

The Peculiarities of The Electrical and Thermoelectrical Properties of p-Type Ag_2Te

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Abstract

The electrical and thermoelectrical properties of p-type Ag_2Te have been investigated. Various peculiarities were observed: the minimum (at $T \approx 65$ K) and maximum (at $T \approx 200$ K) on the temperature dependence of conductivity $\sigma(T)$; the weak dependence of Hall coefficient $R(T)$ (in 200-300 K range) and the maximum (at $T \approx 100$ K and 250 K) on the temperature dependence of thermal power $\alpha_0(T)$. The investigation results were interpreted by two-bands model. It is shown that mentioned peculiarities have been stimulated by the narrow gap of Ag_2Te and its temperature dependence.

1. Introduction

The silver telluride is the narrow-band semiconductor with high electron mobilities and Kane's dispersion law. The electrical properties of p- Ag_2Te were investigated less than n- Ag_2Te . The investigations were made principally in the middle temperatures ($77 \text{ K} \leq T \leq 400 \text{ K}$), but the information was not too exact. To receive more precise data about band parameters it is necessary to investigate the samples of n- and p-types. In this work the electrical and thermoelectrical properties of p- Ag_2Te have been investigated at the temperature range of 4.2-300 K.

2. Experimental Results

The p-Ag₂Te samples were produced with 0.05; 0.25 and 0.75 at % Te surpluses. It was shown previously that the Te surplus in Ag₂Te (less than 1%) leads as shallow acceptor impurity, the display of the second phase and the changes of crystal structure were not observed. Fig. 1 shows the temperature dependencies of the Hall coefficient R for the samples series with different doping levels. It is shown the R independent on T in 4.2 K range, in 50-60 K interval the R abruptly decreases, it changes sign (on n-type). After passing through maximum at T≈80 K the Hall coefficient exponentially decreases up to 180 K, then in 200-300 K range the R(T) is strongly slowed. Fig. 2 shows the characteristic temperature dependence of conductivity σ . It is seen that in 4.2-50 K interval the σ practically does not depend on T, at T≈65 K it passes through minimum, then σ increases with T and at 200 K it passes through maximum. Fig. 3 shows dependent of thermal power on versus temperature. At low temperatures (to 50 K) σ_0 linearly increases with T, in 50-200 K range the $\sigma_0(T)$ -dependence repeats the character of R(T)-dependence. Starting from 200 K the $\alpha(T)$ -dependence increases (different from R(T)) and passes through the maximum at 230 K. We can tell about the next peculiarities of Ag₂Te: 1. The minimum (at 65 K) and maximum (at 200 K) on curve $\sigma(T)$. 2. The faint dependence of R(T) in 200 - 300 K range. 3. Two maximums of $\alpha_0(T)$ at 100 K and 270 K.

3. Discussion

The minimums of $\sigma(T)$ in InSb and Cd_xHg_{1-x} The have been observed [1,2]. The authors have been assuming that the minimum in Cd_xHg_{1-x} has been stimulated by resonance scattering of electrons by the optical phonons, and it InSb has been stimulated by high value of ratio of electrons and holes mobilities ($b=U_e/U_h$). The second model is probably suitable for p-Ag₂Te, but increasing of n(T) will also play an important role as you can see below. The maximum of $\sigma(T)$ has been observed in T≈40-60 K range when at low temperatures there are the degeneration and Rutherford's scattering of charge carries. With T - rising the degeneration degree decreases, the mobility rises, then the scatter by phonons is displayed. These facts lead to decrease of mobility. But the maximum $\sigma(T)$ in Ag₂Te was observed in p-type-sample, i.e. in intrinsic conductivity region. In [3] the $\sigma(T)$ in Ag₂Te was observed also in 300-350 K interval. The authors have been assumed this fact is caused by $\beta_1 \rightarrow \beta_2$ -type phase transition.

In [4] the results of R(T) investigation have been presented in 80-300 K region, and it was noted the R independent on T in 250-300 K interval. According to the theory of intrinsic conductivity the R must decrease, and above - mentioned R(T)-dependence can be presented as anomaly. For explanation this experimental result it is expected the exist of impurity levels at the bottom of conduction band, the second low-field valence band etc.

The next peculiarity is $\alpha_0(T)$ -rise in 200-300 K interval. According to theory in intrinsic region the decrease of α_0 must be continue. In [5] the increase of thermal power

with decrease of T has been analyzed in 200-80 K interval. It is noted this fact has been probably stimulated by phonon drag of electrons.

As shown all ideas explained the nature of observed peculiarities are based on data at $T \geq 77$ K and they have qualitative character. It is guessed that the Te - surplus leads to decrease of electron concentration only and the data have been analyzed in framework of one-band model. There are serious divergences and contradictions in band parameter data, specially about the width of forbidden gap. Thus it is necessary to make the quantitative interpretation of electrical properties of p- and n-Ag₂Te in wide temperature and magnetic field intervals in two-band assumption to receive the final conclusions about mentioned anomalies. This analysis for n-Ag₂Te were made in [6-8]. The band parameters have been obtained; the dispersion law, the principal mechanism of electron scattering, the character of electron-electron and electron-phonon interactions have been found. These results allow to lead quantitative comparison of electrical properties in p-Ag₂Te also (including mixed and intrinsic regions of conductivity).

This comparison in mixed conductivity region is not difficult, consequently we have given here the calculation methods of R, σ and α_0 in weak magnetic fields in the framework of two-band model. According to this model these kinetic coefficients are described by:

$$R = \frac{1}{N_A e} \frac{(1-c)(1-b^2c)}{(1+bc)^2} \quad (1)$$

$$\sigma = N_A e U_e \cdot \frac{1+bc}{b(1-c)} \quad (2)$$

$$\alpha_0 = \frac{\alpha_e \delta_e + \alpha_h \delta_h}{\delta_e + \delta_h} \quad (3)$$

here N_A is acceptor concentration; $b = \frac{U_e}{U_n}$ and $c = \frac{n_e}{n_h}$ are the ratios of mobilities and concentrations of electron (e) and mobility hole (h), respectively; α_e and α_h are the partial thermal powers of electrons and holes; δ_e and δ_h are respective conductivity of carriers. As shown for quantitative calculation of R(T) it is necessary to know the data b(T), $U_e(T)$, and c(T). The value of b has been found from R data in inversion point and at maximum magnitude of the hall coefficient:

$$R_{max} = \frac{(1-b)^2}{4beN_A}, \quad (4)$$

and the value N_A equal to the concentration of electrical active impurities.

Well, in the sample with $n_h^0 = 6.25 \times 10^{16} \text{ cm}^{-3}$, R is independent on the temperature range of 4-40 K and until 60 K exhibits n-type character. After that temperature it becomes p-type. At about 80 K it has a maximum and then decreases gradually until 180 K. In between 200 K and 300 K it is almost independent on temperature. At the temperature, inversion of sign with R occurred, the parameters are b=9; c=0.0124 and after 80 K, are b=8; c=0.125. In mixed conductivity region

$$b = \frac{n_r}{n_{int}} \cdot \frac{n_{int}/n_A + \sqrt{1 + \frac{n_r}{N_A}}}{1 - \frac{n_{int}^2}{n_r N_A}} \quad (5)$$

$$c = \frac{n_{int}}{n_h^0 + n_{int}}, \quad (6)$$

here $n_r = n_h - n_e$, $n_{int}^2 = n_h \cdot n_e$.

As shown the part of calculations requires the determination of $n_{int}(T)$. In narrow-band semiconductors when the valence band is parabolic, the conduction band is parabolic, the intrinsic concentration is determined by

$$n_{int} = (2m_e k_0 T)^{3/2} 3\pi^2 \hbar^3 \cdot I_{3/2,0}^0(\eta_i^*, \beta), \quad (7)$$

here $\eta_i^* = \frac{E_F}{k_0 T}$ is the reduced chemical potential (E_F is the Fermi level), $\beta = \frac{k_0 T}{\epsilon_g}$ is unparabolicity parameter (ϵ_g is width of forbidden band). The value of η_i^* is determined from

$$m_e^{3/2} \cdot I_{3/2,0}^0(\eta_i^*, \beta) = m_h^{3/2} \cdot F(-\eta_i^*), \quad (8)$$

here $I_{3/2,0}^0(\eta_i^*, \beta)$ is two parameter and $F_{3/2}(-\eta_i^*)$ is one-parameter Fermi integrals. Taken into an attention the data of $m_h = 0.12m_0$ (6,8) $m_e = 0.025m_0$ the values of b, c and η_i^* have been calculated. Fig. 4 shows the calculation results of temperature dependencies of b(T), $\eta_i^*(T)$ and c(T). On the basis these data the temperature dependencies of R have been calculated (Fig. 1). The calculations show that the temperature dependence of R is very sensitive for the value of the forbidden band width, especially at the temperature of R-sign inversion and in maximum region. Fig. 1 shows the calculated R(T) - curves for some ϵ_g values. As shown at $T < 200$ K the best accordance of the experimental and calculated data takes place at $\epsilon_g(T) = (0.035 - 7 \times 10^{-5})eV$.

It is noted there are too much information about ϵ_g in literature ($0.7 \pm 0.04eV$). The recent investigations indicate on lower values of ϵ_g in comparison with data from starting works. On Fig. 1 the calculated and experimental data allow to say that the obtained value of ϵ_g and its temperature dependence are more precise.

The analysis of formulae (2) shows that the $\sigma(T)$ -dependence passes through minimum when the condition $n_h = b^2 n_e$ occurs. This condition for the Ag_2Te sample with $n_h^0 = 6.25 \times 10^{16} cm^{-3}$ takes place at $T \approx 60 \pm 5$ K.

The formulae (2) shows that it is necessary to know $U_h(T)$, $U_e(T)$, $n_h(T)$ for quantitative calculation of $\sigma(T)$.

In impurity region of conductivity (4-50 K) the temperature dependence $U_h \sim T$ has been determined by σ and R data. At $T > 50$ K the mobility U_h must decrease according $U_h \sim T^{1.5}$ law (the scatter on acoustic phonons). The electron mobility has been calculated by U_n and b data ($U_e = bU_n$). Figure 5 shows calculated curves of $U_h(T)$ and $U_e(T)$. Fig. 2 shows the calculated dependence of $\sigma(T)$ for the sample with $n_h^0 = 6.25 \times 10^{16} cm^{-3}$

in comparison with experimental data. It is shown the good agreement the experimental and calculated data have been observed.

The analogous calculations have been made for the $\alpha_0(T)$ -dependence and they have been presented on Fig. 3 in comparison with experimental data. It is shown that, besides of T-region where the phonon drag of carriers was proposed, the calculated curve agrees with experimental data.

In this part of the present work we deal with the regions of $R(T)$ and $\alpha_0(T)$ peculiarities, especially with the $R(T)$ dependence at $T=200-300$ K. It is noted in this interval of T the $R(T)$ is not constant (as presented in literature), but it slowly depends on T. The calculations show the slow $R(T)$ dependence has been stipulated by the weak temperature dependence of the intrinsic electron concentration, playing dominant role in this T-region due to them high mobility. The high mobility has been stipulated by the very narrow forbidden band width. Authors: your sentence is incomplete. The $\epsilon_g(T)$ dependence leads to fact that the Ag_2Te is practically gapless ($\epsilon_g \approx 0.008\text{eV}$) at 350 K. Starting from $T \approx 120$ K the Fermi level dipped into the conduction band (see Fig. 4 a), there was degeneration of electron gas the unparabolicity of conduction band starts to play an important role.

The calculations show that the decrease of R with T is no more than 1-10 % in the 200-300 K interval. On the basis of the above-mentioned it may explain the rise of thermal power and decrease of conductivity versus temperature at $T \geq 200$ K. When the concentration is constant the thermal power must increase practically linear with T. The calculations show that the electron deposit in thermal power plays dominant role at weak temperature dependence of α_0 .

The calculations show that the decrease of electron mobility with T is more abrupt and it starts before ($T \approx 50$ K) than for holes (Fig. 5). It leads to a decrease of $b = \frac{U_e}{U_n}$ and σ values in this T-region. But at $T > 60$ K the strong rise of $n_{int}(T)$ leads to an increase of σ , and this fact stipulates the passing of σ through minimum.

4. Conclusions

Similar results belonging to InSb and $\text{Cd}_x\text{Hg}_{1-x}$ are in literature [1,2]. Their characteristic behaviors depend on resonance dispersion of electrons (for $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$) and activity of electrons and holes (for InSb). The second mechanism is more convenient to the explanation of the results given above for p- AgTe . Increasing of $n(T)$ can be interpreted as below. Because of the carrier dispersion at low temperatures, the maximum of $\sigma(T)$ appears at temperatures between 40 K. Through the increasing of the temperature, degeneration of the carriers disappears, but the mobility of the carriers decreases (see Fig. 5). For the p-type crystals, maximum can be seen at 300-350 K. It can be related phase transition. That $R(T)$ is independent of temperature in the range 200-300 K has been shown above. According to self conductivity theory, it can be said this phenomena is an anomaly, so $R(T)$ must decrease in this temperature region. Perhaps it may be related with the admixtures of the levels in the conductivity band or the second low one.

It is also worthwhile to note the increasing of $\alpha(T)$ between 200 and 300 K, while $\alpha(t)$

increases with decreasing temperature in the range 200-300 K, in the self-conductivity band.

It is guessed that the surplus of Tellurium caused a decreasing of electron concentration according to the single band model. There are big differences and contradictions in values of the band parameters, especially in that of the band gap. The results deduced above should be verified by further though tedious work, and comparison experimental data. The double band model must be tested over the wide range of temperatures of magnetic fields. Some properties of n-type AgTe, such as band parameters, dispersion relation of the collision between electrons have been previously studied.

This work allows us to compare the electrical properties of the p-AgTe including mixed and pure bands of conductivity with that of n-AgTe. These calculations are in agreement with the predictions of the double band model.

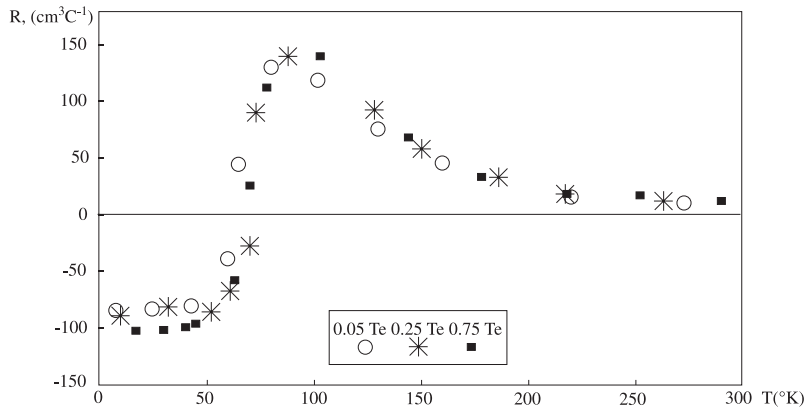


Figure 1. Dependence of the Hall coefficient versus temperature in p-Ag₂Te with Te surplus.

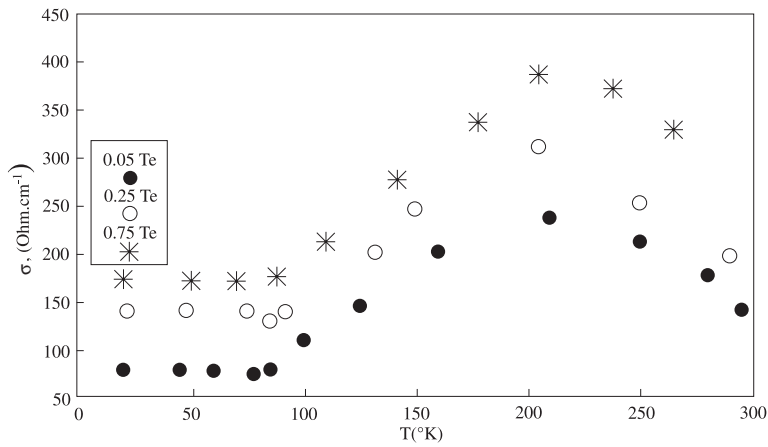


Figure 2. Temperature dependence of conductivity.

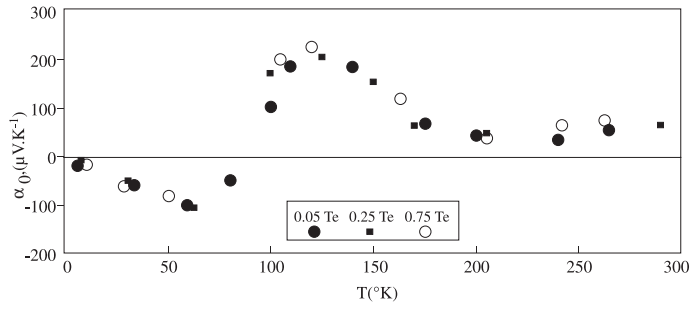


Figure 3. Dependence of thermal power versus temperature.

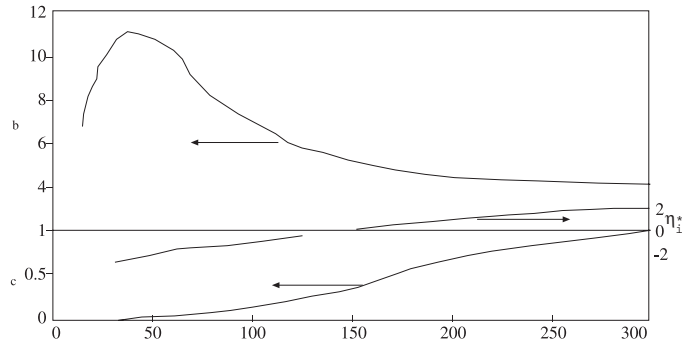


Figure 4. Temperature dependences of the ratio of carrier mobilities $b = U_e/U_n$: (1) the reduced chemical potential η_i^* ; (2) and the ratio of carrier concentrations $c = n_e/n_h$. The lines show the calculations of different ε_{g_0} values (marking as in Figure 1).

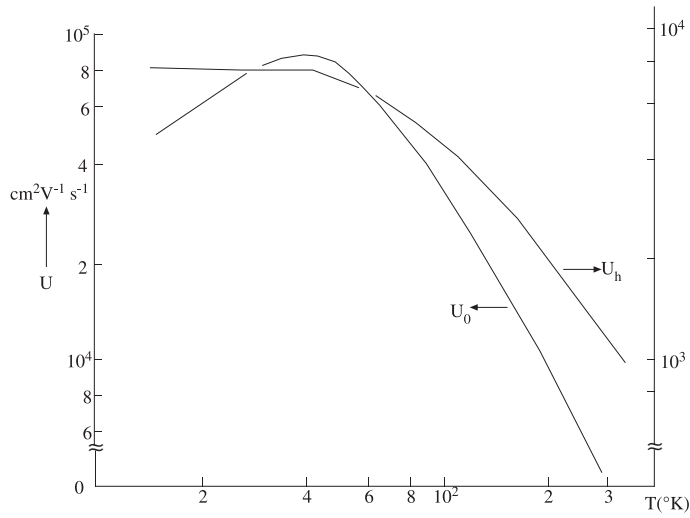


Figure 5. The temperature dependences of the electron and hole mobilities.

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