is an extremely difficult problem because it is impossible to strictly take into account all the factors related to charge transfer in the crystal owing to the strong nonparabolicity of the bands and the complex mechanism of carrier scattering.

However, an experimental study of transport phenomena in these semiconductors provides the most complete information on the kinetics and energy spectrum of charge carriers over a wide range of variation in the charge carrier concentration, impurities, and temperature.

2. Results and Discussion

The quality requirements for the samples under study are very high in order to obtain reliable experimental results: the volume distribution of the components must be uniform, and mechanical defects must be reduced to minimum. The most effective technique for preparing homogeneous $Pb_{1-x}Sn_xTe$ single crystals is the gas-phase growth method. We have developed a special technology for gas-phase growth of single crystals using high-purity Pb, Sn, and Te of the OSCh-0000 grade as initial materials (Te was purified by multiple zone recrystallization). Microstructural and spectral studies and Hall-effect measurements have confirmed the high quality of the prepared $Pb_{1-x}Sn_xTe$ (x = 0.18) single crystals.

To determine the concentration, charge sign, and mobility of carriers, measurements of the Hall effect and electric conductivity were conducted. Measurements of the temperature dependence of thermoelectric power, electric conductivity, and Hall effect in the same samples made it possible to calculate the parameters of $Pb_{1-x}Sn_xTe$ (x = 0.18). In our previous studies [1, 2], using $Pb_{0.82}Sn_{0.18}Te$ samples with the same carrier concentrations, the Shubnikov-de Haas oscillations and the temperature dependences of thermopower were examined. Based on the data, using the formulas given in [3–5], a number of kinetic coefficients were calculated (Table 1).

Table 1. Characteristics of $Pb_{1-x}Sn_xTe$ (x = 0.18) at 77 K

Sample	Carrier concentration p, 10^{17} cm^{-3}	Carrier mobility μ, cm^2/(V s), 10^4	Fermi energy, E_f, eV	$\frac{m_{eff}}{m_0}$, 10^2
3	5.2	0.37	0.03	3.1
4	2.6	1.91	0.017	1.8
5	0.52	2.34	0.066	0.6

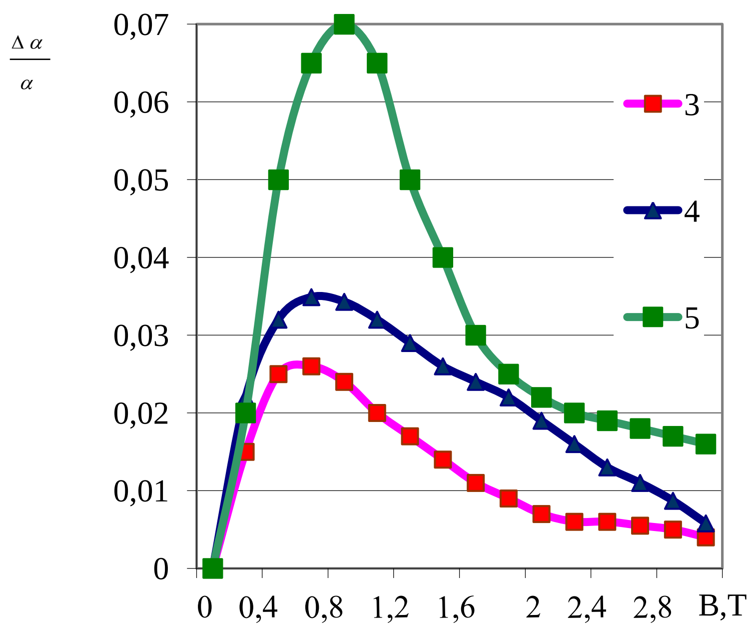

Fig. 1. Field dependences of differential thermopower $\frac{\Delta\alpha}{\alpha}$ on magnetic field induction B for three $Pb_{0,82}Sn_{0,18}Te$ samples with different charge carrier concentrations. Hole concentration, cm^{-3} ,77 K, 10^{17} : 3-5.2; 4-2.6; 5-0.52.

In this study, field dependences of the thermopower of $Pb_{0.82}Sn_{0.18}Te$ samples at different carrier concentrations ($0.52 \cdot 10^{17}$ to $5.2 \cdot 10^{17}$ cm^{-3}) have been examined. The results have shown that the thermopower heavily depends on charge carrier concentration (Fig. 1)

Using the experimental data shown in Fig. 1, the field dependences of differential thermopower $\frac{\Delta\alpha}{\alpha}$ of $Pb_{0,82}Sn_{0,18}Te$ at different carrier concentrations were calculated. The theoretical calculations were based on the following analytical dependences of $\frac{\Delta\alpha}{\alpha}$ on magnetic field induction *B*:

$$\frac{\Delta\alpha(B)}{\alpha(0)} = k[1 + \frac{\Omega^2\tau^2(\delta - 2) - \delta}{(1+\Omega^2\tau^2)(\delta + \Omega^2\tau^2)}] \tag{1}$$

$$k = \frac{3\left(1 + 2\frac{E_f}{E_g}\right)}{2\left(1 + \frac{E_f}{E_g}\right)} - \beta \tag{2}$$

$$\Omega = \frac{eB}{m_{eff}} \tag{3}$$

where Ω is the cyclotron frequency, τ is the charge carrier lifetime, E_f is the Fermi energy, E_g is the bandgap, β is an adjustable parameter associated with the dependence of relaxation time τ and effective mass m_{eff} on the Fermi energy, and δ is the parameter that takes into account the energy spectrum anisotropy.

Equation (1) implies that the function of $\frac{\Delta\alpha}{\alpha}$ has a maximum at

$$(\Omega\tau)^2 = \frac{\delta + (\delta - 1)\sqrt{2\delta}}{\delta - 2} \tag{4}$$

Thus, the experimental data on $\frac{\Delta\alpha}{\alpha}$ shown in Fig. 1 make it possible to calculate the charge carrier lifetime τ and determine the δ value from two magnetic field inductions at which the $\frac{\Delta\alpha}{\alpha}$ values are equal. Table 2 lists the τ values calculated according to the experimental data.

Table 2. Carrier concentration, differential thermopower and charge carrier lifetime of $Pb_{1-x}Sn_xTe$ (x = 0.18) at 77 K

Sample	Carrier concentration p, 10^{17} cm^{-3}	$\frac{\Delta\alpha}{\alpha}_{max}$ B, T	τ, 10^{-12} s
3	5.2	0.058	1.65
4	2.6	0.06	0.992
5	0.52	0.08	0.24

From the relationship $\frac{\Delta\alpha(B_1)}{\alpha} = \frac{\Delta\alpha(B_2)}{\alpha}$, according to formula (1), the δ value was found to be 4.22. At known τ and δ, considering k as an adjustable parameter, according to formula (1), the field dependences of differential thermopower $\frac{\Delta\alpha}{\alpha}$ of $Pb_{0,82}Sn_{0,18}Te$ at different charge carrier concentrations were calculated; the results are shown in Fig. 2.

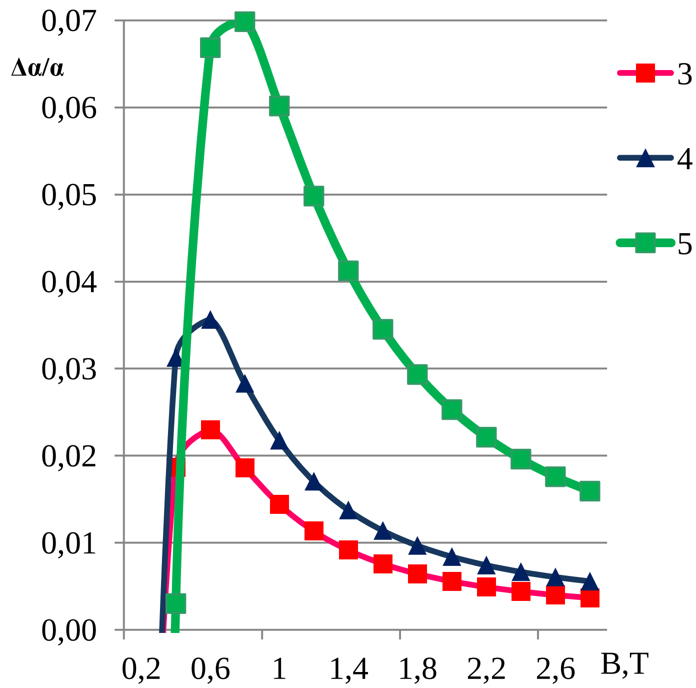

Fig. 2. Calculated field dependences of differential thermopower $\frac{\Delta\alpha}{\alpha}$ on magnetic field induction B for three $Pb_{0,82}Sn_{0,18}Te$ samples with different charge carrier concentrations. Hole concentration, cm^{-3}, 77 K, 10^{17} : *3*-5.2; *4*-2.6; *5*-0.52.

Comparison of the data in Figs. 1 and 2 shows satisfactory agreement between the experimental and calculated data.

A comprehensive study of the temperature dependence of thermoelectric power, electric conductivity, and Hall effect and the dependence of thermoelectric power on magnetic field induction conducted using the same samples has made it possible to calculate a number of kinetic parameters of three $Pb_{1-x}Sn_xTe$ ($x = 0.18$) samples with different charge carrier concentrations.

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