INVESTIGATION OF THE STRUCTURE OF THE CONDUCTION BAND AND THE VALENCE BAND OF GaAs

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INVESTIGATION OF THE STRUCTURE OF THE CONDUCTION BAND AND THE VALENCE BAND OF GaAs

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The infrared reflection spectrum in the wavelength region $\lambda = 1\text{-}35\,\mu$ in GaAs crystals with unknown characteristics was first studied in work ([1]); on the basis of it, the effective ion charge e^* and the high-frequency dielectric constant ε_∞ were estimated. Further investigations ([2,3]) showed that the values of e^* and ε_∞ are not in agreement with the data of work ([3]). The values of the effective mass of current carriers in the valence band, found by optical ([4]) and thermal ([10]) methods, were not in agreement with one another.

The aim of the present work was to study the optical properties of GaAs and to determine the effective ion charges and the effective masses of holes in various branches of the valence band of GaAs.

The infrared reflection spectrum in the wavelength range from 1 to $40\,\mu$ was studied on gallium arsenide crystals of n- and p-type with various concentrations of charge carriers (see Table 1). Te and Zn were used as dopants.

Figure 1 gives the dependence of the reflection coefficient on wavelength for 8 n-type samples and two p-type samples. From these curves it is seen that for 4 samples with electron concentration $4.6 \cdot 10^{16}$-$3 \cdot 10^{17}$ cm^{-3} a minimum was observed at $35\,\mu$. The position of this minimum does not change with change in concentration. For samples with impurity concentrations $4.6 \cdot 10^{16}$-$3 \cdot 10^{17}$ cm^{-3}, the Fermi level lies below the conduction band, and

Table 1

	n and p, cm^{-3}	m^*_{op}/m_0	e^*/e_0	$\lambda_{\min}$, μ
n-GaAs	$n = 4.4 \cdot 10^{16}$	–	0.476	35
n-GaAs	$4.6 \cdot 10^{16}$	–	–	–
n-GaAs	$6 \cdot 10^{16}$	–	–	35
n-GaAs	$8.6 \cdot 10^{16}$	–	–	35
n-GaAs	$3.0 \cdot 10^{17}$	–	0.475	35
n-GaAs	$6 \cdot 10^{17}$	0.068	–	31 ± 0.1

Fig. 1. Dependence of the reflection coefficient R on wavelength λ.

Figure 1: Fig. 1. Dependence of the reflection coefficient R on wavelength λ.

	n and p, cm^{-3}	m^*_{op}/m_0	e^*/e_0	$\lambda_{\min}$, μ
n-GaAs	$8 \cdot 10^{17}$	0.070	–	28
n-GaAs	$1.08 \cdot 10^{18}$	0.072	–	27
p-GaAs	$p = 1.7 \cdot 10^{20}$	0.59 ± 0.03	–	6.7
p-GaAs	$2 \cdot 10^{20}$	0.62 ± 0.02	–	6

the influence of free carriers on the dielectric susceptibility is not detected. If it is assumed that this minimum is associated with lattice vibrations, then the value $35\,\mu$ is in good agreement with the data of work ([1]).

For ionic crystals with a simple cubic structure, the effective ionic charge on an atom is expressed by the equation ([2])

$$e = \frac{3\omega_t}{\varepsilon_\infty + 2}\left[\frac{M(\varepsilon_0 - \varepsilon_\infty)}{4\pi n_0}\right]^{1/2}, \tag{1}$$

where ε_∞ is the high-frequency (optical) dielectric constant; according to our data it is equal to 11.6; ε_0 is the static dielectric constant, equal to 12.5 ([2]); n_0 is the number of ion pairs per unit volume for GaAs, $n_0 = 2.23 \cdot 10^{22}$ cm^{-3}; M is the mass of ion pairs for GaAs, $M = 6.00 \cdot 10^{-23}$ g; ω_t is the fundamental frequency of transverse vibrations (of the optical type).

Fig. 1. Dependence of the reflection coefficient R on wavelength λ. 1, 2 – p-GaAs; 3, 4, 5 –n-GaAs.
1 –$p = 2 \cdot 10^{20}$ cm^{-3}; 2 –$p = 1.7 \cdot 10^{20}$; 3 –$n = 1.08 \cdot 10^{18}$; 4 –$n = 8 \cdot 10^{17}$; 5 – $n = 4.6 \cdot 10^{16} \div 3 \cdot 10^{17}$ cm^{-3}. $T = 300$°K

The vibration frequency in our experiments corresponds to a wavelength $\lambda = 35.0 \pm 0.5$ μ (determined from Fig. 1). The frequency of transverse vibrations is related to the frequency of longitudinal vibrations by

$$\omega_t = \omega_l\left(\frac{\varepsilon_\infty}{\varepsilon_0}\right)^{1/2} = \frac{2\pi c}{\lambda}\left(\frac{\varepsilon_\infty}{\varepsilon_0}\right)^{1/2}.$$

Hence we obtain $\omega_t = 5.5 \cdot 10^{13}$ s^{-1}. Substituting these values into formula (1), we obtain $e^* = 0.475\,e_0$. This result agrees well with the data of work ([2]), is somewhat lower than in work ([3]), and higher than the data of ([1]).

It is seen from Fig. 1 that, with increasing concentration of current carriers (as the conduction band is filled with free carriers), the minimum in the spectrum shifts into the short-wavelength region.

It is known that the effective mass of current carriers m^*_{op}, the concentration of electrons n and holes p, the dielectric constant of the crystal ε_∞ under conditions in which it does not depend on free carriers, and the wavelength $\lambda_{\min}$ at which the minimum occurs in the reflection spectrum are related by the relation ([7,8,14])

$$\frac{m^*_{op}}{m_0} = \frac{e^2 N \lambda^2_{\min}}{\pi c^2 m_0 (\varepsilon_\infty - 1)}.$$

On the basis of Fig. 1, the optical effective mass m^*_{op} was determined by the method of ([7,8,14]) (the values of m^*_{op} are given in Table 1).

The values of the effective mass of holes (see Table 1) are close to the data of work ([4]). The effective density-of-states mass of holes, estimated by V. G. Sidorov ([10]), has values $1.8\,m_0$, $0.9\,m_0$, and $0.97\,m_0$, respectively, for hole concentrations 10^{17}, 10^{19}, and $2\cdot 10^{20}$ cm^{-3}.

For the sample with $p = 2\cdot 10^{20}$ cm^{-3}, the Fermi level falls below the top of the valence band by $E_F = 0.29$ eV, so that $\Delta \geq E_F$ for a concentration $2\cdot 10^{20}$ cm^{-3}, and, probably, free holes may be present in the split-off band due to thermal excitation. Let us take from the theoretical calculation ([16]) the effective mass of heavy holes $m^*_{p1} = 0.68\,m_0$, of light holes $m^*_{p2} = 0.12\,m_0$, and for holes in the band split off due to spin-orbit interaction,

$m^*_{p_3} = 0.2m_0$. One can calculate the effective density-of-states mass for all valence bands $m^*_{d_{123}}$, for the two upper branches (heavy and light holes) of the valence band $m^*_{d_{12}}$, and the optical mass m^*_{op} from the formulas

$$\frac{m^*_{d_{123}}}{m_0} = \left[\left(\frac{m^*_{p_1}}{m_0}\right)^{3/2} + \left(\frac{m^*_{p_2}}{m_0}\right)^{3/2} + \left(\frac{m^*_{p_3}}{m_0}\right)^{3/2}\right]^{2/3} = 0.90,$$

$$\frac{m^*_{d_{12}}}{m_0} = \left[\left(\frac{m^*_{p_1}}{m_0}\right)^{3/2} + \left(\frac{m^*_{p_2}}{m_0}\right)^{3/2}\right]^{2/3} = 0.76,$$

$$\frac{m^*_{op}}{m_0} = \frac{m^{*3/2}_{p_1} + m^{*3/2}_{p_2}}{m^{*1/2}_{p_1} + m^{*1/2}_{p_2}} = 0.50.$$

The result obtained for m^*_{op} (see Table 1) is close to the calculated value $m^*_{op} = 0.50m_0$ and is considerably smaller than the experimental and theoretical values of the density-of-states mass m^*_d, which may be explained by the complexity of the structure of the GaAs valence band.

Fig. 2. Dispersion law $(dE/dk)_F \sim f(k)$.
a—our results; *b*—from ([6]); *c*—from ([11]); *g*—from ([12]); *d*—from ([13]); *e*—theoretical curve.

Fig. 2 and Fig. 3

Figure 2: Fig. 2 and Fig. 3

Fig. 3. Dispersion law $E(k^2)$ of the GaAs conduction band.
1–$E \sim k^2$; 2–Kane theory; 3–experiment.

To calculate the dispersion law of the conduction band, values of the effective electron mass found for our n-type GaAs samples from reflection measurements were used, together with our previously published data ([5],[6]) and data of other authors ([11–13]). For comparison with the experimental results, a theoretical dependence was constructed in the atomic system of units $m_0 = \hbar = e_0 = 1$,

$$dE/dk = k_F/m^* = (3\pi N)^{1/3}/m_n^*,$$

where the effective mass m_n^* was calculated, for the strongly degenerate case ($n > 3 \cdot 10^{18}$ cm^{-3}), by formula (9)

$$m_n^* = m_B \left[1 + \frac{2(2\pi)^{2/3}\hbar^2 n^{2/3}}{m_B E_g}\right]^{1/2};$$

here $m_B = 0.070 m_0$; $E_g = 1.39$ eV; the values of the effective mass for $n < 3 \cdot 10^{18}$ cm^{-3} were taken from ([15]).

The results of the calculation are presented in Fig. 2, where the experimental dependence, drawn as a solid line on the basis of exper-

experimental points and the theoretical curve. From Fig. 2 it is seen that the theoretical curve lies above the experimental one. To compare the theoretical dependence of the dispersion law $E(k^2)$ with the experiment and with parabolic dependences, the curve $(dE/dk)_F = j(k)$ (Fig. 2) was integrated graphically and the dependence $E(k^2)$, shown in Fig. 3, was constructed.

From a comparison of the dependences $E(k^2)$ in Fig. 3 it is seen that the degree of nonquadraticity of the empirical dispersion law $E(k^2)$ is somewhat greater than according to Kane.

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Note: Figure translations are in progress. See original paper for figures.