

Optical Coefficients of Nonuniform Semiconductor Layers

A brief discussion of determination of optical coefficients in uniform absorbing layers is given. Next a method of determining the absorption coefficient as well as of the complex refractive index in nonuniform semiconductor layers is proposed. The applications of the derived formulae to the analysis of the measurement results obtained for epitaxial $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layers of molar composition changing with the thickness are described.

1. Introduction

Determination of the spectral dependences of refractive and reflection indices provides an extremely important information about energy states of electrons in semiconductors. This enables, in particular, to determine both the energy gap width at a Γ point and the energy of interband transitions at other characteristic points of the relation $E(k)$.

The properties of nonuniform mixed crystals such in which band parameters (energy gap, effective mass and mobility of carriers and so on) are functions of their position in the crystal have been thoroughly studied in the recent years. Because of so highly interesting properties these crystals find a number of practical applications, e.g. to radiation detectors working in a predetermined spectral range; the fitting to the given spectral range is achieved, by changing the molar composition in the material, which is a relatively simple procedure. The above semiconductors are of particular interest as far as the production of infrared detectors working in the region of *atmospheric window* i.e. in the 8–14 μm wavelength range is concerned.

The interaction of the radiation with the uniform absorbing layer was widely discussed in the fundamental literature (see papers [1–7]). The case of nonuniform absorbing layer was considered in [8] but in a way highly restricted due to the accepted boundary condi-

tions; assuming that the refractive indices on the both surfaces of the layer are equal to the refractive indices of the surrounding medium.

The paper suggests a method of determining the absorption and refractive indices for various regions of semiconductor layer nonuniform optically, based on measurement of reflection and transmission indices. The results of application of the obtained dependences to investigations of the optical properties of the epitaxial $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layers, with molar composition evarying with the layer thickness have been also briefly discussed.

2. Determination of optical coefficient of uniform semiconductor layers

The absorption index α and the complex refractive index $n^* = n + ik$ are the basic quantities characterizing the optical properties of a uniform semiconductor layer; the transmission index T and the refraction index R , being the parameters usually measured. The literature dependence between T and R , on the one hand, and the thickness d of the semiconductor layer and the refractive and absorption indices, on the other one, differ among one another.

HEAVENS [4] gave an expression for the reflectivity R and transmittivity T which is valid in the case of a uniform absorbing layer deposited on a transparent substrate. The method of calculation of refractive and absor-

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ption indices of the layer suggested by this author [4] is rather difficult, though its accuracy may be relatively high, depending on the fitting of wavelength to the given layer thickness.

Generally, the relations, between T and R , and n^* and a are given in the form of

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}, \quad (1a)$$

$$T = \frac{(1-R)^2 \cdot \exp(-ad)}{1 + R^2 \cdot \exp(-2ad)}, \quad (1b)$$

respectively.

Formula (1b) has been derived for one-dimensional absorbing layer of thickness d by taking into account multiple internal reflections. In the above form this relation is given among others by MOSS [1], JOHNSON [6] VAVILOV [2], MADELUNG [3] and TAUC [5]. By inserting the equation (1a) into (1b) and solving the latter with respect to a for the spectral range, in which $n^2 \ll k^2$ we get

$$a = \frac{1}{d} \ln \frac{B + \left[B^2 - 4T^2 \left(\frac{n-1}{n+1} \right)^4 \right]^{1/2}}{2T}, \quad (2)$$

where

$$B = \frac{16n^2}{(n+1)^4}.$$

This formula is valid in the case, when the both media surrounding the layer have the same refraction index, i.e. $n_0 = n_2 = 1$. The case when $n_0 = 1$ (air) and $n_2 > 1$ (e.g. glass, mica, NaCl, and so on) have been considered e.g. in [1] and its applications given in [11], and [12] to Cd_3As_2 and to Zn_3As_2 layers respectively. For a uniform layer, in which $k^2 \ll n^2$, and for maximum transmission the coefficients of absorption and reflection may be written in the form

$$a = \frac{1}{d} \ln \times \frac{(A + 2r_1 r_2) + [(A + 2r_1 r_2)^2 - 4T^2 r_1^2 r_2^2]^{1/2}}{2T}, \quad (3a)$$

and

$$R' = \left(\frac{n-1}{n+1} \right)^2$$

or

$$R'' = \left(\frac{n-n_2}{n+n_2} \right)^2. \quad (3b)$$

In strong absorption region (high absorption indices) or large spectral widths of the incident light beams the expression for the transmission takes an averaged form, while the expression for a has the form

$$a \cong \frac{1}{d} \ln \frac{A + (A - 4T^2 r_1^2 r_2^2)^{1/2}}{2T}. \quad (4)$$

In the formulae (3) and (4) r_1 denotes the complex Fresnel coefficients at the air-layer boundary and r_2 the layer-substrate boundary. They are given by the formulae

$$|r_1|^2 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}, \quad (5)$$

$$|r_2|^2 = \frac{(n_2 - n)^2 + k^2}{(n_2 + n)^2 + k^2},$$

whereas

$$A = \frac{16(n^2 + k^2)n_2}{[(1+n)^2 + k^2][(n+n_2)^2 + k^2]}. \quad (6)$$

As it may be easily verified the formula (2) may be obtained by letting $n_2 = 1$ in the formulae (4), (5) and (6).

The papers [13] and [14] present a method of estimation of the coefficients n and k (n and a) based on dispersion relation for the reflectance spectrum. This method requires only the measurement of reflection coefficient and will not be discussed hereafter.

3. Optical coefficient of a nonuniform semiconductor layers

The case of nonuniform layer discussed in paper [8] has been restricted by the assumptions explained in Fig. 1. If $n_1 = n_0$ (on one side) and $n_2 = n_g$ (on second side) then according to (3b) the reflection indices are equal to

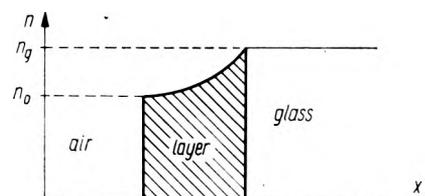


Fig. 1. A simplified case of a nonuniform layer

$R' = R'' = 0$. This situation is rather exceptional however.

Let us now discuss the case characteristic of the nonuniform mixed crystal layers presented schematically in Fig. 2. The refractive

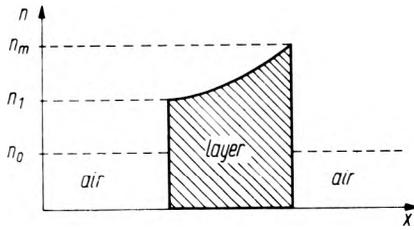


Fig. 2. Nonuniform absorbing layer discussed in the paper

indices in the planes bounding the layer from the both sides fulfill the inequality $n_0 < n_1 \leq n(x) \leq n_2 > n_0$, while the relation between the refractive index of the layer and the thickness x of the latter, i.e. $n(x)$, may be pretty well described by a diminishing or increasing function.

The discussion will be developed under the following assumptions:

1. A plane wave of intensity I_0 travelling along the X axis falls perpendicularly on a semiconductor layer located in vacuum or air surrounding. The variation in optical parameters occurs also along the X -axis.

(ii) For each X the layer is optically uniform in the Y and Z axes.

(iii) The layer may be divided into an arbitrary large number of plane parallel slices of thickness dx . Within the distance dx the optical

parameters are assumed to be constant (this idea is illustrated by Fig. 3).

(iv) No internal reflections occur at the boundaries between the slices. This corresponds to the real situation in the semiconductor crystals with a continuous change of $R(x)$.

(v) The influence of the beam reflected from the both boundary planes of the layer may be neglected due to a high value of the absorption index (usually within the whole range of the radiation spectrum used in the measurements).

The trace of radiation within the layer (consisting of m slices) is shown schematically in Fig. 3. As seen from Fig. 3 the successive reflection coefficients may be written as follows:

$$R_1 = \frac{(n_1 - 1)^2 + k_1^2}{(n_1 + 1)^2 + k_1^2},$$

$$R_2 = \frac{(n_2 - n_1)^2 + k_2^2}{(n_2 + n_1)^2 + k_2^2},$$

$$\dots$$

$$R_c = \frac{(n_m - 1)^2 + k_m^2}{(n_m + 1)^2 + k_m^2}.$$

Consequently, the intensity of radiation emerging from the layer may be expressed as

$$I_m = (1 - R_1)(1 - R_2) \dots (1 - R_c) I_0 \times \exp\left(-\sum_{m-1}^m \alpha_m dx\right), \quad (8)$$

assuming that $dx_1 = \dots = dx_m = dx$ and considering the condition (v). In view of the con-

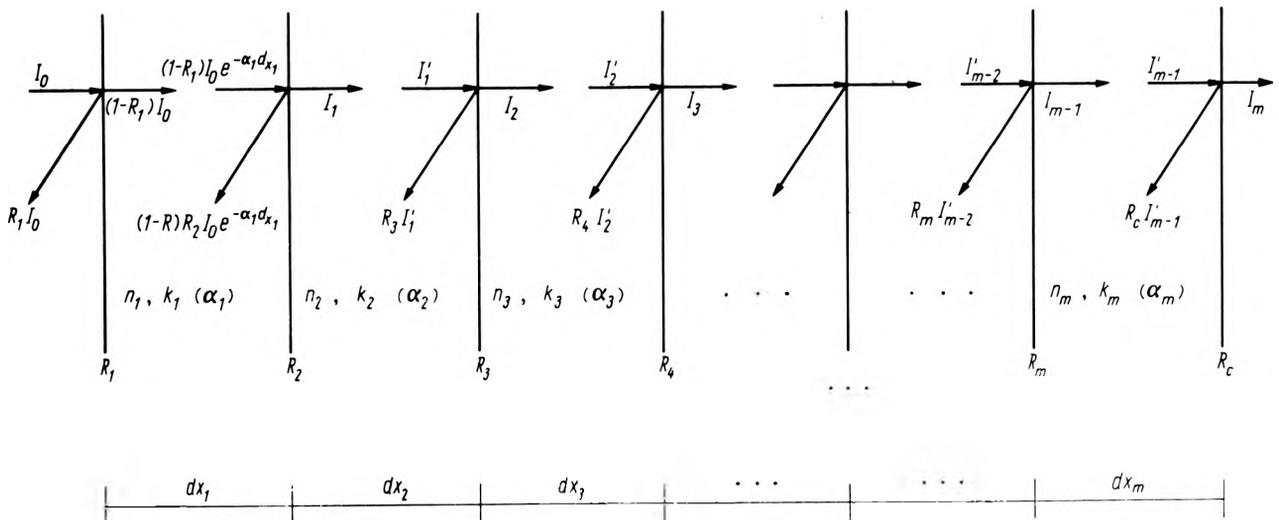


Fig. 3. The ray travelling along a nonuniform layer with perpendicular radiation incidence

ditions (iii) and (iv) the formula (8) (for a layer consisting of m slices) takes the form

$$\begin{aligned}
 I_1 &= (1 - R_1)(1 - R_2)I_0 \exp(-a_1 dx), && \text{for } m = 1, \\
 I_2 &= (1 - R_1)(1 - R_3)I_0 \exp[-(a_1 + a_2)dx], && \text{for } m = 2, \\
 I_3 &= (1 - R_1)(1 - R_4) \exp[-(a_1 + a_2 + a_3)dx], && \text{for } m = 3, \\
 &\dots\dots\dots && \dots\dots\dots \\
 I_m &= (1 - R_1)(1 - R_c)I_0 \exp\left(-\sum_{m=1}^m a_m dx\right), && \text{for } m = m.
 \end{aligned} \tag{9}$$

Thus transmission values for separate slices will be given by the following formulae

$$T_1 = \frac{I_1}{I_0}, \quad T_2 = \frac{T'_2}{T_1} = \frac{I_2}{I_1},$$

where $T'_2 = \frac{I_2}{I_0}$,

$$T_3 = \frac{T'_3}{T_1 T_2}, \tag{10}$$

where $T'_3 = \frac{I_3}{I_0} \dots$, while, as it is easy to show, the transmission of the whole layer T_c is equal to

$$T_c = T_1 \cdot T_2 \dots T_m = \frac{I_m}{I_0}, \tag{11}$$

(see Fig. 3 and the conditions (iii), (iv) and (v)).

3.1. Determination of the absorption index as a function of the layer thickness

To determine the absorption coefficient of a nonuniform layer with respect to its thickness the following procedure is proposed:

The layer should be prepared for the measurements in the way illustrated in Fig. 4. The thickness of the jumps (Fig. 4a) or of the slices etched consecutively (Fig. 4b) must be selected so that the energy gap width (and other band parameters) be changed along this thickness in a way imperceptible for the measuring set-up. Their thicknesses moreover, should not be smaller than the wavelength of the radiation used in the measurements (lower bound limitation) and not greater than the

value of dx , for which $adx \approx 5$ [19] (upper bound limitation). Simultaneously, the slices should be of possibly the same thickness. For a sample prepared in such a way the measurement of reflection and absorption are made in the given wavelength range for the successive surfaces of the stepwise increasing layer. The performed series of measurements yields a sequences of values I_1, I_2, \dots, I_m (the intensities of the transmitted beams) and $I_1^R, I_2^R, \dots, I_m^R$ (the intensities of the reflected beams) in function of the wavelengths corresponding to reflection and transmission of the layer at different thicknesses. In view of these results and employing the relations given above for each slice, separately, the spectral transmission characteristics $T(\lambda)$ may be determined from the formulae (10) and (11), the reflection characteristics $R(\lambda)$ being given by the following relations (see Fig. 4):

$$R_1(\lambda) = \frac{I_1^R}{I_0}, \quad R_2(\lambda) = \frac{I_2^R}{I_0}, \dots, \quad R_c(\lambda) = \frac{I_c^R}{I_0}.$$

Consequently, R and T may be determined as functions of the thickness, the molar composition, etc.

The calculation of the absorption coefficient may be now performed with the help of two methods described below.

3.1.1. Calculation of $a(h\nu)$ by using the effective thickness of absorption

As mentioned in section 3, semiconductor layer consisting of m slices should be treated as a set of m uniform (but differing among one another) absorbing semiconductor slices. This assumption enables to estimate the absorption coefficient by applying formula (2) or (3) which are valid for homogeneous samples estimation.

It remains to define the quantity d appearing in this formula. By d we mean either a part of the slice (jump, at Fig. 4) or the whole slice or two, three or more slices, depending on particular conditions. The method described in this section consists in the estimation of an *effective thickness* d_{ef} of portion of the layer, which takes an essential part in the absorption process.

The values of $T(\lambda)$ and $R(\lambda)$ as respective functions of the layer thickness being known the participation of particular regions of the layer in total absorption of the incident radia-

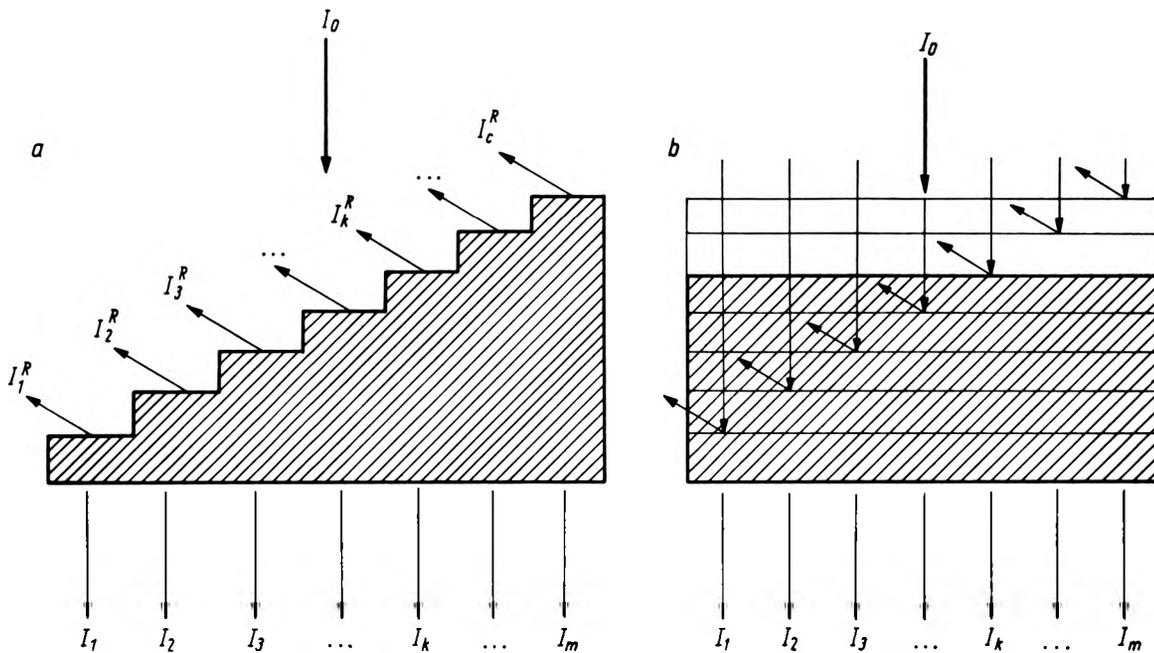


Fig. 4. Preparation of a nonuniform layer to the optical measurements *a* – production of jumps; *b* – successive etching of slices

tion can be estimated consecutively. An example of such an estimation is presented in Fig. 5, where typical dependences of $T(\lambda)$ and $(1-T-R)$ on the layer thickness are shown graphically. On the base of a graph shown in Fig. 5b it is possible to evaluate an effective

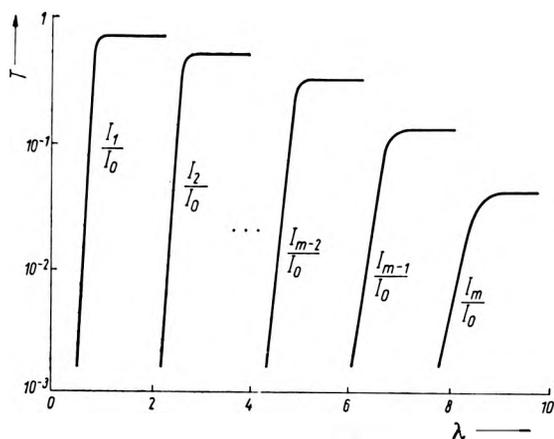


Fig. 5a. Spectral dependence I_k/I_0 typical of nonuniform semiconductor layer (exemplified by a $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layer) in arbitrary units. For notation see Fig. 3 and 4

thickness of the absorbing layer d_{et} as the thickness along which the transmission diminishes significantly, e.g. by 1 or 2 orders of magnitude. The coefficient of absorption is then defined from the following relations (e.g. for the ra-

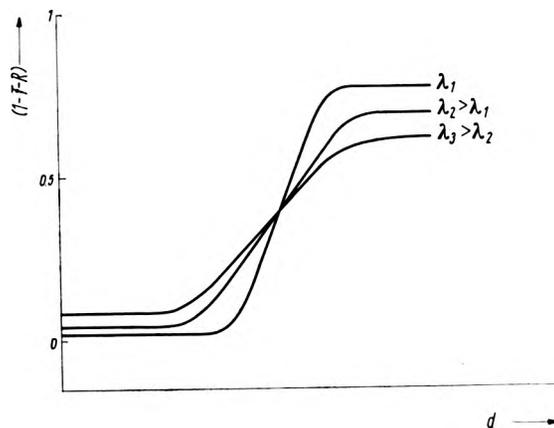


Fig. 5b. An example of the participation of separate regions of nonuniform semiconductor layer (exemplified by a $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layer) in absorption

diation falling on the k -th surface – see Fig. 4):

$$\alpha_k = \frac{1}{d_{\text{et}k}} \ln \frac{(1-R_k)(1-R_1)}{T'_k}, \quad (12)$$

which may be obtained from the formula (1b) and the condition (v) by substitution of the qualities R_1 and R_k gives by formula (7) for R . The value T'_k is determined according to the formula (10), for a layer containing k slices.

3.1.2. Evaluation of $\alpha(h\nu)$ from the transmission of successive slices

This manner based on a simple comparison of transmission of two slices of different thickness, (see e.g. [7]), has been proposed for the $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layers by DUDZIAK [15]. If the values I_1, \dots, I_m and R_1, R_2, \dots, R_c are known for each wavelength, then the transmission of one slice and of two consecutive slices can be compared. By employing the formulae (1b) and (9) jointly with the condition (v) we get (e.g. for the two first slices)

$$\frac{I_1}{I_0} : \frac{I_2}{I_0} = \frac{(1-R_1)(1-R_2)}{(1-R_1)(1-R_3)} \times \exp[(-a_1 dx) + (a_1 + a_2) dx], \quad (13)$$

and

$$\frac{I_1}{I_2} = \frac{1-R_2}{1-R_3} \exp(a_2 dx), \quad (14)$$

whence the value of $a_2(h\nu)$ may be easily estimated. The equation (14) may be generalized for two arbitrary consecutive constant-thickness slices of a layer.

3.2. Determination of the refractive index as a function of the layer thickness

The real and imaginary parts of a complex refraction index $n^* = n + ik$ may be determined from the measurement which have been shown schematically in Fig. 4. The spectral characteristics of the imaginary part of n^* may be determined from the previously determined $\alpha(h\nu)$ described above with the help of a well-known formula $k = \frac{\lambda\alpha}{4\pi}$. The real part of n^* may be determined from the formula (1a), which may be usually written in form of (3b), since for the semiconductors within that part of radiation spectrum which is usually of interest (i.e. in the vicinity of the fundamental edge) we have $n^2 \gg k^2$.

4. On the application of the proposed methods to the analysis of the measurements made on epitaxial layers

The discussion presented above and the relations obtained have been used in the analysis of the experimental results for the epitaxial

$\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layers [16]. The measurements were carried out on the samples prepared according to Fig. 4b. The values of refraction coefficient $R_1 = 0.31$ for $x \cong 0.1$ and $R_c = 0.22$ for $x = 1$ (measured outside the characteristic points corresponding to the interband transitions of energy $E_0, E_0 + \Delta E_0, E_1 + \Delta E_1$ and so on, see [16]) indicate that this coefficient depends on molar composition rather weakly.

The values of the absorption coefficient were calculated by using the two methods described above, i.e. according to formulae (12) and (14). It has been stated that the difference between the results obtained in the both ways cannot be ascribed to experimental error. To illustrate this fact the minimum values of the absorption coefficient a_{\min} (corresponding approximately to the least values of α for the absorption edge) evaluated by the both methods have been presented in Fig. 6 as functions of

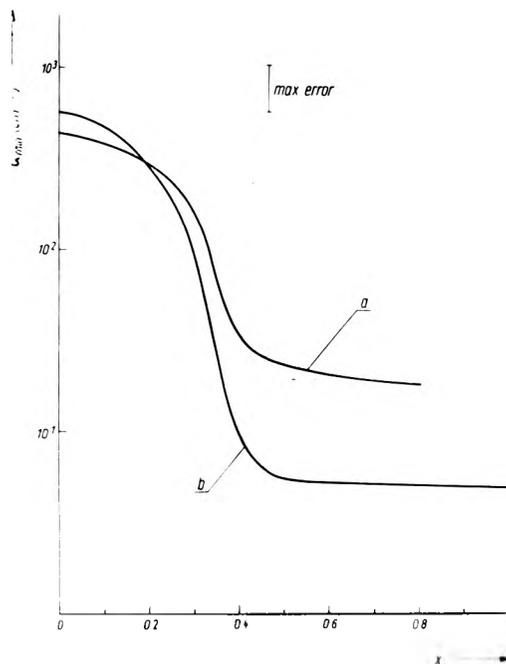


Fig. 6. Spectral dependence of the minimal value of the absorption coefficient for an epitaxial layer $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ upon the molar composition a - calculated from (12), b - calculated from (14)

the molar composition of the examined semiconductor. In this figure the maximum experimental error has been also marked. For each slice the average molar fraction of cadmium was determined from the formula

$$\bar{x} = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} x(t) dt, \quad (15)$$

for known dependence of α on the actual layer thickness t . A significant difference in the calculated values of α_{\min} were in particular obtained for low values of the absorption coefficient i.e. for a high cadmium content in the layer. This was probably due to the following reasons:

1. Insufficient measurement accuracy in determining the absolute values of transmissions (e.g. due to instability of the radiation source, to differences in dimensions of slits used in the monochromator, and the like). This accuracy is especially important at measurements performed in the regions of small relative changes in T values, i.e. just in the high transmission-region.

2. The differences in the values of molar composition (representative of a given slice) determined from the formula (15).

3. The error committed in evaluation of the effective thickness d_{ef} of the absorbing layer.

4. Error in the measurement of thickness of jump (Fig. 4a) or of etched slices (Fig. 4b).

It may be estimated preliminarily that the most important source of the said discrepancy is the reason given in item 1. Therefore the measurements should be performed according to the scheme 4a rather than to 4b, and the stability improved of both the source and the detector.

In case of high cadmium content a considerable error in calculation of $\alpha(x)$ (performed by the both method) is due to reason 2.

It is worth noting that the both calculation methods discussed in sections 3.1.1. and 3.1.2 suffer from some shortcomings, independent of restrictions resulting from the assumptions (i)-(v). When carrying out the computations, as in section 3.1.1, we obtain the averaged value of the absorption coefficient

$$\alpha = \frac{1}{d_{\text{ef}}} \int_0^{d_{\text{ef}}} \alpha(x) dx, \quad (16)$$

characterizing the region in the layer down to the depth d_{ef} from the layer surface (considering the surface with smaller energy gap). In the $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layers examined in our laboratory [16] the thickness of this region was in general not greater than that at which the molar composition x (and hence E_g) changed markedly. For large x (large E_g) the thickness d_{ef} was comparable with or even less than the thickness of jumps or etched slices. In this region the

method described in section 3.1.2. suffers from relatively greater errors, as the absorption of the radiation is not constant along the whole slice thickness. This method is more sensitive to the measurement errors of the absolute radiation intensity.

The values of the real and imaginary parts of the refractive index calculated by the method described in the section 3.2. are presented (for several molar compositions) in Fig. 7. The

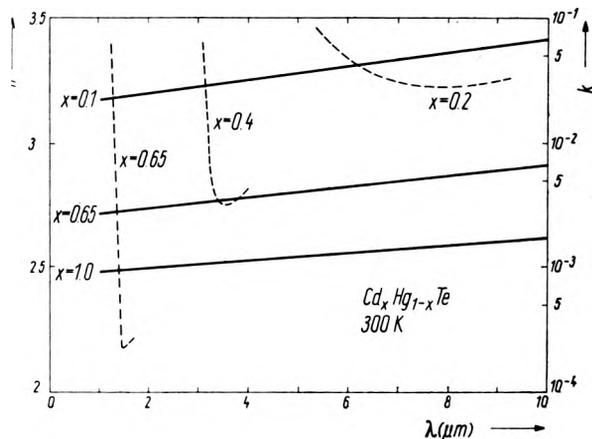


Fig. 7. The real (solid line) and imaginary (dashed line) parts of the complex refractive index of an epitaxial $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ layer in the vicinity of the fundamental edge (for several molar compositions)

obtained values of the refractive index are satisfactorily consistent with those published by the others authors. E.g. for $\text{Cd}_{0.23}\text{Hg}_{0.77}\text{Te}$ crystal have been obtained $R = 0.33 \pm 0.02$, hence (for $n^2 \gg k^2$) $n = 3.7$ (cf. [17]). For the molar composition $x = 0.1$ we have $\epsilon_r = 12.5 \pm 2$ in the long wavelength range, which is consistent with the value $\epsilon_r = 12.6$ given in [18].

The results obtained allow to state that the suggested method of calculation of the absorption and refraction indices applied to the non-uniform semiconductor layer allows to evaluate the optical parameters of the separate regions of this layer. Practical aspects of these results have been widely discussed in the paper [16].

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Note added in proof

The application of transmission measurements to estimation of optical band gap profile as well as absorbed photon distribution in $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ graded-gap structures was also given by COHEN-SOLAL and MARFAING [20]. The suggestion discussed in this paper is based on experimental determining of "theoretical absorption plane" (T.A.P.) position which correspond to the coordinate t_0 of such a homogeneous plane in crystal, for which the band gap value is equal to the energy of the incident photons. The distribution of absorbed photons is then represented by the function $(t-t_0)$.

This method, however, cannot be successfully recommended for experimental investigation of such layers of semiconductor with the energy gap gradient $\partial E_g/\partial t$, in which the gradient value is relatively low. The main reason is (besides the problem of non-uniformity of the composition within T.A.P. plane) a finite spectral width of radiation beam generated by the used monochromator $\Delta(h\nu)$.

For typical layers obtained by us the gradient of E_g ranged from about 0.25 eV mm^{-1} (for molar composition with small x) to about 100 eV mm^{-1} nearer the surface reach in Cd. For $\Delta(h\nu) = 0.01 \text{ eV}$ this gives the value of T. A. P. width about $40 \mu\text{m}$ with $x \cong 0.1$. On the other hand, for negligible low $\Delta(h\nu)$ and for high gradient values of E_g the method presented in [20] can be successfully used.

Les coefficient optiques d'une couche hétérogène de semi-conducteur

On a déterminé des coefficients optiques des couches d'absorption homogènes. On a proposé une méthode de détermination du coefficient d'absorption et du coefficient complexe de réfraction pour les couches hétérogènes du semi-conducteur. On a décrit l'application des formules obtenues à l'analyse des résultats des mesures épitaxiales des couches dont la composition molaire était $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$ changeant en fonction de largeur.

Оптические коэффициенты неоднородного слоя полупроводника

Определены оптические коэффициенты однородных поглощающих слоев. Предложен метод определения коэффициента поглощения и комплексного коэффициента преломления для неоднородных слоев полупроводника. Описано применение полученных формул для анализа результатов эпитаксиальных измерений слоев с молярным составом $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$, меняющимся в зависимости от толщины.

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