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Absorption Coefficient of the Zn_3As_2 Thin Films

The results of calculation of the absorption coefficient of semiconductor compound Zn_3As_2 thin films obtained with the aid of the vacuum evaporation technique, have been presented. Results of measurements of these layers, when covered with a protective coating of SiO_x and treated thermally, are also given.

1. Introduction

The spectrum relationships of the absorption and reflection coefficients as well as the optical measurements leading to their determinations play an important part in investigation of the basis properties of the semiconductors and, in particular of their band structures. Some interesting data on the subject are available in paper [1].

The band structure of Zn_3As_2 was theoretically calculated in paper [2]. The width of the energy gap — the minimum distance between the valence band and the conductance band — determined in [2] appeared to be equal to 0.9 eV. The energy gap for the solid Zn_3As_2 determined from the optical measurements at $T = 300$ K amounts to $\Delta E = 1.1$ eV due to [3] and to $\Delta E = 0.93$ eV due to [4]. From the electrical measurements ΔE was evaluated as equal to $\Delta E = (0.86-5.5\cdot10^{-4}\cdot T)$ eV [5] and $\Delta E = 1.1$ eV [3]. The energy gap for the thin Zn_2As_3 films obtained from the optical measurements performed at the temperature $T = 300$ K is equal to $\Delta E = 0.95 + + 0.05$ eV [6], while that estimated from the electrical measurements amounts to $\Delta E = 1.00 \pm 0.05$ eV [7].

In the present paper an attempt has been made to analyse the shape of the curve representing the dependence of the absorption coefficient on the radiation energy for the Zn_3As_2 thin films deposited on the substrate at room temperature as well as on the substrates heated up to the temperature 190–270 °C. The same will be done for the layers heated under the protective coating of SiO_x.

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2. The Experimental Part

Thin Zn_3As_2 layers were deposited in a vacuum unit under the pressure of the order of 10^{-5} Tr on the substrate of BK-7 glass and NaCl respectively. The thickness of the examined layers determined with the help of a weighing method as well as the interference method ranged between 0.6 and 3.2 μm. The measurements of transmittance of the layers evaporated on the glass substrate have been performed with the help of the SP-700 UNICAM spectrometer within the wavelength range 0.4–2.5 μm. The measurements for the films deposited on the NaCl substrate were made with the UR–10 spectrophotometer within the wavelength interval 2–20 μm.

The absorption coefficient α for the Zn_3As_2 layers was calculated on the ODRA 1003 computer. For the case of high absorption coefficients and lack of interference effect the computer was programmed according to the formula (1), while for the case in which the interference appears, the absorption coefficient was evaluated from formula (2) (see [8]).

$$\alpha = \frac{1}{d}\ln\frac{A+\sqrt{A^2-4T^2r_1^2r_2^2}}{2T}, \tag{1}$$

where

$$r_1 = \frac{n_0-n_1}{n_0+n_1}, \quad r_2 = \frac{n_1-n_2}{n_1+n_2},$$

$$A = \frac{16n_1^2n_2}{(n_0+n_1)^2\cdot(n_1+n_2)^2}.$$

$$\alpha = \frac{1}{d}\ln\frac{(A+2r_1r_2)+\sqrt{(A+2r_1r_2)^2-4T^2r_1^2r_2^2}}{2T}. \tag{2}$$

The input data for the computer contained the following quantities given for the discrete values of λ:

- T — transmittance for the system with a $Zn_3\,As_2$ layer,
- n_0 — refractive index for the air or the SiO_x layer respectively,
- n_1 — refractive index for the examined semiconductor layer,
- n_2 — refractive index of the substrate (glass or NaCl).

The value of the refractive index for the air was assumed to be equal to $n_0 = 1.0003$ within the whole measurements range. The values for the index of refraction n_2 were read out from the dispersion curves for BK-7 glass (comp. [9]) and for NaCl (comp. [10]).

In Fig. 1 the transmittance spectrum is presented typical for the Zn_3As_2 films deposited on the glass substrate and heated up to the temperature 500 K. The changes in transmittance typical for the same layers also deposited on glass and heated up to the temperature 500 K but under the protective SiO_x coating of tens nm thickness are shown in Fig. 2.

3. Discussion of Results

The results obtained from the calculations of the absorption coefficient are presented in Fig. 3–5. Fig. 3 contains the results for the Zn_3As_2 films evaporated

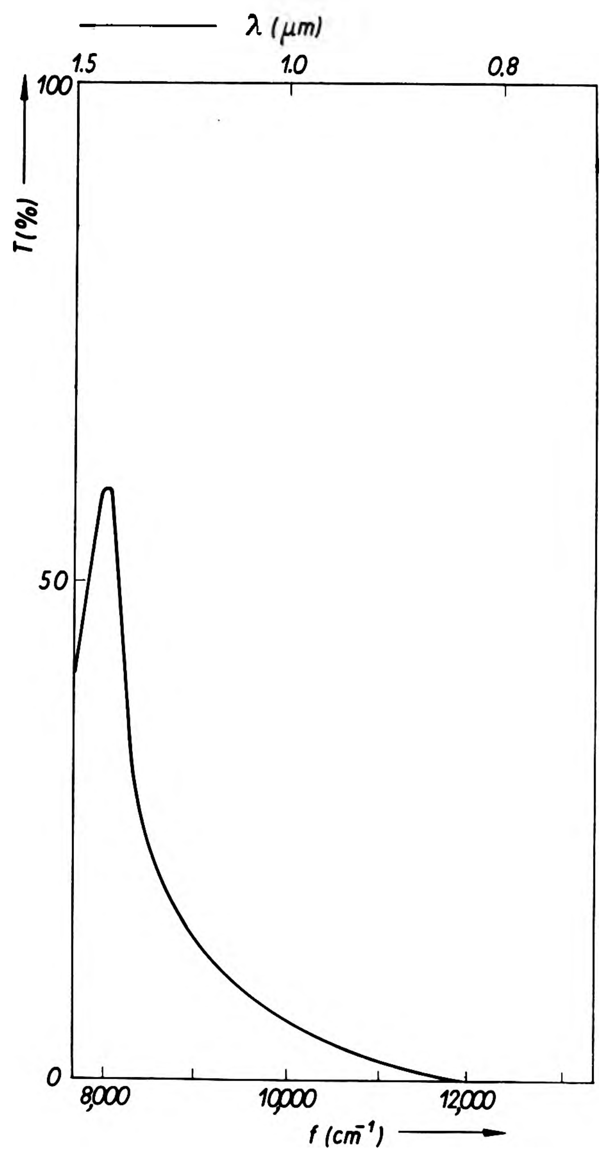

Fig. 1. Dependence of the transmittance T on the wavelength λ and the wave number f for the Zn_3As_2 film deposited on the heated substrate

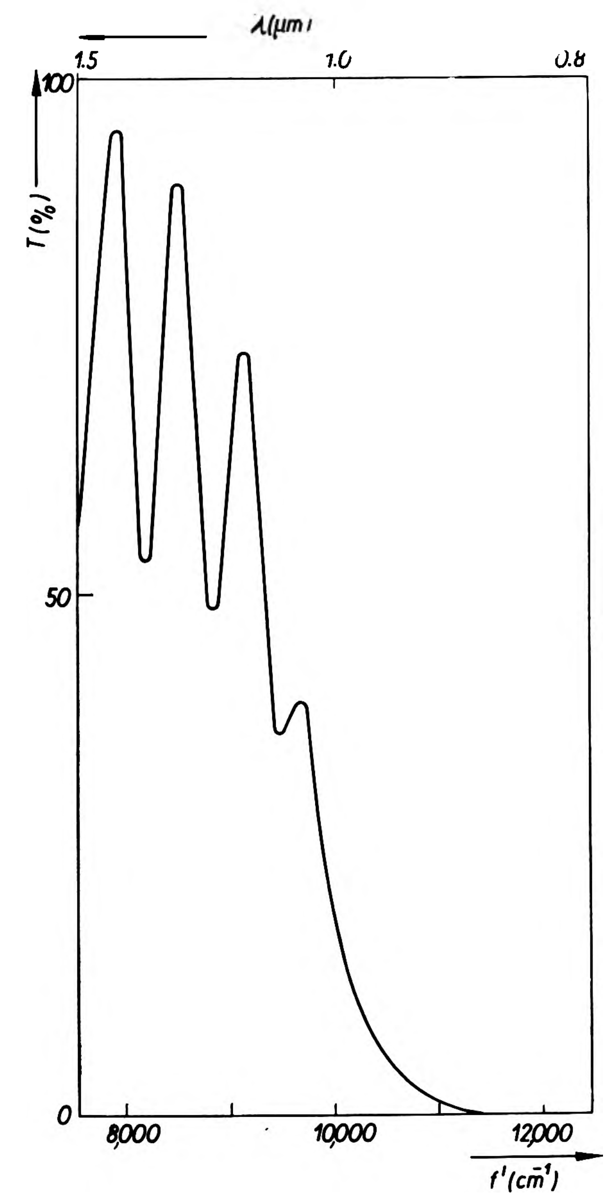

Fig. 2. Dependence of the transmittance T on the wavelength λ and the wave number f for the Zn_3As_2 films heated under the protective coating of SiO_x

on the substrate at room temperature, while Fig. 4 shows the results for the Zn_3As_2 films deposited on the substrate at temperature between 190 °C and 270 °C. In Fig. 5 the results for the Zn_3As_2 films heated under the protective SiO_x coating are presented.

The absorption coefficient α for the allowed direct transitions with the photon only and without change of the electron wave vector $\vec{k}_{min} = \vec{k}_{max}$ may be described with help of an equation

$$\alpha = B\cdot(h\nu - \Delta E)^{1/2} \tag{3}$$

for $h\nu > \Delta E$ where ΔE is the smallest permissible activation energy of the carriers. The constant B may be expressed as

$$B = \frac{\pi\cdot e^2(2m_r)^{3/2}}{\varepsilon_0\cdot c\cdot m\cdot h^2\cdot n}\cdot f_{ij}, \tag{4}$$

where e, ε_0, c, m, h are constant and denote an electron charge, dielectric constant in vacuo, light velocity in vacuo, rest mass of electron and Planck constant, respectively, n denotes the real part of the complex refractive index, $\hat{n} = n+ik$, while f_{ij} is a factor of

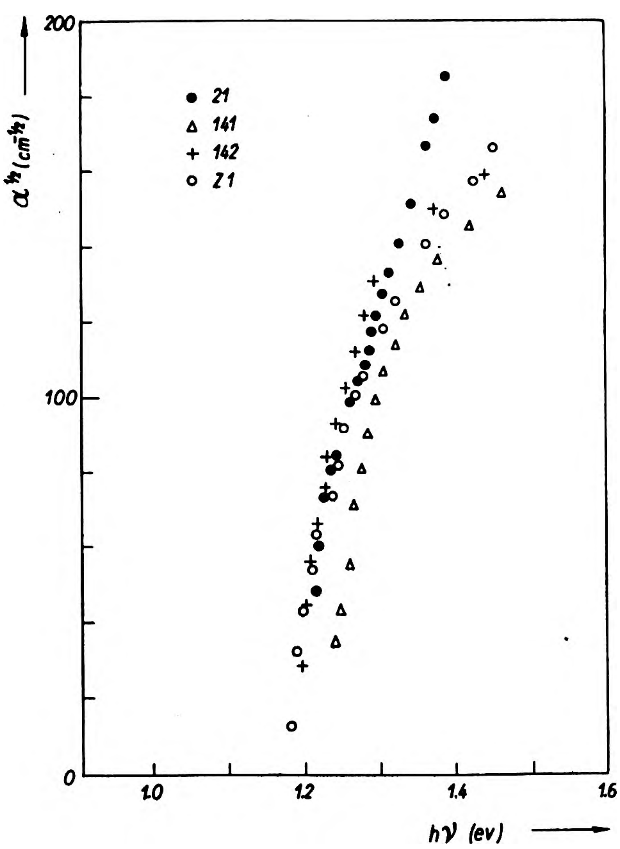

Fig. 3. Dependence of the absorption coefficient α on the radiation energy $h\nu$ for the Zn_3As_2 films evaporated on the substrate at temperature $t_p = 20$ °C

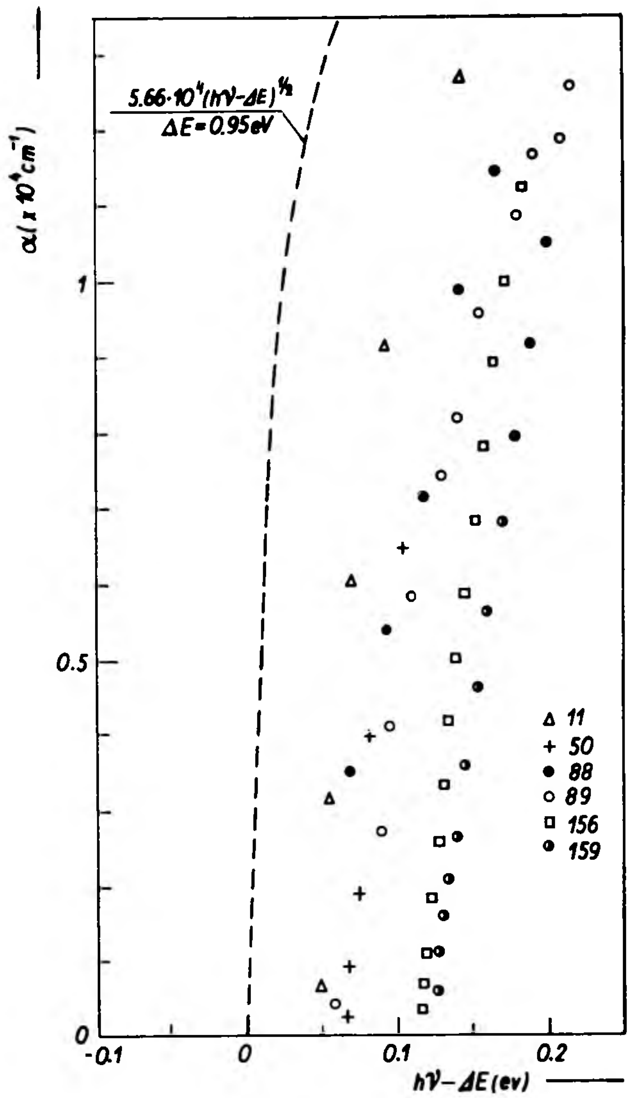

Fig. 4. Dependence of the absorption coefficient α on the radiation energy $h\nu$ for the Zn_3As_2 films evaporated on the substrate at temperature $t_p = 190$–270 °C

value approximately equal to unity, m_r is the reduced mass (which takes account of the change of $E(\vec{k})$ in the conduction band) given by equation (5)

$$\frac{1}{m_r} = \frac{1}{m_e} + \frac{1}{m_h}, \tag{5}$$

where m_e and m_h denote electron and hole mass respectively. If we assume for Zn_3As_2 the values

$$m_e = 1.6\text{m} \quad \text{and} \quad m_h = 0.66\text{m},$$

and if the average value of the refractive index in the vicinity of the absorption edge [6] will be assued to be equal to $n = 4.2$ then we obtain a dependence

$$\alpha = 5.66\cdot 10^4(h\nu - \Delta E)^{1/2}\,[\text{cm}^{-1}]. \tag{6}$$

This relationship has been presented in Fig. 4 for $\Delta E = 0.95$ eV.

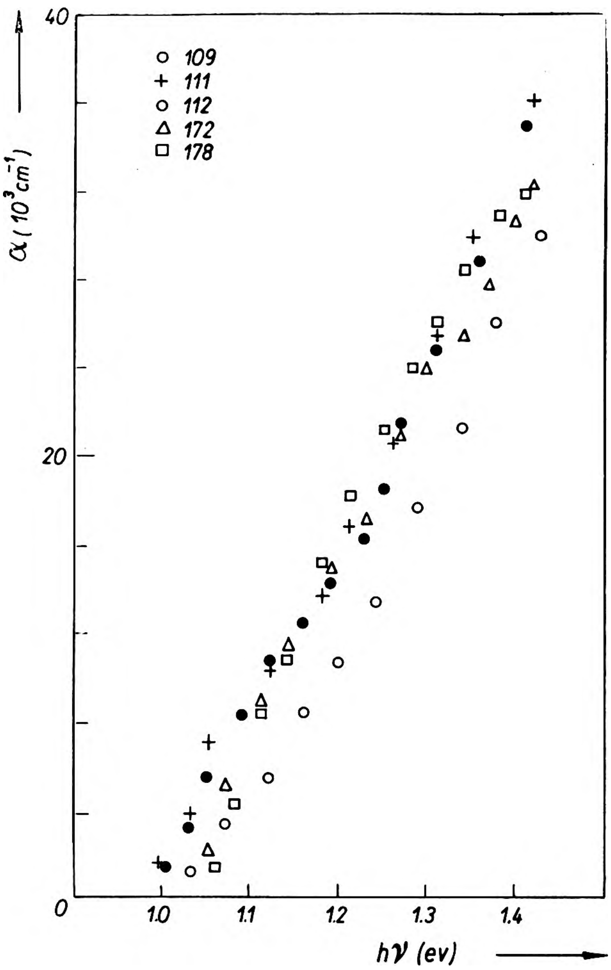

Fig. 5. Dependence of the absorption coefficient $\alpha(h\nu)$ for the Zn_3As_2 films heated under the protective coating of SiO_x

Equations (4) and (6) are valid only for a limited range of values $h\nu - \Delta E$. For small values of $h\nu$ and in particular for $h\nu \to \Delta E$ the basic absorption does not tend to zero but is transformed into absorption connected with the higher excited states of excitons and the absorption on the free carriers.

The error in determining the coefficient α is the smallest in the spectrum range, which fullfilms the condition

$$0.5 < (\alpha \cdot d) < 3$$

(see [11]).

The product $(\alpha \cdot d)$ is being changed in the vicinity of the absorption edge by at least one order and consequently the error appearing by determining α may exceed 10 percent.

To obtain the real course of $\alpha(h\nu)$ the measurements of absorption in the layer of thickness of order μm up to cm should be performed and these points selected, for which $\alpha \cdot d = 1$.

Because of technology applied to producing the Zn_3As_2 films the exact fulfilment of the said requirements was impossible. From the above considerations it may be concluted that the error of estimation of α was equal to about 12%, while that for the small absorption coefficients (of the order of 10^2 cm^{-1}) increased to about 25%.

When plotting the relationships $\alpha^2(h\nu)$ and $\alpha^{1/2}(h\nu)$ we expect to obtain straight lines for the direct and indirect transitions. The Zn_3As_2 layers deposited on the substrate of 20 °C temperature exhibit the dependence of the absorption coefficient on the energy close to that given by the formula $\alpha^{1/2}(h \cdot \nu)$ characteristic to the indirect transitions (Fig. 3), whereas the layers deposited on the substrates heated up to the temperature from the range 190–270 °C show the dependence of the type $\alpha^2(h \cdot \nu)$, which is characteristic for the direct transitions (Fig. 4). From the course of the curves $\alpha(h \cdot \nu)$ the width ΔE_0 of the energy gap for the thin layers of Zn_3As_2 has been determined. The corresponding data are presented in table I.

Table I

Energetic gap width ΔE_0 in the thin Zn_3As_2 films as determined experimentally

Films deposited on substrates at temperature $t_p = 20$ °C		$t_p = 190-270$ °C		
Film number	ΔE_0 300 K [eV]	Film number	t_p [°C]	ΔE_0 300 K [eV]
21	1.19	11	270	1.00
141	1.21	50	250	1.02
142	1.17	88	190	1.01
Z-1	1.18	89	190	1.04
		156	220	1.07
		159	220	1.08

In table II the values ΔE_0 are shown, being estimated from the graph of the absorption coefficient ver-

Table II

Values of ΔE_0 for the layers protected by a SiO_x coating and heated. The values have been obtained from absorption measurements

Film number	Coating thickness SiO_x [nm]	ΔE_0 300 K [eV]
109	40	0.98
111	40	0.98
112	40	1.01
172	50	1.03
178	50	1.05

sus the energy $h\nu$ (Fig. 5) for the Zn_3As_2 films protected by a SiO_x coating and submitted to the thermal treatment.

On the base of the analysis of the graphs $\alpha(h\cdot\nu)$ it may be assumed that the transitions of the optically activated carriers are most probably of transition type for the thin layers deposited on the heated substrate or treated thermally, which by the same means are of policrystalic (but ordered to some extent structure). The energy necessary for these transitions is from the range 1.00 to 1.1 eV.

The authors realize that the results mentioned above are only of preliminary value ant that the study of the structure of the Zn_3As_2 films should be continued. They hope to receive some further informations after having elaborated the measurement results obtained for the reflection from the thin Zn_3As_2 layer. It should be emphasized that though the optical investigations of the semiconductor in the form of thin deposited layers has some priorities the interpretation of the experimental results is difficult because of the (usually) policrystalic structure of the layers.

The authors express their gratitude to Doc. Dr. W. Żdanowicz for suggesting the topic of these investigations.

Etude du coéfficient d'absorption des couches minces de Zn_2As_3

On a présenté dans ce travail les résultats du calcul du coefficient d'absorption des couches minces du composé semiconducteur Zn_2As_3, obtenues par la méthode de vaporisation sous vide. On a également donné les résultats des mesures sur les couches dont la surface est protégée par un revêtement de SiO_x et qui sont soumises à un traitement thermique.

Коэффициент абсорбции тонких пленок арсенида цинка Zn_3As_2

В работе представлены результаты расчета коэффициента абсорбции тонких пленок полупроводникового соединения Zn_3As_2, полученных методом вакуумного настаивания. Приводятся также результаты измерений пленок, поверхностно защищенных покрытием из SiO_x и подвергнутых термообработке.

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