EXPERIMENTAL AND THEORETICAL TEMPERATURE DEPENDENCES OF THE THERMOPOWER OF $Pb_{0.82}Sn_{0.18}Te$

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Abstract

In this study, the temperature dependences of the thermopower of five samples of $Pb_{0.82}Sn_{0.18}Te$ at different carrier concentrations ($0.52 \cdot 10^{17}$ to $15 \cdot 10^{17}$ cm^{-3}) were analyzed. The results showed that the thermopower heavily depends on charge carrier concentration. At low concentrations of charge carriers, the temperature dependences of thermopower exhibit a nonmonotonic behavior and have a maximum. A two-band Gottwick model with a linear temperature term was used to interpret the experimental data. In this approximation, it is assumed that a Lorentz resonance takes place near the Fermi surface. This model makes it possible to determine the Fermi energy, as well as the position and width of the resonance, from experimental data.

Significant interest in studying the properties of narrow-gap semiconductors, particularly lead telluride–tin telluride single crystals, is attributed to wide possibilities of their practical use 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.

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.

In this study, the temperature dependences of the thermopower of five $Pb_{0.82}Sn_{0.18}Te$ samples at different carrier concentrations ($0.52 \cdot 10^{17}$ to $15 \cdot 10^{17}$ cm^{-3}) have been examined. The results have shown that the thermopower heavily depends on charge carrier concentration. For low concentrations of charge carriers, the temperature dependences of the thermopower are nonmonotonic and exhibit a maximum.

Figure 1 shows the derived typical temperature dependences of the thermopower of $Pb_{1-x}Sn_xTe$ ($x = 0.18$) at different concentrations of charge carriers. Samples with a low carrier concentration exhibit the thermopower sign reversal, which is indicative of the transition to the intrinsic conduction region (curves *4* and *5* in Fig. 1). The thermopower sign reversal for samples with a lower concentration of charge carriers is observed at lower temperatures.

Generally, it is fairly difficult to calculate the kinetic coefficients in semimetals and narrow-gap semiconductors because it is impossible to strictly take into account all the factors associated with the charge transfer in the crystal owing to strong nonparabolicity of the bands and

the complex mechanism of carrier scattering. Nevertheless, experimental studies of transport phenomena in these semiconductors provide the most complete information on the kinetics of charge carriers and their energy spectrum under a wide variation in temperature and concentrations of charge carriers and impurities.

The derived experimental data were interpreted using a two-band model with a linear temperature term proposed by Gottwick [1-4]. This approach assumes that Lorentzian resonance occurs in the vicinity of the Fermi surface. This model makes it possible to determine the Fermi energy and the position and the width of the resonance from experimental data.

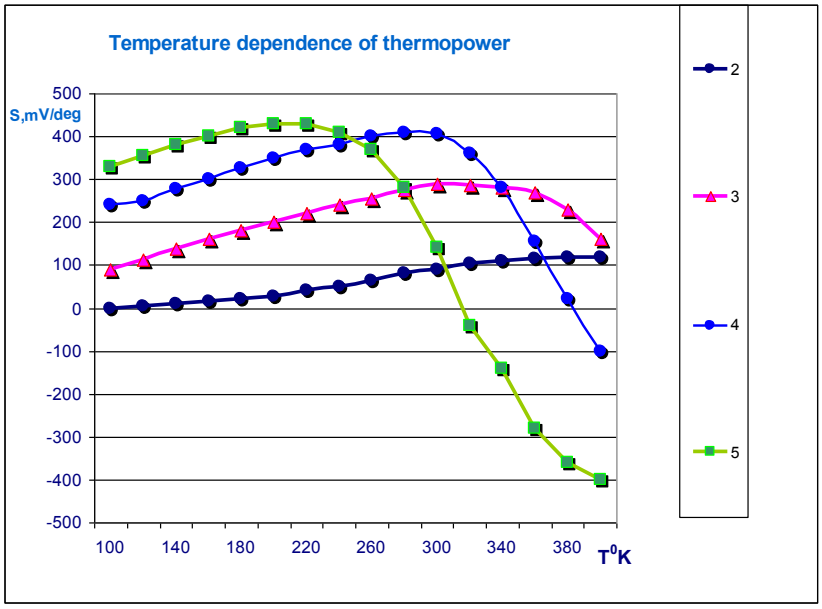

Fig. 1. Temperature dependence of the thermopower of $Pb_{0.82}Sn_{0.18}Te$ at different carrier concentrations: hole concentration, 10^{17} cm^{-3}, 77 K.

2	3	4	5
15	5.2	2.6	0.52

For theoretical analysis in terms of this model, we use the following formulas:

$$S(T) = \frac{AT}{B^2 + T^2} \tag{1}$$

$$A = \frac{2(E_0 - E_F)}{e} \tag{2}$$

$$B^2 = 3\frac{(E_0 - E_F)^2 + \Gamma^2}{\pi^2 k_B^2}, \tag{3}$$

where S(T) is the thermopower, T is the temperature, and A, B are constant coefficients.

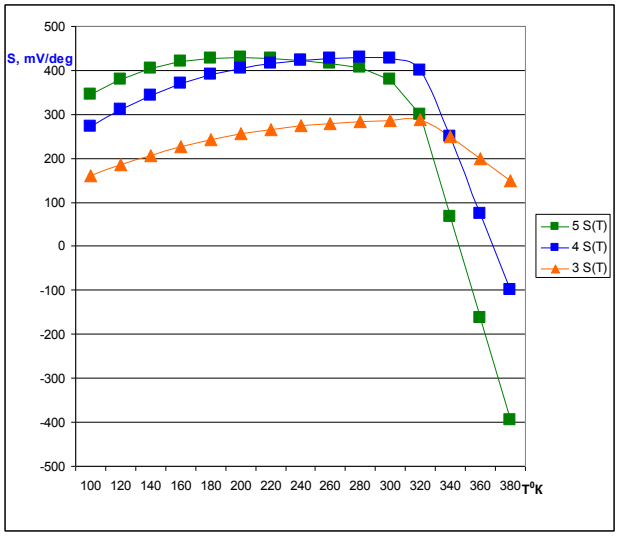

Fig. 2. Calculated temperature dependences of the thermopower of $Pb_{0.82}Sn_{0.18}Te$ at different carrier concentrations:

hole concentration,	10^{17} cm^{-3}, 77 K	
3	4	5
5.2	2.6	0.52

The table 1 lists parameters A, B, E_0, and Γ calculated by formulas (1)–(3).

Table 1. Parameters A, B, E_0, and Γ calculated by formulas (1)–(3)

	$S(T)_{max}$	B, K (B=T)	A, eV/C	E_F, eV	E_0, eV	Γ, eV
5	430	200	$5.38 \cdot 10^{17}$	0.066	0.043	0.021
4	410	280	$7.18 \cdot 10^{17}$	0.017	0.057	0.016
3	288	300	$5.40 \cdot 10^{17}$	0.03	0.043	0.0449

where C is coulomb.

The E_0 and Γ (gamma) are determined by the position of the center and the width of the resonance on the energy axis, respectively.

The resonance peak defined by formula (1) adequately describes the temperature dependence S(T). The thermopower passes through a maximum at the T = B point. Thus, we can determine B and calculate A, E_0, and Γ. The calculated temperature dependences of the thermopower of $Pb_{0.82}Sn_{0.18}Te$ at different carrier concentrations are shown in Fig. 2.

References

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