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The calculation of free charge carrier intrinsic concentration values in indium antimonide

A. G. Belov¹, R. Yu. Kozlov^{1,2}, E. O. Zhuravlev^{1,2,*}, E. V. Molodtsova¹, N. G. Khikheev¹,
N. A. Sarkisov³, M. A. Pankov³ and V. B. Kulikov⁴

¹ Giredmet, JSC, Moscow, 111524 Russia

* E-mail: EOZhuravlev@yandex.ru

² National University of Science and Technology MISiS, Moscow, 119049 Russia

³ RD&P Center ORION, JSC, Moscow, 111538 Russia

⁴ Joint Stock Company "Central Scientific-Research Institute "Cyclone", Moscow, 107497 Russia

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The calculations of free charge carrier intrinsic concentration values, n_i , in indium antimonide for $T = 295$ K and $T = 77$ K have been made, taking into account the nonparabolism of conduction band. It was shown, that $n_{i_{295}} = (2.14 \pm 0.01) \times 10^{16} \text{ cm}^{-3}$ and $n_{i_{77}} = (2.47 \pm 0.01) \times 10^9 \text{ cm}^{-3}$.

The comparison of $n \times p_i$ product and n_i^2 -values has been made, and they were shown to differ from each other. It has been suggested, that these differences are due to conduction band nonparabolism. Literary data have been analyzed (the results of experiments to determine n_i -values in wide temperature range). The results of calculation are shown to be in satisfactory agreement with experimental data. It is suggested that results obtained will be used in the future for optimization of technological processes of InSb single crystal growth and doping.

Keywords: indium antimonide; intrinsic free charge carrier concentration.

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Introduction

The intrinsic free charge carrier concentration (IFCCC) is a fundamental characteristic of any semiconductor material and one of the key parameters used in calculating distributions of electrons and holes. It is impossible to correctly determine dopant masses and growth conditions for semiconductor materials without information on IFCCC.

As for indium antimonide, the literature provides the IFCCC values pertaining to the temperature range of $T \geq 150$ K, while information on the IFCCC values at the temperatures close to the boiling point of liquid nitrogen is hardly available.

We have attempted to fill this gap. The aim of this paper is to calculate the IFCCC values for indium antimonide at $T = 295$ K and $T = 77$ K, as

well as to analyze literature data concerning methods for determining IFCCC values. The results obtained are expected to be used to optimize processes for producing and doping InSb single crystals.

Theoretical calculations

The band structure of indium antimonide is shown in Fig. 1 [1].

According to the formula (see summary [1]) for calculating the band gap width vs. the temperature in the temperature range of $(0 < T < 300 \text{ K})$:

$$E_g = 0.24 - 6 \times 10^{-4} \times T^2 / (T + 500), \text{ eV}; \quad (1)$$

we get $(E_g)_{295} = 0.17 \text{ eV}$; $(E_g)_{77} = 0.23 \text{ eV}$.

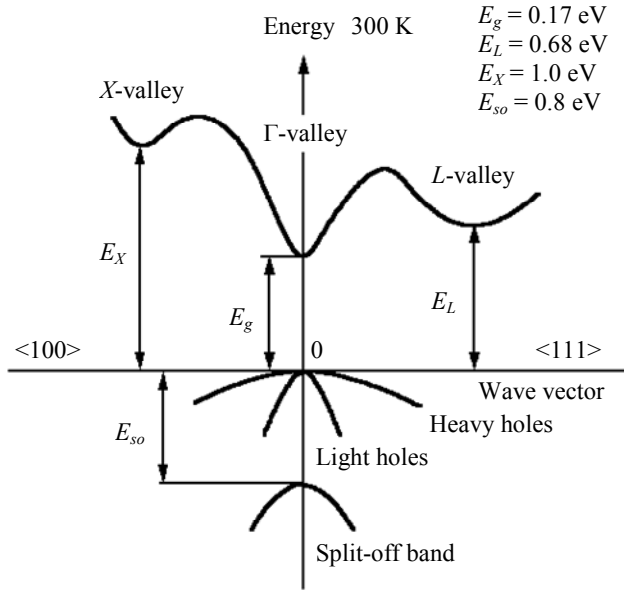


Fig. 1. Band structure of InSb

The following relations [2] are applicable to the concentrations of electrons (n), light (p_L) and heavy (p_H) holes:

$$n = \frac{\sqrt{3}}{2\sqrt{2}\pi^2} \times \frac{(kTE_g)^{\frac{3}{2}}}{P_{cv}^3} \times {}^0L_0^{\frac{3}{2}}(\eta, \beta); \quad (2)$$

$$p_L = \frac{\sqrt{3}}{2\sqrt{2}\pi^2} \times \frac{(kTE_g)^{\frac{3}{2}}}{P_{cv}^3} \times {}^0L_0^{\frac{3}{2}}\left[\left(-\frac{1}{\beta} - \eta\right), \beta\right]; \quad (3)$$

$$p_H = \frac{8\pi}{3h^3} \times (2m_{pH} kT)^{\frac{3}{2}} \times F_{\frac{3}{2}}\left(-\frac{1}{\beta} - \eta\right), \quad (4)$$

where $\eta = \frac{E_F}{kT}$ is reduced Fermi energy level;

$\beta = \frac{kT}{E_g}$ is nonparabolicity parameter of the conduction band and light holes in Kane model [3]:

Here, E_g is the semiconductor band gap width; $k = 1.38 \times 10^{-16}$ erg/K is Boltzmann's constant; $\hbar = \frac{h}{2\pi}$, where $h = 6.62 \times 10^{-27}$ erg·s is Planck's constant; $m_{pH} = 0.43 m_0$ [1] is the effective mass of heavy holes ($m_0 = 9.11 \times 10^{-28}$ g is the free electron mass); $P_{cv} = 8.7 \times 10^{-8}$ eV·cm [4] is the array element for the interaction between the light-hole valence band and

conduction band (considered to be independent of the temperature and identical for all A_3B_5 compounds).

The bottom of the conduction band is taken as the zero energy reference; the positive direction is upward; our concern is values of $\eta \leq 0$.

Formulas (2) and (3) use two-parameter Fermi integrals:

$${}_mL_k^n(\eta, \beta) = \int_0^\infty \left(-\frac{\partial f_0}{\partial x} \right) \frac{x^m (x + \beta x^2)^n}{(1 + 2\beta x)^k} dx \quad (5)$$

The two-parameter integral ${}_0L_0^{\frac{3}{2}}(\eta, \beta)$ transforms into the one-parameter integral $F_{\frac{3}{2}}(\eta)$

(4) when $\beta \rightarrow 0$, that is, when the nonparabolicity of the band can be neglected.

$$F_{\frac{3}{2}}(\eta) = \int_0^\infty \left(-\frac{\partial f_0}{\partial x} \right) x^{\frac{3}{2}} dx, \quad (6)$$

where

$$f_0(x, \eta) = [1 + \exp(x - \eta)]^{-1} \quad (7)$$

The algorithm for determining IFCCC is as follows.

1. A specific value of parameter η is selected, and concentrations of electrons, light holes, and heavy holes are calculated using formulas (2), (3), and (4).

2. A different value of the mentioned parameter is selected, and the calculation procedure is repeated (and so on).

3. Dependencies of free charge carrier concentrations vs. reduced Fermi level are plotted on the logarithmic scale.

4. The intersection point of these dependencies is found, along with the corresponding free charge carrier concentration values. This will be the IFCCC value sought.

All calculations were performed for temperatures $T = 295$ K and $T = 77$ K. Let us consider both cases in more detail.

$$T = 295 \text{ K}; E_g = 0.17; kT = 25.4 \times 10^{-3} \text{ eV};$$

$$\beta = 0.149; \frac{1}{\beta} = 6.69.$$

Formulas (2), (3), (4) will look as follows:

$$n = 2,676 \times 10^{16} \times {}^0L_0^{\frac{3}{2}}(\eta; 0,149) \quad (8)$$

$$p_L = 2.676 \times 10^{16} \times {}^0L_0^{\frac{3}{2}}(-6.69 - \eta; 0,149) \quad (9)$$

$$p_H = 5.185 \times 10^{18} \times F_{\frac{3}{2}}(-6.69 - \eta) \quad (10)$$

Within the range of the reduced Fermi level that interests us ($-6.69 \leq \eta \leq 0$), the Fermi integrals in formulas (9) and (10) differ only

slightly from each other, whereas their coefficients are approximately 190 times different. In other words, $\frac{p_L}{p_H} \approx \frac{1}{190}$, the concentration of heavy holes is more than two orders of magnitude greater than the concentration of light holes. Therefore, the contribution of the latter to the IFCCC value can be neglected, and the n_i value can be calculated based on the relation:

$$n = p_H. \quad (11)$$

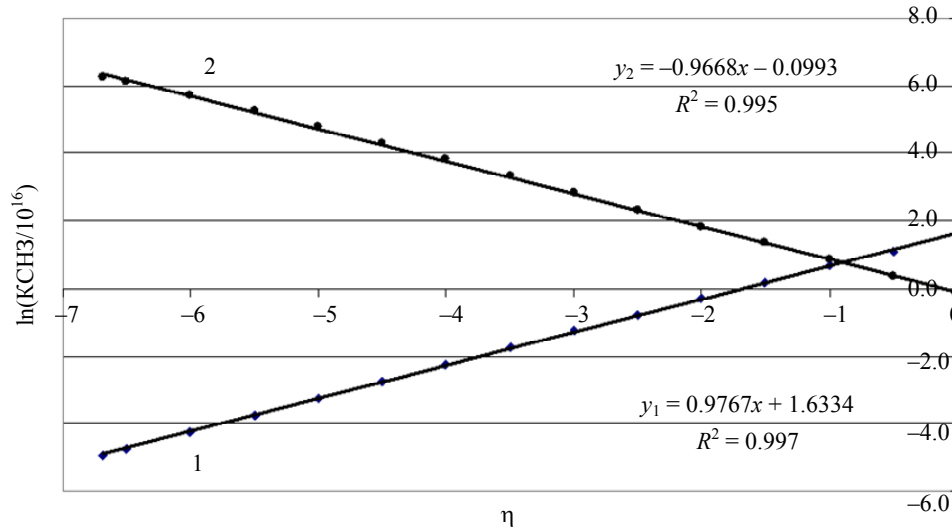


Fig. 2. $(n/10^{16})$ and $(p_H/10^{16})$ vs. reduced Fermi level on the logarithmic scale for $T = 295$ K: 1 – electrons; 2 – heavy holes

Figure 2 shows the calculated dependencies of IFCCC vs. reduced Fermi level on the logarithmic scale for $T = 295$ K. Both dependencies are seen to be well described by linear functions. The intersection point has the coordinates: $\eta_i = -0.8915$, $\ln(n/10^{16}) = 0.7627$, which corresponds to an intrinsic carrier concentration $n_i = (2.14 \pm 0.01) \times 10^{16} \text{ cm}^{-3}$.

Now let's consider the case of low temperatures.

$$T = 77 \text{ K}; E_g = 0.23 \text{ eV}; kT = 6.62 \times 10^{-3} \text{ eV};$$

$$\beta = 0.0288; \frac{1}{\beta} = 34.7.$$

Let's assume that the effective mass of heavy holes does not depend on the temperature and is equal to $0.43 m_0$.

Relations (2)–(4) for $T = 77$ K will look as follows:

$$n = 5.620 \times 10^{15} \times {}^0L_0^{\frac{3}{2}}(\eta; 0,0288) \quad (12)$$

$$p_L = 5.620 \times 10^{15} \times {}^0L_0^{\frac{3}{2}}(-34.7 - \eta; 0,0288) \quad (13)$$

$$p_H = 6.914 \times 10^{17} \times F_{\frac{3}{2}}(-34.7 - \eta) \quad (14)$$

Given that Fermi integrals in formulas (13) are (14) are scarcely different from each other, we will get that $\frac{p_L}{p_H} \approx \frac{1}{120}$.

The dependencies for $T = 77$ K similar to those listed above are shown in Fig. 3. Like in the previous example, both dependencies are well described with straight lines intersecting at the point with the coordinates: $\eta_i = -14.94$, $\ln(n/10^{15}) = -12.91$, which corresponds to an intrinsic carrier concentration $n_i = (2.47 \pm 0.01) \times 10^9 \text{ cm}^{-3}$.

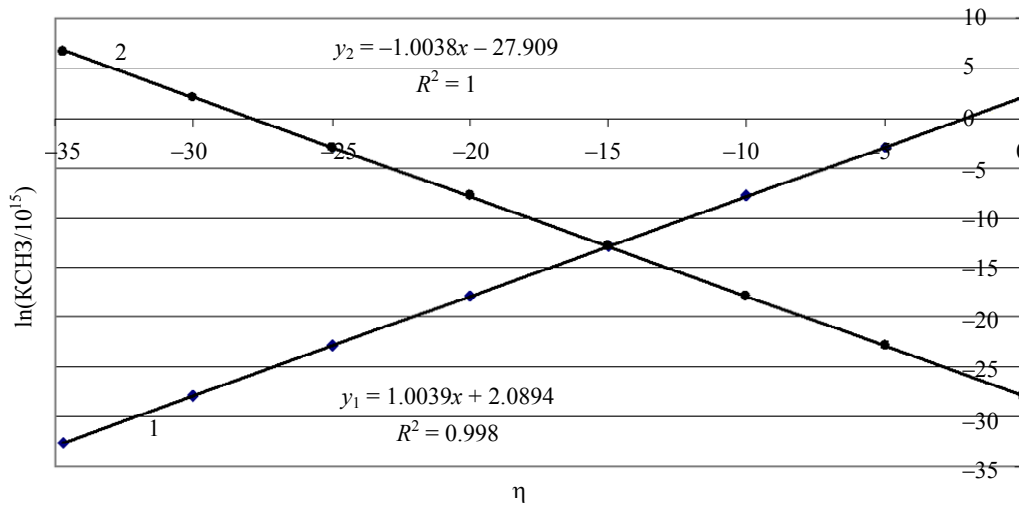


Fig. 3. $(n/10^{15})$ and $(p_H/10^{15})$ vs. reduced Fermi level on the logarithmic scale for $T = 77$ K: 1 – electrons; 2 – heavy holes

Note that η_i at $T = 295$ K lies within the band gap, not far from the bottom of the conduction band, whereas at $T = 77$ K, the corresponding value is close to the middle of the band gap ($\eta_{\text{mid}} - 17.35$). In other words, as the temperature decreases, the Fermi level shifts from above towards the middle of the band gap – a fact well-documented in the literature (see, for example, in [5]).

Is a common knowledge that relation

$$n \times p_L = n_i^2 \quad (15)$$

shall be valid for nondegenerated semiconductors [5]. Let's verify whether this is true in the cases

under consideration. Figures 4 and 5 show the curves of the product of electron and heavy hole concentrations vs. reduced Fermi level for $T = 295$ K and $T = 77$ K, respectively; the horizontal line indicates the value n_i^2 .

As can be seen in Figures 4 and 5, relation (15) is only approximately satisfied, with maximum deviation of $n \times p_H$ values from n_i^2 being +5.7 % at $T = 295$ K and +6.9 % at $T = 77$ K. It should be noted that at $T = 77$ K, the $n \times p_H$ curve has a segment parallel to the horizontal line n_i^2 (see Fig. 5), whereas the $n \times p_H$ curve at $T = 295$ K has a distinctly bell-shaped form (see Fig. 4).

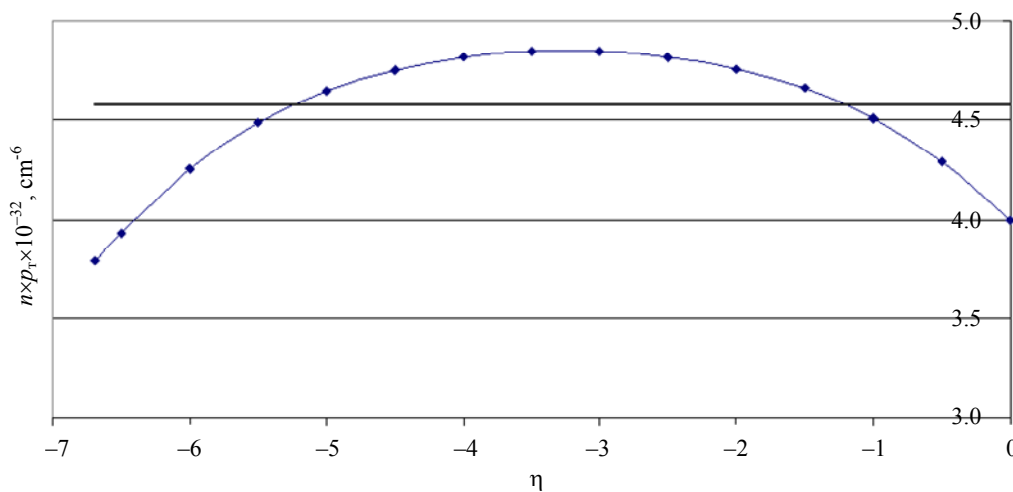


Fig. 4. Product $n \times p_H$ vs. reduced Fermi level for $T = 295$ K. Horizontal line corresponds to value $n_i^2 = 4.58 \times 10^{32} \text{ cm}^{-6}$

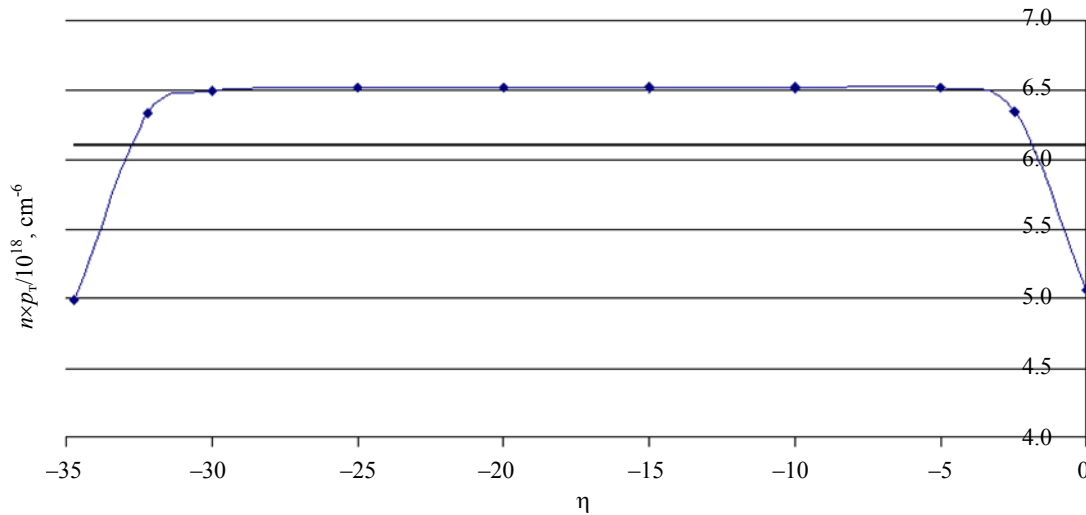


Fig. 5. Product $n \times p_H$ vs. reduced Fermi level for $T = 77$ K. Horizontal line corresponds to value $n_i^2 = 6.10 \times 10^{18} \text{ cm}^{-6}$

We attribute these differences to the nonparabolicity of the conduction band, which is significantly greater at the room temperature: $\beta_{295} = 0.149$; $\beta_{77} = 0.0288$.

Discussion of experimental results

Let's now proceed to discussing the literature data concerning the experimental determination of IFCCC values. IFCCC values are usually derived from the curve of the Hall coefficient, R (on the logarithmic scale), vs. the inverse temperature, $10^3/T$ (temperature factor $\sim T^{-\frac{3}{2}}$ is also taken into account). One shall find a linear segment on this curve and attribute it to the intrinsic concentration region [6, 7]. However, the method for determining the free charge carrier concentration using the Hall coefficient invites some questions.

To begin with, when determining the IFCCC value, the authors of papers [6, 7] do not account for the influence of light holes. It is assumed that they can be neglected in an intrinsic semiconductor, and that relation (11) is valid.

In the most general case (charge carriers of three types: electrons, light holes, and heavy holes), the expression for the Hall coefficient in weak magnetic fields ($\mu^2 B^2 \ll 1$) can be written as:

$$R = \frac{1}{e} \times \frac{\left(p_H \mu_{p_H}^2 + p_L \mu_{p_L}^2 - n \mu_n^2 \right)}{\left(p_H \mu_{p_H} + p_L \mu_{p_L} + n \mu_n \right)^2}, \quad (16)$$

where μ_{p_H} , μ_{p_L} , μ_n are mobilities of heavy holes, light holes and electrons, respectively. Formula (16) can be transformed as follows:

$$R = \frac{1}{e p_H} \times \frac{\left(1 + \frac{p_L}{p_H} \times \frac{\mu_{p_L}^2}{\mu_{p_H}^2} - \frac{n}{p_H} \times \frac{\mu_n^2}{\mu_{p_H}^2} \right)}{\left(1 + \frac{p_L}{p_H} \times \frac{\mu_{p_L}}{\mu_{p_H}} + \frac{n}{p_H} \times \frac{\mu_n}{\mu_{p_H}} \right)^2} \quad (17)$$

Now let's estimate contributions of free charge carriers of various types into the Hall coefficient for intrinsic concentration $n = p_H = n_i$. Let's choose the values of parameters from formula (17) for the purpose of estimation:

$$T = 295 \text{ K}: \quad \frac{p_L}{p_H} = \frac{1}{190} \quad (\text{see above});$$

$$\mu_{p_H} = 850 \text{ cm}^2/(\text{V}\cdot\text{s}) \quad [1]; \quad \mu_{p_L} = 17,000 \text{ cm}^2/(\text{V}\cdot\text{s}) \quad (\text{let's consider relation } \frac{\mu_{p_L}}{\mu_{p_H}} \text{ not to depend on the temperature and equal to 20 [8]}); \mu_n = 25,000 \text{ cm}^2/(\text{V}\cdot\text{s}). \text{ Then, we will get the following from formula (17):}$$

$$R = \frac{1}{e n_i} \times \frac{(1 + 2.1 - 865)}{(1 + 0.105 + 29.4)^2} \quad (18)$$

$$\text{Similarly, for } T = 77 \text{ K we have: } \frac{p_L}{p_H} = \frac{1}{120} \quad (\text{see above}); \quad \mu_{p_H} = 5,000 \text{ cm}^2/(\text{V}\cdot\text{s}) \quad [1];$$

$\mu_{p_L} = 100,000 \text{ cm}^2/(\text{V}\cdot\text{s})$; $\mu_n = 200,000 \text{ cm}^2/(\text{V}\cdot\text{s})$.
We will get the following from formula (17):

$$R = \frac{1}{en_i} \times \frac{(1 + 3.33 - 1600)}{(1 + 0.167 + 40)^2} \quad (19)$$

As can be seen from formulas (18) and (19), contributions by light and heavy holes are of the same order of magnitude, but when put together they are much lower than the contribution of electrons. In other words, the simple formula used by the authors of papers [6, 7]

$$R = -\frac{1}{n_i e} \quad (20)$$

can be considered to be quite justified in the above context.

It should be noted that formula (20) is only valid for the weak magnetic fields when the below condition is satisfied for all types of free charge carriers:

$$(\mu B)^2 \ll 1 \quad (21)$$

where B is the magnetic field induction (taken in terms of T, while μ – in terms of $\text{m}^2/(\text{V}\cdot\text{s})$).

It can be seen that this condition is not satisfied for electrons even at $T = 295 \text{ K}$; for $B = 0.4 \text{ T}$ [7], we have $(\mu B)^2 = 1$, and even more this condition is not satisfied at $T = 77 \text{ K}$: $(\mu_n B)^2 = 64$. Consequently, when calculating n_i values using the Hall coefficient, it is necessary to use more complex relations that account for the influence of the magnetic field (see, for example, [2]).) instead of formula (20). Formula (20) can lead to significant errors in determining n_i values, which cannot be estimated in advance.

The literature provides for various formulas for calculating IFCCC values over a wide temperature range. All of them are derived from the curves of the Hall coefficient vs. temperature. Without giving these relations here, we will only

provide n_i values calculated with the use thereof for $T = 295 \text{ K}$: $2 \times 10^{16} \text{ cm}^{-3}$ [1]; $1.63 \times 10^{16} \text{ cm}^{-3}$ [4]; $1.81 \times 10^{16} \text{ cm}^{-3}$ [6]; $1.75 \times 10^{16} \text{ cm}^{-3}$ [7]. To these, we add the value $n_i \approx 1.9 \times 10^{16} \text{ cm}^{-3}$ obtained by the helicon wave interference method [9].

It can be seen that all these values are lower than our calculated value of $(2.14 \pm 0.01) \times 10^{16} \text{ cm}^{-3}$. This slight discrepancy with the experimental data may be due to the incorrect interpretation of the curve of the Hall coefficient vs. temperature (see above).

Regarding the temperature $T = 77 \text{ K}$, data on IFCCC values here are very scarce and contradictory. As an example, the data obtained in [8] can be given: extrapolation of the straight line for n_i to the low-temperature region (Fig. 3) gives an approximate value of $2 \times 10^9 \text{ cm}^{-3}$, which is consistent with the results of our calculations: $(2.47 \pm 0.01) \times 10^9 \text{ cm}^{-3}$.

Conclusion

1. Calculations of the free charge carrier intrinsic concentration in InSb have been made for temperatures $T = 295 \text{ K}$ and $T = 77 \text{ K}$. It was shown that:

$$n_{i_{295}} = (2.14 \pm 0.01) \times 10^{16} \text{ cm}^{-3}$$

$$\text{and } n_{i_{77}} = (2.47 \pm 0.01) \times 10^9 \text{ cm}^{-3}.$$

2. Values of $n \times p_H$ product and n_i^2 have been compared. The maximum difference between these curves has been shown to be 5.7 % for $T = 295 \text{ K}$ and 6.9 % for $T = 77 \text{ K}$.

3. Values $n_{i_{295}}$ and $n_{i_{77}}$ have been compared to the literature data obtained experimentally. The calculated data have been shown to be consistent with the experimental findings.

4. The results obtained are expected to be used to optimize processes for growing and doping InSb single crystals.

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About authors

Belov Alexander Georgievich, Cand. Sci. (Phys.-Math.), Leading Research Scientist, Giredmet, JSC (111524, Russia, Moscow, Elektrodnyaya Ulitsa, 2, bld. 1). E-mail: IADenisov@rosatom.ru SPIN code: 9546-0477, AuthorID: 38536

Kozlov Roman Yurievich, Giredmet, JSC (111524, Russia, Moscow, Elektrodnyaya Ulitsa, 2, bld 1), National University of Science and Technology MISiS (119049, Russia, Moscow, Leninsky Prospekt, 4, bld. 1). E-mail: RYKozlov@rosatom.ru SPIN code: 7324-5403, AuthorID: 1302882

Zhuravlev Evgeny Olegovich, Research Assistant, Giredmet, JSC (111524, Russia, Moscow, Elektrodnyaya Ulitsa, 2, bld 1), National University of Science and Technology MISiS (119049, Russia, Moscow, Leninsky Prospekt, 4, bld. 1). E-mail: EOZhuravlev@yandex.ru SPIN code: 5492-0419, AuthorID: 1297975

Molodtsova Elena Vladimirovna, Candidate of Technical Sciences, Leading Research Scientist, Giredmet, JSC

Khikheev Nikolay Germanovich, Engineer, Giredmet, JSC (111524, Russia, Moscow, Elektrodnyaya Ulitsa, 2, bld 1), National University of Science and Technology MISiS (119049, Russia, Moscow, Leninsky Prospekt, 4, bld. 1).

Sarkisov Nikita Andreyevich, Engineer of 2nd Category, RD&P Center ORION, JSC (111538, Russia, Moscow, Kosinskaya, 9). E-mail: nsarkisov@mail.ru

Pankov Mikhail Aleksandrovich, Cand. Sci. (Phys.-Math.), Head of Laboratory, RD&P Center ORION, JSC (111538, Russia, Moscow, Kosinskaya, 9). E-mail: mpa.off@gmail.com. SPIN code: 7160-9289, AuthorID: 145651

Kulikov Vladimir Borisovich, Dr. Sci. (Eng.), Head of Department, Joint Stock Company "Central Scientific-Research Institute "Cyclone" (107497, Russia, Moscow, Shchelkovskoe Shosse, 77). E-mail: v.kulikov@cyclone-jsc.ru SPIN code: 2840-0055, AuthorID: 1017695