PHYSICS

1964

SovietRxiv

Abstract

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PHYSICS

S. A. Abagyan, V. K. Subashiev

THE STRUCTURE OF THE CONDUCTION BAND OF GaP

(Presented by Academician B. P. Konstantinov, January 7, 1964)

The band structure of gallium phosphide has so far been studied relatively little. By analogy with silicon, from experiments on the effect of pressure on absorption and electrical conductivity [1,2], it was concluded that the absolute minimum of the GaP conduction band lies in the ⟨100⟩ direction. As a result of a study of the optical properties [3], a model of the band structure with two minima in the conduction band was proposed. The first minimum lies in the ⟨100⟩ direction, while the second is located at the point $k = 0$ and is 0.35 eV above the first. This picture of the GaP band structure, with one indirect transition at 2.2 eV and a direct transition near 2.55 eV, has been used up to the present time.

However, from the dependence of the forbidden-band width on composition in the GaP–GaAs system [7], it follows that direct transitions in GaP should begin at energies of approximately 2.7 eV.

To test the picture of the GaP band structure, we carried out a detailed measurement and analysis of the edge of intrinsic absorption in the region 2–2.75 eV. Transmission measurements were performed on plane-parallel samples 5 to 200 μ thick, obtained naturally in the course of crystal growth or prepared by the usual grinding and polishing technique. The plane-parallelism and thickness of the crystals were monitored from the interference pattern in the transmission spectrum in the region 2–25 μ, recorded on a UR-10 automatic spectrophotometer. Analysis of the interference periods for samples of known thickness made it possible to determine the refractive index, which in the region 2–20 μ proved to be 2.95 ± 0.10. In the range 0.7–2.75 eV, transmission was measured by the "sample inserted–removed" method; a germanium photoresistor or an FEU-36 photomultiplier was used as the detector. The optical part of an SF-4 spectrophotometer served as the source of monochromatic light. To eliminate errors introduced by scattered light from the monochromator, the beam incident on the sample was passed through light filters cutting off the long-wavelength part of the spectrum immediately near the wavelength being measured. On the same apparatus the reflection spectrum of GaP was also studied. The absorption coefficient was calculated from a formula taking multiple reflection into account.

The measurement results are shown in Fig. 1, where α and $h\nu$ are the absorption

Fig. 1

Figure 1: Fig. 1

coefficient and photon energy. From Fig. 1, 1′, which shows the dependence of $\alpha^{1/2}$ on $h\nu$, it is seen that in the region from the edge to $\simeq 2.51$ eV

$$\alpha \sim (h\nu - Eg_1)^2.$$

Such a frequency dependence coincides with that theoretically calculated for indirect allowed transitions [4]. The forbidden-band width Eg_1, determined from measurements of this kind for a large number of crystals, was found at room temperature to be 2.21 ± 0.01 eV.

The linear section may also indicate that the assumptions of parabolic bands in this energy interval are valid (i.e., to a depth of 0.3 eV from the band edges).

It may be assumed that the deviations from the straight line $\alpha^{1/2} \sim (h\nu - Eg_1)$ are caused by transitions of electrons into the minimum of a higher branch of the conduction band.

of mobility. Then, assuming that the bands remain parabolic thereafter as well, one can, by subtracting from α the values α_1 lying on the continuation of the rectilinear portion of the dependence of $\alpha^{1/2}$ on $h\nu$, obtain the energy dependence of the absorption coefficient for processes of electron transition from the valence band to the next minimum of the conduction band.

Fig. 1. Dependence of $\alpha^{1/2}$ (1) and $(\alpha - \alpha_1)^{1/3}$ (2) on the photon energy $h\nu$

It turned out, as is seen from Figs. 1 and 2, that the quantities $\alpha - \alpha_1$ in the region 2.55-2.7 eV depend on the photon energy in the form

$$\alpha - \alpha_1 \sim (h\nu - Eg_2)^3,$$

which is characteristic of allowed indirect transitions. The energy corresponding to the position of the second minimum, Eg_2, was found to be 2.51 eV. From the same graph it follows that a sharp, approximately exponential, increase of α begins at energies of about 2.7 eV and, apparently, is caused by direct transitions. It may be noted that in GaAs, where the absolute minimum of the conduction band is located at $k = 0$, the absorption coefficient in the region of the intrinsic-absorption edge also depends exponentially on the photon energy ([5]).

Thus, the edge of intrinsic absorption in GaP is well explained on the basis of a band-structure model in which there are two indirect transitions and one direct transition.

With regard to the position of the second minimum in k-space, two assumptions can be made: either it is located in the $\langle 100 \rangle$ direction, i.e., approximately at the

Fig. 2

Figure 2: Fig. 2

same point of k-space as the first minimum, or in the $\langle 100 \rangle$ direction. In the first case one might think that the i.-f. absorption band in n-GaP ([3]) is associated with direct interband transitions from the first minimum to the second. Indeed, the energy gap between the first and second minima coincides with the long-wavelength edge of the band; the weak dependence of the position of the band on pressure and temperature ([1],[3]) is explained by the fact that both minima shift in approximately the same way when pressure or temperature changes. However, in ([6]), on the basis of a study of photoluminescence and absorption spectra, it is considered that the cause of the i.-f. absorption band is donor levels lying 0.4 eV below the bottom of the conduction band. In addition, if both minima were located at one and the same point of k-space, a strong interaction between them would have to appear because of the small energy gap separating them. Therefore the assumption that the second minimum lies in the $\langle 111 \rangle$ direction seems more plausible.

Fig. 2. Proposed picture of the band structure of GaP

The result seems somewhat strange: that the transition to the first minimum is allowed, whereas to the second it is forbidden, since if a virtual transition to $k = 0$ is allowed for the first minimum, then it should also be allowed for the second. It is possible, however, that the scheme for the transition of an electron from the top of the valence band to the $\langle 100 \rangle$ minimum differs from the scheme for the transition to the $\langle 111 \rangle$ minimum; i.e., in the transition to the $\langle 111 \rangle$ minimum the electron first virtually passes from the valence band to the $\langle 111 \rangle$ minimum, transitions between which are forbidden, and then scattering of the remaining hole in the valence band occurs. It is also possible that the second indirect transition is allowed and that the cubic dependence of $\alpha - \alpha_1$ on $h\nu$ is caused by the nonparabolicity of the first minimum or by the nonconstancy of the matrix element for the transition probability in this energy region.

Thus, the band diagram of gallium phosphide is represented in the form shown in Fig. 2.

The authors consider it their pleasant duty to express gratitude to A. V. Lishina for providing the crystals and to P. Singhal for assistance with the measurements.

Institute of Semiconductors
Academy of Sciences of the USSR

Received
30 XII 1963

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