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The Transmittivity of Epitaxial Cd$_x$Hg$_{1-x}$Te Layers

The epitaxial Cd$_x$Hg$_{1-x}$Te layers have been obtained by isothermic deposition of HgTe on CdTe monocrystal. Transmission measurements have been performed at 77 and 300 K within spectrum range 1–15 μm. The absorption coefficient of the layers etched deep from the surface (i. e. for different molar compositions) has been determined and the dependence of energy gap and molar composition on the layer thickness estimated. The effect of the change in the type of conductivity and temperature on the position of the absorption edge has been examined.

1. Introduction

Epitaxial Cd$_x$Hg$_{1-x}$Te layers, because of much interesting applications have been recently investigated intensively (see e.g. [1–51]). Usually they are obtained by depositing HgTe (or more rarely Cd$_x$Hg$_{1-x}$Te) from gaseous phase on CdTe monocrystal under isothermic conditions or with a small temperature gradient between the source of vapours and the substrate. The process may be also carried out in a mercury atmosphere, additionally supplied (see e.g. [3, 4]).

Some interesting results of transmission measurements performed on epitaxial Cd$_x$Hg$_{1-x}$Te layers obtained by means of the mentioned above methods are given in [1, 2], but the results presented there were given for the whole layers which had not been thinned. The authors of [2], have stated that the p-layers with mole composition on the surface $x \cong 0.2$ are much opaque for all wavelengths, while for the layers doped in mercury vapours into n-type a sharp absorption edge and a high value are obtained in transmission. According to the authors this high absorption in p-type layers is probably due to a high absorption inside them i.e. within the Cd$_x$Hg$_{1-x}$Te region, in which the molar fraction of Cd is higher than on the surface. As far as the layer of n-type is concerned, the authors express their opinion that the absorption depends to a great extent on a surface layer which is not very thick.

An attempt to determine the molar fraction from the transmission measurements was undertaken earlier by ALMASI and SMITH in [1]. The results presented in their paper were obtained from the measurements of transmission taken for two examplary layers differing in technological conditions. The first was obtained for molar fraction of the source $x = 0.25$, and the second for $x = 0.58$, the transmission threshold amounted to 0.25 eV and 0.65 eV, respectively. The authors suggest that the composition of the source used for production of the layer was also representative for the layer itself (i.e. at least for its surface), and they compare the energy gap values obtained from transmission measurements with the results of earlier investigations concerning the dependence of energy gap on molar fraction. The values of the source molar fraction assumed by the authors as representative for the surfaces of the obtained layers are disputable. In view of the above, the profile of energy gap in epitaxial Cd$_x$Hg$_{1-x}$Te layers, estimated by the authors of [1] is probably misguided.

Technology and some electric properties of the epitaxial Cd$_x$Hg$_{1-x}$Te layers produced by the authors have been described in the previous papers [6, 7]. The purpose of the present paper was to study the transmission of epitaxial Cd$_x$Hg$_{1-x}$Te layers in order to determine the absorption coefficient for the layers etched deep from the primary surface, and to determine the contribution of separate regions of the layer to the absorption of incident radiation. The next purpose of the paper was to estimate the profile of energy gap and mole fraction of our layers. The experimental work includes also investigations on the effect of changes in conductivity type of the layers (from p to n type

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obtained by heating of p-layers in mercury vapours), on the position of basic absorption edge. Finally the shift of the absorption edge due to temperature has been determined.

2. Experimental part

Epitaxial $Cd_xHg_{1-x}Te$ layers have been obtained applying the method of gas transport in closed space under isothermal conditions, by deposition of HgTe on monocrystalline CdTe substrate. As-grown layers were p-type, annealing in Hg vapour yielded n-type layers. The experiment has been described in details in papers [6, 7]. Depending upon technological conditions (temperature and duration of the process, in particular) the thickness of the obtained layers ranged from tenth μm to about 500 μm. Molar fraction x (i.e. molar content of cadmium) in the layers studied varied from pure CdTe, i.e. $x = 1$ to x approaching zero (on the layer surface). In order to study the transmission for different contents of x in a single layer, the layers were polished mechanically and then etched (deep from the primary surface) in $5^0/_0$ Br solution in ethylene alcohol.

Transmission measurements have been carried out in a cryostat with KRS-5 windows at 77 and 300 K. The scheme of measuring arrangement is shown in Fig. 1. Global with
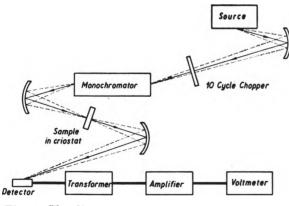

Fig. 1. The diagram of measuring arrangement

temperature about 1.600 K was used as a source of radiation. The radiation modulated mechanically with 10 Hz frequency was directed to monochromator with NaCl prisme. Signal from detector was measured with a selective nanovoltometer UNIPAN-233 with a transfor-

mer and preamplifier. The layer thickness was measured on a skew microsection ($a = 1.5°$) with help of a microscope with a micrometric eye-piece calibrated with an accuracy better than 2 μm. The reflectivity measurements have been made by the method, described in [13].

3. Results and discussion

The transmission of the layers etched deep from the primary surface, i.e. of the layers thinned started with molar fractions with small x. Transmission spectra at 300 K for the exemplary p-type 3A-61 layer are shown in Fig. 2. Technological parameters were the
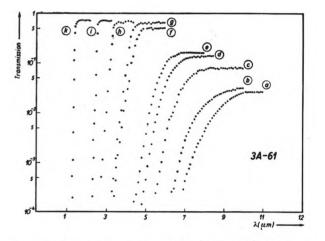

Fig. 2. Transmission spectra of the epitaxial $Cd_xHg_{1-x}Te$ layer

following: temperature of epitaxy 870 K, time of epitaxy 25 hr, total thickness 235 μm. The additional data have been presented in Table. The transmission spectra shown in Fig. 2 is typical of our layers in the sense that the observed difference between the layers concerning only the absolute value of maximum transmission were probably related to a different thickness of the layers and different concentration as well as the extent to which the crystalline structure was ordered within separate layers. As it follows from the Fig. 2 the value of maximum transmission increased with the decreasing thickness of the layer and was easily measured for all layers whose thickness did not exceed 150 μm. The measurements became more difficult when the thickness of layer ranged within about 150–250 μm and for thickness exceeding 250 μm the results were

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Data of the epitaxial p-type 3A-61 layer

Denotation of etched layer surface	Layer thickness μm	Mole fraction on surface x
a	104	0.15
b	96	0.17
c	83	0.19
d	75	0.20
e	69	0.23
f	57	0.28
g	52	0.30
h	42	0.38
i	35	0.42
j	15	0.65

charged with relatively far greater error. The spectral shift of the transmittivity maximum with etching of consecutive slices of the layer proves the effect of the surface slice on the optical transmission of the whole layer. The same observations might be made for both n and p-types of our layers.

The results obtained in the present work do not fully agree with the results of [2] for the p-type layer. It seems that the high absorption in p-type layers observed in [2] needs not be related to absorption occurring inside the layer for large x, (large E_g), but may be e.g. due to heavy non-stoichiometry and molar composition on the surface somewhat lower than determined by the electron-beam microprobe, as well as due to large electron concentration. The effect of other factors cannot be excluded, either. The lack of full data does not allow to express a decisive opinion in this matter.

Results of transmission measurements performed in the examined $Cd_xHg_{1-x}Te$ layers, similar to those shown in Fig. 2, have allowed to estimate qualitatively the contribution of separate regions of the layer in absorption of incident radiation. The result is shown in Fig. 3 as a (1-T-R) function of the layer thickness for various wavelengths. The performed measurements allowed to take into consideration the effect of reflection. It has been stated that its value slightly depended on molar composition within the investigated range of wavelengths. The obtained results were presented graphically in Fig. 4 for two molar compositions in $Cd_xHg_{1-x}Te$ and for pure CdTe. The obtained results are approximate and were used only in calculation of absorption coefficient.

Fig. 3. Intensity of absorption radiation versus $Cd_xHg_{1-x}Te$ layer thickness

The result shown in Fig. 3 (especially for $\lambda \geqslant 10$ μm) allows to state that for the p-type $Cd_xHg_{1-x}Te$ layers the radiation absorption is also conditioned by a relatively thin region of surface layer. The thickness of this region depends on the mole fraction gradient, i.e. on
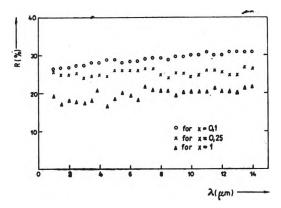

Fig. 4. Reflection spectra of the $Cd_xHg_{1-x}Te$ and CdTe

the gradient of energy gap in surface region of the layer, in which the reaction with radiation takes place (for the given wavelength). For example for molar fractions with a low content of Cd the intensity of the absorbed radiation (with wavelength corresponding to band-to-band generation) decreases two times in a surface layer about 40–60 μm thick, and for a high Cd content analogical change in

intensity occurs on a thickness of about 20–35 µm. Results presented in Fig. 3 have enabled the estimation of the thickness of the surface layer slice, taking a dominant part in absorption. The estimated values have been used to calculate the absorption coefficient.

In view of the obtained results the absorption coefficient of epitaxial layers can be calculated from the well-known relation

$$T = \frac{(1-R)^2 \exp(-at)}{1-R^2\exp(-2at)},\qquad(1)$$

where T — is transmission, R — coefficient of reflection, a — absorption coefficient and t — thickness of sample.

In case when the transmission for two consecutive slices is to be compared, we obtained [8]:

$$\frac{T_2}{T_1} = \frac{1-R_2}{1-R_1}\exp(a_2\Delta t),\qquad(2)$$

where Δt is a slice thickness.

To calculate from eq. (1) the value of t was taken from the graph, as shown in Fig. 3 plotted for each layer. The assumed value of t in eq. (1) was the effective thickness corresponding to that at which transmission dropped below $1^0/_0$. Coefficient a was also calculated from the formula (2). It has been noted that the difference in results obtained by the two methods is greater than experimental error. The problem of the optical indices for nonuniformity semiconductor and proposal of transmittivity measurements for non-homogenous semiconductor layer have been analyzed in [8] and the reasons of this error have been discussed.

The function $a(h\nu)$ calculated from the formula (1) is represented in Fig. 5 for the layer shown in Fig. 2. Analogic relations $a(h\nu)$ for other layers had the same character. In order to determine the energy gap from the dependence of absorption coefficient on energy for n-type layers, the position of Fermi level should
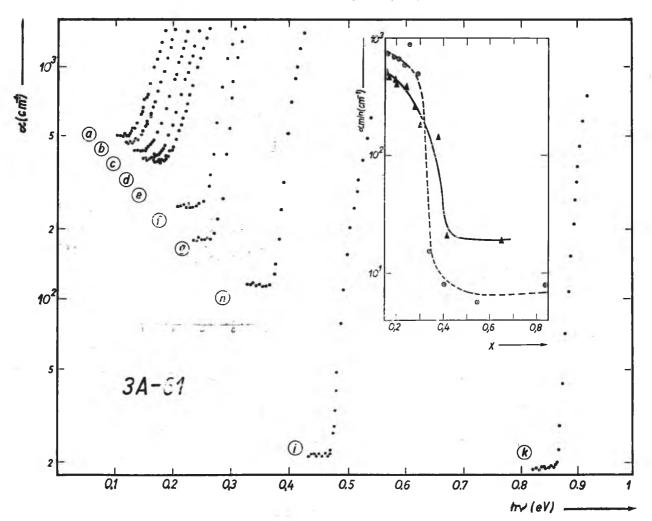

Fig. 5. Absorption coefficient of the epitaxial $Cd_xHg_{1-x}Te$ layer for different mole fractions in near-surface layer. Inset presents $a_{min}(x)$ from eq. (1) and (2), denoted by solid and dashed lines, respectively

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be estimated for a known concentration of carriers in the sample. Such an estimation has been performed in [9] for 4.2, 77 and 300 K, using a generalized Fermi integral and Sommerfeld approximation. The heavy hole effective mass not varies with the energy gap. In this case due to the high heavy hole density of states, the Burstein shift is very small.

It has been assumed that the value of energy gap is the value of the energy $(h\nu)$ corresponding to the point of the curve $\alpha(h\nu)$ at which absorption coefficient increases distinctly. Energy gap function of the layer thickness, estimated for the layer 3A-61 in a way described above, is shown in Fig. 6a.

3.1. Determination of mole fraction

Using the results of measurements shown in Fig. 6a molar composition of the layer may be estimated by means of relation given by SCOTT [10]

$$E_g(x, T) = -0.303 + 1.73x + \frac{dE_g}{dT} \times$$
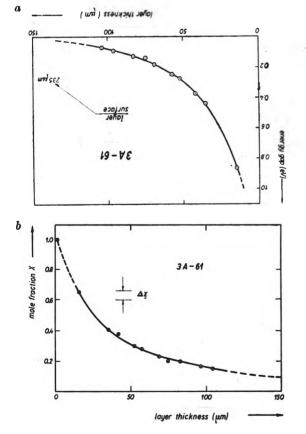$$\times T + 0.25x^4 \ldots, \quad (3)$$

Fig. 6. The energy gap (a) and mole fraction (b) versus the layer thickness

where dE_g/dT varies linearly with the composition from 5.6×10^{-4} eV/K for HgTe, to -5.6×10^{-4} eV/K for CdTe, or it may be calculated from the relation given by STANKIEWICZ and GIRIAT [11]

$$E_g(x, T) = -0.303 + 1.91x + \frac{dE_g}{dT} \times$$
$$\times (1 - 2x)T, \quad (4)$$

where $\dfrac{dE_g}{dT} = 5.25 \times 10^{-4}$ eV/K.

In the present paper molar fraction has been determined from the eq. (3). According to [11] the relation (4) holds if and only if molar fraction of Cd does not exceed $x \simeq 0.25$. Molar composition as a function of layer thickness, determined (for the layer from Fig. 6a) from the formula (3) is given in Fig. 6b. Value Δx marked in Fig. 6a (as well as in Fig. 7)
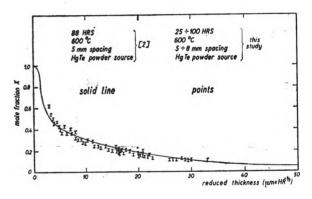

Fig. 7. The compositional profile of epitaxial Cd_xHg_{1-x} Te layers from transmittivity measurements

denotes the maximal difference in molar composition determined from the measurements at 77 and 300 K. The profile of molar fractions of layers obtained at 870 K and different times of epitaxy is shown in Fig. 7. To make the results uniform X-axis representes a reduced layer thickness i.e. the thickness divided by the square root of epitaxy duration. For comparative reasons the curve of composition obtained in [2] by electron-beam microprobe for similar technological conditions has been also shown. The profile of the composition performed in the way described above is now verified by means of reflection measurements [12], performed in the laboratory of Professor A. Kisiel (Institute of Physics, Jagiellonian University) and in our laboratory. The so far obtained results are in qualitative agreement with the results of transmission obtained by us.

It should be, however underlined, that the measurements of reflection allow to relate the molar composition of the layer to the maxima in reflection spectrum, corresponding to the transitions E_1 and $(E_1 + \Delta E_1)$ with the accuracy better than 1% [13].

The compositional profile obtained by us from the transmission measurements has been compared with the results of investigations performed in [2] by means of electron-beam microprobe. It may be easily seen from Fig. 7 that a good agreement has been obtained for the layers produced under analogic (as far as possible) technology conditions. In next part of this paper the curves in Fig. 7 will be used for mole fraction estimation of the layer based on precise measurements of the layer thickness.

3.2. The effects of changes in conductivity type and temperature on the absorption edge

An attempt has been made in the present paper to estimate the effect of heating in mercury vapours on the position of absorption edge. The heating was performed in order to obtained n-type layers (being applied in p-n junctions IR detectors). The method of heating
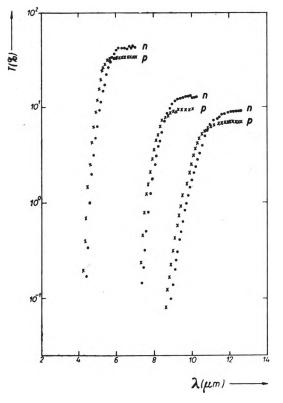

Fig. 8. The optical transmission for three epitaxial layers with various molar composition on surface depending on the change in the conductivity type

and technological conditions have been described in [14, 15]. Fig. 8 presents the absorption edges shift due to doping of epitaxial p-type $Cd_xHg_{1-x}Te$ layer. This shift was not greater than 15 meV.

It may be assumed that the molar composition at the layer surface remained unchanged (with the accuracy of experimental error).

While studying the effect of temperature on the position of absorption edge it has been observed that for the compositions (at the layer surface) $x \leqslant 0.45$ the absorption edge is shifted toward higher energy, and for $x \geqslant 0.55$ it is shifted toward lower energy, at the temperature varying from 77 to 300 K. This relationship is shown in Fig. 9 for three epitaxial $Cd_xHg_{1-x}Te$ layers. The above results is in conformity with the earlier works, in which the transmission of $Cd_xHg_{1-x}Te$ monocrystals (e.g. [10]) has been investigated. It confirms also indirectly our method of calculation of molar fraction which has been based on the relations, in which thermal coefficient of energy gap is a function of molar composition [10]. The obtained results have allowed to calculate the thermal coefficient of the change in energy gap, for the temperature changed from 77 to 300 K. The coefficient has been shown in Fig. 10 as a function of molar composition. The maximal error of the mole fraction estimation is also denoted. Despite a certain dispersion of the results this function remains in qualitative conformity with the results presented in [10].

4. Conclusions

Transmission of epitaxial $Cd_xHg_{1-x}Te$ layers etched inside from the primary surface (i.e. for different molar compositions) has been investigated. It has been stated, that:

1° The radiation incident on the layer is mostly absorbed by surface region its thickness however must be such a one that the value of its molar composition (and hence of energy gap) on both its edges be significantly different. This is true for $Cd_xHg_{1-x}Te$ layers of both n and p-types.

2° The results of transmission measurements allow to estimate the compositional profile of epitaxial $Cd_xHg_{1-x}Te$ layer, although the accuracy of this method may be relatively worse than that given by the measurements of reflectivity.

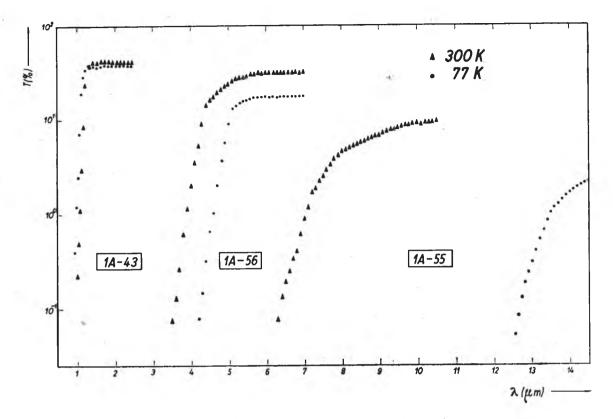3° The profile of molar composition of the layers determined in the present paper is in

Fig. 9. The effect of temperature on optical transmission for different mole fraction on surface of the three layers
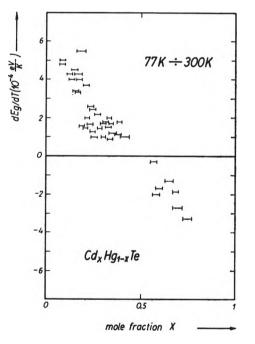

Fig. 10. The dE_g/dT coefficient for $Cd_xHg_{1-x}Te$ obtained from transmittivity measurement in epitaxial layers

a way described in [14, 15] changes the type of conductivity into n, not visibly changing, however, the molar composition at the layer surface.

5° Thermal coefficient of energy gap depends on the molar composition and changes the sign for $0.45 < x < 0.55$. Because of insufficient data linear change dE_g/dT with the change of molar fraction suggested in [10] can be neither confirmed nor denied. Further measurements of transmission and of photoelectric effect will provide us with additional data.

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a good conformity with the results of measurements performed by means of electron-beam microprobe [2].

4° Heating of p-layers in mercury vapours in order to improve the stechiometry and to change the type of conductivity, performed in

Светопроницаемость эпитаксиальных слоев $Cd_xHg_{1-x}Te$

Эпитаксиальные слои $Cd_xHg_{1-x}Te$ получены изотермическим осаждением HgTe на монокристалл CdTe. Измерения прозрачности производились при температурах 77

и 300 К, в области спектра 1–15 μм. Определен коэффициент поглощения слоев, травимых вглубь (то есть для разных молярных составов), и дана оценка зависимости ширины энергетической щели и молярного состава от толщины слоя. Исследовано влияние изменения типа проводности и температуры на расположение края поглощения.

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