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Electric and thermoelectric properties of the $In_{0.5}Ga_{0.5}Sb$ equimolar composition

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ABSTRACT: *The temperature dependences of the Hall coefficients, electrical conductivity, and thermal emf of $In_{0.5}$ $Ga_{0.5}Sb$ temperature range of 80-600 K have been studied. The data obtained is interpreted in the framework of the three-band model, ie, based on a complex model of the valence band, states from two overlapping subbands with different density states and conduction band. It was determined the value of the energy gap between the subbands (Δ = 0.005 ± 0.001 eV) and its adopted temperature coefficient ($d\Delta / dT$ = -2.6 •10^{-4}eV / K) the effective mass of heavy and light holes and electron have been calculated.*
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A^{III} B^{V} compounds have recently been widely used in the manufacture of various semiconductor devices. Therefore, an intensive study of the properties of compounds led to the discovery of a number of fundamentally new phenomena of great importance for the technique of electronic devices and contributed to the substantial development of solid-state physics. An intensive study of this type of compound is due to their features, which differ from previous semiconductors. In this sense, the investigation of InhGa0xSb solid solutions attracts a lot of researchers interest/

It is known that [1,2] in these solid solutions, the width of the forbidden band Eg varies from 0.7 eV (GaSb) to 0.23 eV (InSb). The author [3] studying the change in the band structure and concluding that solid solutions of In1-xGaxSb have a complex band structure. Of particular interest is the study of the band structure in the isomolar composition (x = 0.5) and its effect on the kinetic properties of the crystal. For this purpose, the temperature dependences of the electrical conductivity (σ), the Hall coefficients (R) and the thermal emf (α) in the sample In0.5Ga0.5Sb were investigated.

The solid solution In0.5Ga0.5Sb is obtained by band equalization at various speeds [4]. The measurements of σ, R and α were carried out on samples with ohmic contacts at constant current [5] and constant magnetic fields up to 1400 A / m. The measurement error is not exceeded ~ 5%.

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I. Experimental Results.

Figure 1 shows the temperature dependence of the Hall coefficient R. It is seen that R (T) to T ~ 110 K is independent of T, then increases with increasing temperature to T ~ 250 K and at T ~ 350 K changes sign to negative, reaches of the maximum modulo / R / at T ~ 450 K and then gradually decreases with the onset of intrinsic conductivity. Figure 2 shows the temperature dependence of the thermal emf α, which increases approximately linearly to T ~ 200 K, and then changes the sign of p to n. At T ~ 200 and T ~ 350 K, the maxima appear on the α (T) curve. Figure 3 shows the temperature dependence of the electrical conductivity σ. As can be seen from Fig.3, σ (T) to T ~ 350 K monotonically decreases and starting from T ~ 400 K with the onset of intrinsic conductivity it exponentially increases.

II. Theoretical Analysis.

The complex behavior of R (T), σ (T), and α (T) is analyzed in the framework of the three-band model (two kinds of holes and electrons), according to which [6]

$$R = \frac{1}{e}\frac{n U_n^2 - P_L U_L^2 - P_h U_h^2}{(\sigma_n + \sigma_L + \sigma_h)^2} \quad (1)$$

$$\alpha = \frac{\alpha_h \sigma_h + \alpha_L \sigma_L - \alpha_n \sigma_n}{\sigma_n + \sigma_L + \sigma_h} \quad (2)$$

$$\sigma = e(nU_n + p_h U_h + p_L u_{L)} = \sigma_n + \sigma_h + \sigma_L \quad (3)$$

where pL, ph, n - concentration of light, heavy holes and electrons, σ_L, σ_h, σ_n and α_L, α_h, α_n - partial electrical conductivity and thermal emf.

Plateau in R (T) up to ~ 90 K means that conductivity is provided by one type of charge carriers (light holes). This makes it possible to determine the effective mass of light holes. In the case of a quadratic dispersion law, at any degree of degeneracy, the thermal emf in a classically strong magnetic field is described by the formula [6]

$$\alpha_\infty = -\frac{\kappa_0}{e}\left[\frac{5F_{3/2}(\mu^*)}{3F_{1/2}(\mu^*)} - \mu^*\right], \qquad (4)$$

Where μ *- is the reduced chemical potential, F (μ*) is the one-parameter Fermi integral. It is known that a thermal emf with a strong magnetic field is expressed

as $\alpha_\infty = \alpha + \Delta\alpha_\infty$, where $\Delta\alpha_\infty$ is the magneto-thermoelectric emf in a classical strong magnetic field. In semiconductors, $\Delta\alpha_\infty$- is 10-12% of α [7]. By the method of numerical solution of equation (4), μ* is determined with allowance for α_∞.

The Hall coefficient in a strong magnetic field (R_∞) is determined only by the concentration of charge carriers

$$R_\infty = \frac{1}{p_L e}, \qquad (5)$$

From the formula (5) it is possible to determine the concentration of light holes which is expressed in terms of μ* and m_L^*

$$p_L = 4\pi\left(\frac{2m_L^* k_0 T}{h^2}\right)^{3/2} F_{3/2}(\mu^*), \qquad (6)$$

where m* is the effective mass of light holes.

From (6) it is possible to determinem_L^* ($m_L^* = 0.040m_0$) from the known p_L, T and μ*.

Other parameters entering in (1-3) are defined as follows: since at the maximum / R / the condition [8] is determined

$$/R/_{max} = R(1+b)^2/4b, \qquad (7)$$

Where **b** - the ratio of lung mobility to heavy holes R can be calculated from R = f (T) when R does not depend on temperature, then according to formula (7) it is possible to determine the ratio of lung mobility to heavy holes (**b** = 8.6), and from the dependence lg (Δ / R) = f (103 / T), it is possible to find the Δ-energy gap between the subbands (Δ = (0.05 ± 0.01) eV (Fig.4a) If **b** and Δ are known, one can find (m_L^*) from the formula [9]

$$\Delta R/_R = (1-b)^2\left(\frac{m_L^*}{m_h}\right)^{3/2}\exp -\Delta/k_0 T, \qquad (8)$$

It was found that m_h ^ = 0.340m0. The values ofm_L^* , $m_h^*$and Δ determine the concentration of heavy holes in the following form [9]

$$\frac{p_h}{p_h+p_L} = \left[\left(\frac{m_L^*}{m_h^*}\right)^{3/2} e^{\Delta/k_0 T} + 1\right]^{-1}, \qquad (9) \quad \text{где } \mu^* = 2$$

In this case, **b** depends weakly on temperature (here $r_L = r_h$ (r_L, r_h scattering factors), this occurs when the relaxation time for both charge carriers is independent of energy [6]), since the variation of R (T) in mainly due to the redistribution of carriers in the conduction band and the subbands of the valence band, i.e. R = f (n, p_h, p_L). The electron concentration is determined as follows: the statistics of charge carriers in intrinsic semiconductors with two types of holes and the neutrality condition for the three-band model have the form [6]

$$n = p_h + p_L, \qquad (10)$$

or $$m_n^{*3/2}\exp(\mu^*) = (m_L^{*3/2} + m_h^{*3/2})\exp(-\mu^* - E_g^*), \qquad (11)$$

где $E_g^* = E_g^T/k_0 T$ (E_g=0.36 эВ [10]) , m_n^*- effective mass of electrons.

In semiconductors with a complex band structure, the light valence band and the conduction band are usually mirror images [9, 11], i.e $m_L^* \approx m_n^*$. To confirm this fact in $In_{0.5}Ga_{0.5}Sb$, the effective mass of electrons was calculated as follows. Under the condition $n = p_L + p_h$, determination of the electron concentration in the intrinsic semiconductor takes place [12]

$$n_i = \frac{\left(2\sqrt{m_L^* m_h^*}\cdot k_0 T\right)^{3/2}}{4\pi^{3/2}\hbar^3}\left[1 + \left(\frac{m_h^*}{m_L^*}\right)^{3/2}\right]^{1/2}\exp -\left(\frac{E_g}{2k_0 T}\right), \qquad (12)$$

where for Eg = (0.36-2.6 • 10-4) eV, assuming here the temperature coefficient Eg, dEg / dT = -2.6 • 10-4 eV / K.

It can be seen from Fig.1 that at T ~ 350 K the intrinsic conductivity of the Hall coefficient R begins, and with good accuracy is determined by the relation

$$n_i = \frac{1}{eR_i}, \qquad (13)$$

Substituting the values of at T ~ 450 K in formula (12) and using the value of Eg m_L^*, m_h^*, and one can determine ($m_n^* = 0.038m_0$) and it is obtained that $m_n^* \approx m_L^*$,

The data on m_L^*, m_h^*, m_n^* obtained by us do not differ significantly from the data obtained by the authors [13]
From (11) we obtain

$$\mu^* = \frac{E_g^*}{2} + \frac{3}{2}k_0 T\, ln\left(\frac{m_h^*}{m_n^*}\right)^{3/2} + \frac{3}{2}k_0 T ln\left[1 + \left(\frac{m_L^*}{m_h^*}\right)^{3/2}\right], \qquad (14)$$

The electron concentration is determined according to formula (6)

$$n = 4\pi\left(\frac{2m_n^* k_0 T}{h^2}\right)^{3/2} F(\mu^*), \qquad (15)$$

For any degree of degeneracy and a mixed mechanism by charge-carrier scattering, the thermal emf. (partial) is defined [6] as

$$\left.\begin{aligned} \alpha_n &= -\frac{k_0}{e}\left[\frac{G_3(\gamma)}{G_1(\gamma)} - \mu_n^*\right], \\ \alpha_{p_L} &= -\frac{k_0}{e}\left[\frac{G_3(\gamma)}{G_1(\gamma)} - \mu_L^*\right], \\ \alpha_{p_n} &= -\frac{k_0}{e}\left[\frac{G_3(\gamma)}{G_1(\gamma)} - (\mu_L^* + \Delta^*)\right] \end{aligned}\right\} \qquad (16)$$

where $\gamma = \frac{F_3(\mu^*)}{F_1(\mu^*)}$, $G_1(\gamma) = \int_0^\infty \frac{x^3 e^{-x}}{x^2+\gamma^2}\, dx, G_3(\gamma) = \int_0^\infty \frac{x^4 e^{-x}}{x^2+\gamma^2} dx$, $\Delta^* = \Delta/\kappa_0 T$ $\chi = \frac{\varepsilon}{k_0 T}$
$\gamma = U_1/U_2$ where U_L and U_i- respectively, the mobility of charge carriers, due to scattering by phonons and impurity ions.
For not too large values of γ, it is expressed in terms of the integral sine and cosine:

$G_1(\gamma) = 1 + \gamma^2(cos\gamma ci\gamma - sin\gamma si\gamma)$, $G_3(\gamma) = 2 - \gamma^2 + \gamma^3(sin\gamma ci\gamma + cos\gamma si\gamma)$, (17) где $si\gamma = \int_\gamma^\infty \frac{sint}{t} dt$ и $ci\gamma = -\int_\gamma^\infty \frac{cost}{t} dt$

It is seen from (17) that when γ = 0 (scattering by phonons) G_3 / G_1 = 2, and as γ → ∞ (scattering by ions is imparted) G_3 / G_1 = 4.
As seen from (16), an insignificant change in G_3 / G_1 strongly affects the effective mass m*.
For very large values of the parameters γ? 10 of the function G (γ), the asymptotics has the form [14]

$$G_1(\gamma) \approx \frac{6}{\gamma^2}\left(1 - \frac{20}{\gamma^2}\right), \quad G_3(\gamma) \approx \frac{24}{\gamma^2}\left(1 - \frac{30}{\gamma^2}\right)$$

The temperature dependence of the mobility is determined in the form

$$U = \frac{e}{m^*}\tau(T), \qquad (18)$$

where τ is the relaxation time of charge carriers.
In the case of a mixed carrier scattering mechanism, the mobility is expressed by the effective relaxation time [6]

$$U = \frac{e}{m^*}\tau_{ef}(T), \qquad (19)$$

With the existing mechanisms of scattering of charge carriers by ions and acoustic phonons with parameters τ_i τ_{ac}, the effective relaxation time has the form [6]

$$\tau_{ef}(T) = \frac{\tau_i(T)\tau_{ac}(T)\left(\frac{\varepsilon}{k_0 T}\right)^{\gamma_{ac}-1/2}}{\tau_i(T) + \tau_{ac}\left(\frac{\varepsilon}{k_0 T}\right)^{\gamma_{ac}-\gamma_i}}, \qquad (20)$$

The charge carrier relaxation time involved in scattering by ions and acoustic phonons is determined as follows [6]

$$\tau_i(T) = \frac{\chi_0 (2m^*)^{1/2}(k_0 T)^{3/2}}{\pi e^4 N_i F}, \qquad (21)$$

where χ_0 is the dielectric constant of the crystal

$F = \ln(1+\xi) - \frac{\xi}{1+\xi}$; $\xi = 4kr$

Here r is the screening radius, which for nondegenerate semiconductors is defined as

$$r = \frac{k k_0 T}{4\pi e^2 n}$$

where N_i is the concentration of impurity ions

$$\kappa = \frac{(6k_0 T m^*)^{1/2}}{\hbar}$$

The expression τ_{ac} (T) for the standard zone has the form

$$\tau_{ac}(T) = \frac{\rho U_0^2 \hbar^4}{C^2 (2m^* k_0 T)^{3/2}}\left(\frac{\varepsilon}{\kappa_0 T}\right)^{-1/2}, \qquad (22)$$

Where **C** is the interaction constant of charge carriers with lattice vibrations, U_0 is the speed of sound in the crystal, and ρ is the density of the crystal. It is established that **C** is related to the deformation potential constant: $E_d = 2/3$ C. Taking into account the value of $x_0 = 15$, ρ = 5.66 g / cm^3 $U_0 = 3.4 \cdot 10^5$ cm /s, Ed = 4 eV,

τ_{ac} (T). After determining τ_i (T) and τ_{ac} (T), taking into account their numerical values, τ_{ef} is determined according to (20). Then, mobility of the charge carriers is calculated using (19).

As can be seen from Figs. 1-3, taking into account the contribution of the scattering by the impurity ions and on the acoustic vibrations of the lattice does not give a satisfactory agreement with the experimental results.

To continue the discrepancy between the calculated and experimental data, new scattering centers must be taken into account. In this case, the calculation of U2 (T) for any degree of degeneracy is given as follows:

$$U_2 = (\frac{1}{U_{i,ac}} + \frac{1}{U_o})^{-1} \quad , \qquad (23)$$

here U0 is the mobility with allowance for the scattering of charge carriers by optical phonons, which was calculated as follows, under condition $\gamma = \left[\frac{\chi_0 h^2}{4m^* e^2} (\frac{\pi}{3h})^{1/2}\right]^{1/2}$

and for $k_0T \gg \hbar\omega_0$ the relaxation time for scattering by optical phonons [6]

$$\tau_o(T) = \frac{\sqrt{2}}{4\pi} \frac{M\Omega_0(\hbar\omega_0)^2}{e^4(m^* k_0 T)^{1/2}} (\frac{E}{k_0 T})^{1/2} \quad , \qquad (24)$$

where $M=\frac{m_1 m_2 m_3}{m_1 m_2 + m_2 m_1 + m_1 m_3}$ - the reduced mass of ions in the unit cell, the Ω_0-volume of the unit cell, and $\omega_0 = 2.8 \cdot 10^{13}$ s^{-1} the limiting frequency of the longitudinal phonon.

Substituting (24) into (18), we can determine the temperature dependence of the mobility of the charge carriers under the mechanism on optical phonons. Taking into account the values of Uo in (23), we can determine U^2 (T) and substitute the values of U^2 (T) in (1-2) for R (T), α (T) and σ (T) (Fig.). As can be seen, in both cases the calculated curves are located somewhat higher than the experimental ones; taking into account scattering of charge carriers by ions, impurities of acoustic and optical lattice vibrations leads to a convergence of the experimental and calculated curves.

III. Analysis Of The Results.

The calculated calculation for In0.5Ga0.5Sb at a concentration of $\rho_L = 7.8 \cdot 10^{17}$ cm^{-3}, at which the value of the chemical potential up to temperatures T ~ 110 K and below have been determined by the zone with a lower density of states ($m_L^* = 0.040\ m_0$) . Conductivity is dominated by light holes from the zone with a higher density of states ($m_h^* = 0.340\ m_0$).

To determine the contribution of heavy holes to the total concentration of charge carriers, the change in their concentration was taken into account due to a decrease in the energy gap (Δ = 0.05 eV) between valence bands with increasing temperature with a velocity dΔ / dT = $-2.6 \cdot 10^{-4}$ eV / K. The mobility ratio b for this concentration varies with increasing temperature with increasing from 8.6 to 10. Calculation shows that at p_h / $p_L \approx 1.5$, the values of R and α reach a maximum at T~250 K.

Comparison of the calculated and experimental curves shows that with increasing temperature with increasing p_h / p_L growth of R (T) and α (T) is observed. The theoretical and calculated data are in good agreement. At T> 250 K, R and α begin to fall, although, according to the calculated data, only two types of holes are taken into account. (R) and (α) at a temperature of T ~ 450 K once again pass through a maximum and begins its own region. The eigenfunction is also confirmed by σ (τ). Then, according to the slope of the dependence of lg (RT_3 / 2) ~ 103 / T and lg (σ / T) on 1 / T, it is possible to determine the band gap Eg, it was found for Eg ~ 0.37 ± 0.05 and 0.35 ± 0.02 eV. These values of Eg are consistent with the data of [13].

As can be seen from Figs. 1 and 3, the eigenfunction in R (T) begins earlier than on the σ (T) dependence. In addition, the delay is due to the fact that the role of heavy holes in conductivity extends to T ~ 450 K. After this, a large contribution to the conductivity is made by the intrinsic electrons.

The quantitative disagreement between the experimental and calculated curves can be caused by the following reasons:

1. A quantitative comparison of the data shows that the calculated values of the mobility of light holes at T <110 K are greater than the experimental values. This is probably due to the fact that the screening radius in In0.5Ga0.5Sb is larger than the lattice constant (which can not be taken into account in calculations on the calculation). In this case, the scattering of light holes is more intense than the scattering of heavy holes
2. The fall of R (T) at T> 250 K is attributed to the appearance of band transitions. However, at these temperatures in In0.5Ga0.5Sb $p_h + p_L = 3.25 \cdot 10^{17}$ cm^{-3}, the electron concentration is $n \sim 1.25 \cdot 10^{17}$ cm^{-3}, which does not explain the observed drop R (T). It can be seen from the experimental data that at T <110 K, light holes play the main role in conductivity, and at T> 110 K heavy holes and own electrons play. However, their calculated values can not always be correctly found. Therefore, in the calculations of the inversion point, the sign slightly blends into the high-temperature region.
3. Interpretation of R (T) and a (T) shows that these dependences are affected not only by the band parameters, but also by their temperature dependences (especially at T <250 K, the zonal parameters of light holes play a role); and a significant role is played by the scattering mechanism

4. An insignificant reason for the failure of the agreement between the calculated and experimental data may be due to the inaccurate determination of the prevailing scattering mechanism and the band parameters of the charge carriers.
5. Of special interest is a minimum on σ (T) at T ~ 400 K. Calculations show that starting from T ~ 250, charge carriers are intensely scattered by thermal lattice vibrations, so that Uh, U_L, Un, decrease with temperature, which leads to a decrease σ (T). At T> 400 K, due to the appearance of intrinsic conductivity, the generation of electrons from the valence band to the conduction band begins, which leads to an increase in σ (T). Another feature here is the value of the minimum on σ (T) at T ~ 450 K, since in experiment σ decreases by ~ 15%. The calculation shows that, due to a decrease in the mobility σ, ~ 8% decreases. This can be caused simultaneously by an additional scattering mechanism: interband scattering. As has been shown, the relaxation time of light and heavy holes is equalized, and, consequently, greatly decreases the mobility of light holes, where, in scattering by acoustic and optical phonons, $U_L / U_h \sim (m_h^* / m_L^*)^{3/2}$ and $(m_h^* / m_L^*)^{1/2}$ respectively. In the case of scattering by ionized impurities, interband scattering does not play a role. In comparison with other semiconductors, the radius of curvature σ (T) in the region T ~ 350 ÷ 450 K has a large value. This means that in $In_{0.5}Ga_{0.5}Sb$, the band gap is sufficiently large in comparison with other narrow-gap semiconductors[].

Thus, the temperature dependences of R (T), σ (T), and R (α) in $In_{0.5}Ga_{0.5}Sb$ are well explained taking into account certain values of the band parameters by two types of holes and by their own electrons. At high temperatures, the contribution of heavy holes and intrinsic electrons appears in the total conductivity, since the energy gap between the subbands Δ strongly decreases with increasing temperature ($\Delta = 0.05 - 2.6 \cdot 10^{-4}$eV), then U_L U U_h .

Electrical and thermoelectric properties equimolar composition of $In_{0.5}Ga_{0.5}Sb$

The electrical conductivity, Holl coefficient and thermopower of $In_{0.5}Ga_{0.5}Sb$ have been measured between 80 and 600 K. The results have been interpreted in terms of a there-band model which takes into account, in addition to the conduction band, two overlapping valence subbands. We have determined the energy spacing between the subbands ($\Delta = (0.005 \pm 0.001)$eV), accepted its temperature coefficient ($d\Delta/dT = -2.6 \cdot 10^{-4}$ eV/K, have been calculated the effective masses of the heavy and light holes and electrons.

Literature

[1]. I.G. Lang, D.N. Nasledov, S.T. Pavlov, L.D. Radaikina, A.S. Filipchenko. FTT, 16 (1), 92 (1974)
[2]. Sagar, Phys. Ray.117, 93 (1960).
[3]. İ.L Robert .Sol.Stat. Commun.7. 143 (1969)
[4]. V.I. Ivanov-Omsk, B.T. Kolomiets FTT, 1, (6) 913 (1959)
[5]. S.A. Aliyev, D.G. Arasly, Z.F. Agaev, Sh.S. Ismailov, E.I. Zulfigarov. Izv.AN Azerb. USSR.Ser.phiz-tech.i mat.nauk.6. 67 (1982)
[6]. B.M. Askerov. Kinetic effects in semiconductors. (M. Nauka, 1970)
[7]. F. F. Aliev, G. G. Huseynov, G.P. P. Ashayev, G.M. Agamirzoyev, ABMagerramov. Inorganic Matter. 44 (2), 156 (2008)
[8]. F.F. Aliev, E.M. Kerimov, C.Aliyev. ФТП 36 (8) .932 (2002)
[9]. A.A. Andreev, V.N. Radio FTS. 1 (2), 15 (1967)
[10]. S.A. Zeynalov Phys.Stat. Sol. (B) 128. K 139 (1985)
[11]. E.P.Skipetrov, E.A. Zvereva and others FIT 38 (10). 1199 (2004)
[12]. Yu.N. Samples of the ZTF .25 .995.19551
[13]. D. Auvergne, J. Camassel, H. Mathieu and A. Joullie. J.of Phys. and Chemistry of solids. 85 (2) 133 (1974).

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