STUDIES OF THE STRUCTURE OF THE VALENCE BAND OF INDIUM ARSENIDE

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Fig. 1

Figure 1: Fig. 1

Abstract

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STUDIES OF THE STRUCTURE OF THE VALENCE BAND OF INDIUM ARSENIDE

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In InAs crystals the structure of the valence band was first studied by Shtern and Mattos ([1]) from absorption spectra in samples with hole concentrations from $4 \cdot 10^{16}$ to 10^{17} cm^{-3} (the effective masses of heavy and light holes were found). Data on reflection and absorption spectra in p-InAs crystals with hole concentrations $p > 10^{17}$ cm^{-3} are absent from the literature; nor is there information on the shape of the light- and heavy-hole bands.

To clarify the structure of the valence band, in the present work we investigated reflection and absorption spectra in p-InAs crystals with hole concentrations from $1.6 \cdot 10^{17}$ to $4.9 \cdot 10^{19}$ cm^{-3} at 300 and 100°K.

Single-crystal samples were grown by the Czochralski method. Doping was carried out with zinc during growth.

Figure 1 gives the spectral dependences of the reflection coefficient R on the wavelength λ in the region 1-40 μ. At $\lambda = 1$ μ the reflection coefficient for all samples is about 30%. For the sample with $4.9 \cdot 10^{19}$ cm^{-3} the plasma minimum was observed at 9 μ, and for the sample with $4.82 \cdot 10^{19}$ cm^{-3}, at about 9.4 μ. The reflection coefficient at the minimum is 16%. For the sample with $2.50 \cdot 10^{19}$ cm^{-3} the plasma minimum was observed at $\lambda_{\min} \geq 13.5$ μ.

Fig. 1. Dependence of the reflection coefficient R on the wavelength λ for p-InAs.
1 –$p = 4.90 \cdot 10^{19}$ cm^{-3}; 2 –$4.82 \cdot 10^{19}$; 3 –$2.50 \cdot 10^{19}$; 4 –$1.39 \cdot 10^{18}$; 5 – $3.90 \cdot 10^{17} \div 7.70 \cdot 10^{17}$ cm^{-3}. $T = 293$°K.

In samples with hole concentrations $3.8 \cdot 10^{17}$, $7.7 \cdot 10^{17}$, and $1.3 \cdot 10^{18}$ cm^{-3} no reflection minimum was observed. This is connected with the fact that at $p < 10^{19}$ cm^{-3} the Fermi level lies above the top of the valence band and it contains an insignificant number of thermally excited holes.

The minimum in the reflection spectrum (see Fig. 1) is determined from the formula

$$\frac{m^*_{op}}{m_0} = 0.9 \cdot 10^{-15} \frac{N\lambda^2_{\min}}{\varepsilon_\infty - 1} \tag{1}$$

(where N is the concentration of free carriers in the band; ε_∞ is the dielectric constant of the crystal lattice without the contribution of free and bound carriers); it lies in the wavelength region of 50 μ (the limiting

wavelength of our instrument), if the effective mass of the holes is taken to be $0.3m_0$.

In samples with a hole concentration $p > 10^{19}$ cm^{-3}, the Fermi level is lowered below the top of the valence band, and the minimum in the reflection spectrum lies in the wavelength region $\lambda < 50$ μ. From the plasma minimum one can calculate a certain averaged effective mass, since current carriers from the bands of heavy and light holes contribute to the conductivity. The effective mass calculated from formula (1) for $p = 4.9 \cdot 10^{19}$ cm^{-3} was found to be $m^*_p = 0.31m_0$; for $p = 4.82 \cdot 10^{19}$ cm^{-3}, $m^*_p = 0.315m_0$; for $p = 2.5 \cdot 10^{19}$ cm^{-3}, $m^*_p = (0.27 \pm 0.03)m_0$.

The effective mass was also calculated from the more exact quadratic Lyddane formula

$$m^2 - \frac{3\varepsilon_\infty - 1}{4\varepsilon_0(\varepsilon_\infty - 1)} \frac{1/\Omega^2 + 5 + 8\Omega^2}{1 + 3\Omega^2} cm + \frac{3\varepsilon_\infty - 2}{2\varepsilon_0(\varepsilon_\infty - 1)^2} \frac{1 + 2\Omega^2}{1 + 3\Omega^2} c^2 = 0. \tag{2}$$

The following values were obtained for different carrier concentrations at 300° K:

p, cm^{-3}	$2.5 \cdot 10^{19}$	$4.82 \cdot 10^{19}$	$4.9 \cdot 10^{19}$
m_p/m_0	0.360	0.380	0.400

The result obtained agrees well with the value of the mass (within the error limits) calculated from the absorption spectra ([1]) and with the data of Weiss ([6]), who obtained the density-of-states mass $m_d = 0.33m_0$ from thermoelectric-power measurements.

From Fig. 2, which gives the absorption spectrum for the sample $p = 1.6 \cdot 10^{17}$ cm^{-3}, it is seen that in the energy region $h\nu > 0.33$ eV the absorption is caused by interband transitions. In the energy region $h\nu \ll 0.33$ eV the absorption coefficient increases with decreasing photon energy and, at $h\nu = 0.175$ eV, an absorption maximum is observed, which apparently should be attributed to transitions between the branches of light and heavy holes. A similar maximum was observed earlier in Ref. ([1]).

To compare the experimental data with theoretical ones in the region of the intrinsic absorption edge for a crystal with a low hole concentration ($p < 10^{18}$ cm^{-3}), formula ([2]) was used

$$a_c = \frac{k}{h\nu}\left(m_{r_1}^{3/2} + m_{r_2}^{3/2}\right)(h\nu - E_g)^{1/2}, \tag{3}$$

where

$$m_{r_1} = \frac{m_{p_1} m_n}{m_{p_1} + m_n} = 0.0022 m_0$$

is the reduced effective mass of the heavy-hole branch, $m_{p_1} = 0.37 m_0$, and of the conduction band, $m_n = 0.023 m_0$;

$$m_{r_2} = \frac{m_{p_2} m_n}{m_{p_2} + m_n} = 0.0124$$

is the reduced effective mass of the light-hole branch, $m_{p_2} = 0.027 m_0$, and of the conduction band, $m_n = 0.023 m_0$; $E_g = 0.35$ eV at 300° K is the threshold energy.

In Fig. 2 the theoretical curve 5, calculated from formula (3), agrees quite satisfactorily with the experimental points.

Intrinsic absorption in samples with hole concentrations greater than $1.6 \cdot 10^{17}$ cm^{-3} is shown in Fig. 3, where a shift of the edge of optical absorption toward shorter wavelengths with increasing hole concentration (the Burstein-Moss effect) is seen. Here 2 is the theoretical dependence for a sample with hole concentration $p = 3.48 \cdot 10^{18}$ cm^{-3}, calculated from the formula

$$a_N = a_0 \left[1 + \frac{E_F + E_g - h\nu}{(1 + m_n/m_p)kT}\right]^{-1},$$

which takes into account the considerable filling of the valence band with holes ([5]). Here $m_p = 0.37 m_0$. From Fig. 3 it is seen that the experimental curves agree satisfactorily with the calculated data. In discussing the expe-

experimental data for absorption due to the transition between V_1 and V_2, it was assumed that the valence band of InAs is similar to the valence band of germanium; therefore Kane' s formula, derived for $V_1 \to V_2$ transitions in Ge (it is assumed that the dispersion law in these bands is quadratic), was applied:

Fig. 2

Figure 2: Fig. 2

Fig. 3

Figure 3: Fig. 3

$$\alpha_{12} = \frac{16\pi^2(2)^{1/2}e^2\hbar^{1/2}A_{12}^2 m_{p_1}^{1/2} N v^{1/2}}{nc^{1/2}\left[1+\left(m_{p_2}/m_{p_1}\right)^{3/2}\right] m^2\left(m_{p_1}-m_{p_2}\right)^{5/2}(kT)^{1/2}} \times \left[\exp\left(-\frac{hc\nu}{kT}\frac{m_{p_2}}{m_{p_1}-m_{p_2}}\right) - \exp\left(-\frac{hc\nu}{kT}\frac{m_{p}}{m_{p_1}-\right.\right. \tag{4}$$

where $\nu = \Delta E/ch$, $N = 1.6 \cdot 10^{17}$ cm^{-3}; $n = 3.42$; $c = 3 \cdot 10^{10}$ cm $\cdot$ s^{-1}; $e = 4.8 \cdot 10^{-10}$ CGSE; $m_0 = 9.1 \cdot 10^{-28}$; $kT = 0.025 \cdot 1.6 \cdot 10^{-12}$ erg.

The effective mass of heavy holes $m_{p_1} = 0.37\, m_0$ was taken from our data (see above), and values calculated according to Kane' s theory were also used: $m_{p_1} = 0.41\, m_0$, $m_{p_2} = 0.025\, m_0$ at 0°K (1), $m_{p_2} = 0.027$ at 300°K (3). In addition, $m_{p_2} = 0.06$ and $m_{p_2} = 0.13\, m_0$ were chosen arbitrarily.

Substituting all the values found into equation (4) at photon energy $h\nu = 0.18$ eV and taking from the experimental

Fig. 2. Dependence of the absorption coefficient α on the photon energy for p-InAs, $p = 1.6 \cdot 10^{17}$ cm^{-3}, $d = 36$ μ. 1-4–theoretical curves calculated for different values of the effective masses: 1–$m_{p_1} = 0.37m_0$, $m_{p_2} = 0.13m_0$; 2–$m_{p_1} = 0.37m_0$, $m_{p_2} = 0.027m_0$; 3–$m_{p_1} = 0.41m_0$, $m_{p_2} = 0.025m_0$; 4–$m_{p_1} = 0.41m_0$, $m_{p_2} = 0.06m_0$; 5–theoretical curve. Points–experiment.

Fig. 3. Dependence of the intrinsic absorption coefficient α_c on photon energy for p-InAs at different concentrations p: a–$3.8 \cdot 10^{17}$ cm^{-3}; b–$7.71 \cdot 10^{17}$; c–$1.39 \cdot 10^{18}$; d–$3.48 \cdot 10^{18}$ cm^{-3}; 1 and 2–theoretical curves at $p = 3.8 \cdot 10^{17}$ (1) and $p = 3.48 \cdot 10^{18}$ (2). $T = 100$°K.

curves $\alpha_{12} = 370$ cm^{-1}, we calculated the constant A_{12} for 4 cases:

1) $m_{p_1}^* = 0.37\, m_0$, $m_{p_2}^* = 0.13\, m_0$, $A_{12} = 7.6$.
2) $m_{p_1}^* = 0.37\, m_0$, $m_{p_2}^* = 0.027\, m_0$, $A_{12} = 23.8$.
3) $m_{p_1}^* = 0.41\, m_0$, $m_{p_2}^* = 0.025\, m_0$, $A_{12} = 20.6$.
4) $m_{p_1}^* = 0.41\, m_0$, $m_{p_2}^* = 0.06\, m_0$, $A_{12} = 12$.

On the basis of these values of A_{12}, the spectral dependences $\alpha_{12}(h\nu)$ were calculated. From a comparison of the experimental data with the theoretical curves in Fig. 2, it follows that curves 1 and 4 give the best agreement with experiment in the short-wavelength region. With a further decrease in the

photon energy, the calculated curves 1 and 4 deviate from the experimental ones, and their maxima are shifted into the long-wavelength region relative to the maximum of the experimental dependence. This discrepancy between the calculated curves and the experimental data is apparently connected with the fact that Kane' s theory does not take into account the deviation of the dispersion law of the light-hole branch from quadratic behavior. Comparison of calculated curves 2 and 3 with the experimental points gives good agreement in the long-wavelength region of the spectrum. With increasing photon energy, the experimental points deviate from the theoretical dependence, which may be explained by the nonparabolicity of the light-hole band in InAs, as follows from Kane' s theory.

Kane' s theory, which takes into account the nonparabolicity of the light-hole band, cannot yet be applied in the present case, since exact values of the effective masses of light and heavy holes and reliable information on the dispersion law in these branches are lacking. Comparison of experiment with theory shows that the nonparabolicity of the valence band of light holes manifests itself already at a photon energy $h\nu = 0.23$ eV. Analogous comparisons were made by Kane and Kane for Ge. If our results are compared with their data, it turns out that the nonparabolicity of the light-hole bands in InAs is greater than in Ge.

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