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Determination of parameters of cadmium telluride films on silicon by the methods of main angle and multiangular ellipsometry

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Abstract. The multiangular ellipsometric measurements were conducted at two wavelengths 435 and 579 nm on the system that contains cadmium telluride film deposited onto the monocrystalline silicon substrate. The refraction index and the film thickness as well as their distribution over the sample area were determined. It has been shown that the refraction index of the film (2.15…2.35) is less than that of the monocrystalline cadmium telluride (~3) that can testify the porous structure of the film or about roughness of the film surface. Obtained dependences of values of the film optical parameters from the angle of incidence testify weak heterogeneity of film properties along its depth. It was detected that there are the false solutions of the ellipsometric equation for each angle of incidence.

Keywords: multiangular ellipsometry, cadmium telluride films, film thickness.

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1. Introduction

The control of dispersion of the plane-epitaxial structure parameters, coverings, and the state of plate's surfaces and structures obtains the special significance in microelectronics. In this case, useful information can be obtained using ellipsometry due to the high sensitivity of polarization characteristics of reflected light to the condition of surface and its structure in the region of light reflection. Structures based on cadmium telluride get wide applications in the semiconductor electronics. Thus, an actual task is to obtain high-quality films that would have sufficiently good structures, homogeneity of film surface and other characteristics that are important for the practical use.

The aim of this paper was to determine optical parameters and homogeneity over the whole area of the cadmium telluride film obtained on the surface of monocrystalline silicon by using the method that is widely used in epitaxial technology.

2. Experimental details

In this paper, multiangular ellipsometric measurements were performed at various wavelengths using the photometric ellipsometric method [1], where the ellipsometric parameters $\cos\Delta$ and $\mathrm{tg}\psi$ were calculated by measuring the reflected light intensities in different polarizations of the incident light. The cadmium telluride film obtained on the monocrystalline silicon by the "hot-wall" epitaxial method was the investigated object.

Under the deposition conditions, the film thickness varied over the sample area increasing from the periphery to the centre, which was clearly seen due to thin-film interferential colors. Ellipsometric measurements were performed at the light sounding beam reflecting from six areas with different but unknown thicknesses at two wavelengths 579 and 435 nm. The choice of these wavelengths had not a principle meaning, for more certain thickness determination they must differ appreciably.

In Fig. 1, the typical form of angular dependences for the ellipsometric parameters is depicted as an example. The similar curves were obtained for the rest parts and wavelengths. It is obvious that curves have a monotonous form without extrema that are typical for the interference in a thick layer. It means that the thickness of the investigated film was not so large; its value lies within the first periods of ellipsometric parameter changes with thickness.

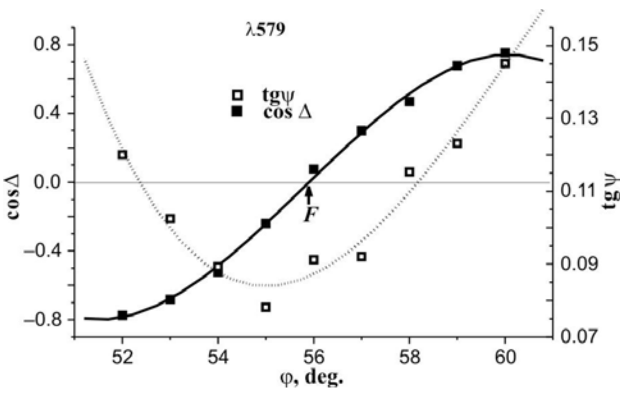

Fig. 1. Dependences of measured ellipsometric parameters cosΔ and tgψ from the angle of incidence φ on one of the central areas on the sample.

We used two following approaches for ellipsometric data interpretation and for determination of the reflective system parameters: the method of fixed incident angle and method of multiangular measurements.

As the ellipsometric equation is non-linear and transcendental relatively to optical constants, so the special calculation procedure based on the iteration methods were used to determine the optical constants [2, 3].

3. Film parameters determination

The well-known ellipsometric function is usually written as follows:

$$\mathrm{tg}\psi e^{i\Delta} = \frac{R_p}{R_s},$$

that is the dependence of the phase difference Δ between *p*- and *s*-components of the electric vector of the light wave and the relation of reflective indexes tgψ in *p*- and *s*-plane of the sample, from the angle of incidence; it carries the full information about the reflective system structure. By measuring this function in a rather wide range of angles, we can calculate the parameters of the system such as optical constants of the environment, layer thicknesses, geometry of interfaces, *etc*.

If the investigated system contains a layer on the semi-infinite medium (as in our case), we have to determine the refraction index n_2 and the absorption index κ_2 of the layer, layer thickness d_2, and optical constants n_3 and κ_3 of the substrate. Even in this rather simple case, for one-valued calculation of parameters measurements must be conducted in a wide range of incident light angles.

There is another method of determination of parameters for this one-layer system: to perform ellipsometric measurements on the sample with a variable thickness of the layer. In this case, measurements could be carried out on different areas of the same sample that has a layer with the variable thickness or on the system of samples with the different thickness. The obtained distribution of experimental points, couple of values of Δ and ψ (or cosΔ and tgψ), each of which corresponds to its own (unknown) thickness, on the diagram of measurement values could be described by the curve of constant values of optical constants of matter from which the layer consists of. If such description is obtained, positions of experimental points on the calculated curve gives us the layer thickness in the sounding area and calculation parameters of ellipsometric curve give us optical constants of this matter. Such approach well operates, if optical constants of the matter layer are equal in areas with different thickness.

Application of these methods to the calculation of film parameters would be described further.

3.1. Method of the fixed angle of incidence

In this method, experimental points obtained at light refraction under the fixed angle of incidence for various areas of the investigated structure were placed on the rectangular diagram of measured values. The angle of incidence could be arbitrary but it would be better to use the experimental data obtained at the main angle Φ (*i.e.*, the angle of incidence when $\cos\Delta = 0$), where the sensitivity of ellipsometric parameters to the system parameters reaches the greatest value.

The main angle as well as values of tgψ at the main angle (ellipticity) were found from the measured dependences of ellipsometric parameters from the angle of incidence (similar to that presented in Fig. 1) using the standard software graphical program ORIGIN.

The distribution of experimental points on the diagram "main angle Φ – ellipticity tgψ" is shown in Fig. 2 for two used wavelengths. It is seen that points are distributed regularly forming certain curves.

It could be assumed that each curve corresponds to permanent values of the film optical constants and to its variable thickness that increase along the curve from some point that corresponds to optical constants of the substrate, *i.e.*, zero thickness of the film.

Optical constants of the substrate (monocrystalline silicon) are known [4, 5], and the task was to find such values of the film optical parameters n_2 and κ_2 that are calculated using this curve when it passes through the experimental points.

This task was solved using the special graphic program that visualized the distribution of experimental data on the monitor screen and the result of calculation of ellipsometric parameters in the form of rectangular diagram Φ–tgψ. At first, the program deposit on the diagram the experimental points, and then, after operator's choosing the optical constants n_2 and κ_2 of the film, it calculates the values of Φ and tgψ for various film thicknesses beginning from zero up to the certain maximum value defined by the operator. When the obtained curve is deposited on the same diagram and on the monitor screen, we can see how the theoretical curve changes with the film optical constant modification. As a result, the couple of values n_2 and κ_2 at which the calculated curve passes through the experimental points is found. The procedure of optical parameters selection is consciously to certain extent because often the area of expected values is known, besides the model calculations have established that the refraction index influences on the inclination of the curve near its origin, and the index of absorption influences on its curvature. In general, determination of theoretical curve parameters by the presented method takes several minutes.

All calculations were performed using the program package [2, 3] that contains the Newton iteration method of solving the main ellipsometric equation relatively to two unknowns and the determination method to solve the equation (to determine the main angle).

Values of optical parameters of substrate (monocrystalline silicon) that are known in the literature [4, 5] were used in our calculation: λ579 – $n_3 = 4.04$, $\kappa_3 = 0.03$; λ435 – $n_3 = 4.86$, $\kappa_3 = 0.185$.

Adjustment of the theoretical results to the experimental data are presented in Fig. 2 as corresponding curves, and the numerical values of optical constants and film thicknesses obtained by the method that was described earlier are presented in Table. Film thicknesses in various areas of the sample were found by the position of corresponding experimental points relatively to the nearest mark on the theoretical curve (its value is given by the cursor).

It is seen from Fig. 2 that the theoretical curves rather well describe experimental results passing through the biggest number of the experimental points, however, points that lie in the peripherical areas (where as it's seen from the interference color the film thickness is the smallest) don't get to the theoretical curve but find their place in that area of diagram where presents considerably smaller refraction index than that for the theoretical curve (see Table). That's why, the film parameters for these areas were determined by the multiangular ellipsometric method (see p. 3.2).

Table. Refraction index n_2, index of absorption κ_2 and thickness d_2 of the film in different areas of the sample.

Number of the area	λ579			λ435		
	n_2	κ_2	d_2, nm	n_2	κ_2	d_2, nm
1	2.03	0.335	43	2.28	0.287	42
2	2.163	0.361	61	2.356	0.333	61.5
3	2.159	0.353	64.7	2.342	0.354	66
4	2.158	0.366	80	2.381	0.330	79
5	2.158	0.366	80	2.376	0.328	79.5
6	2.156	0.350	82	2.343	0.332	81
Mean values of optical constants	2.159	0.359		2.360	0.335	

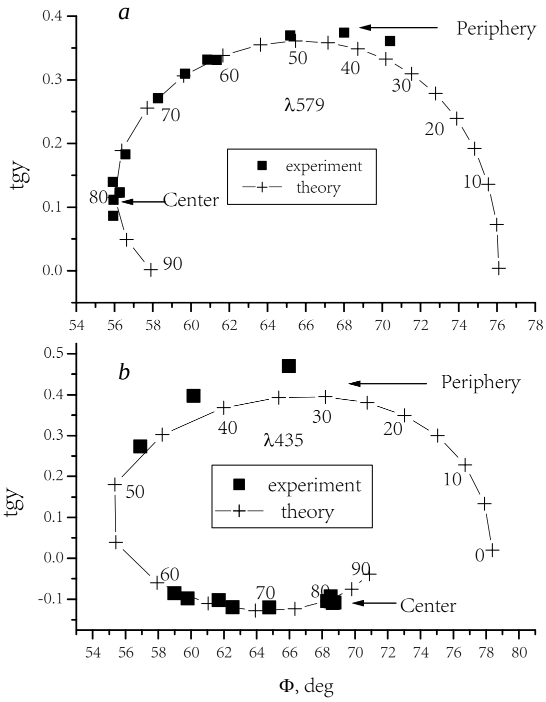

Fig. 2. Values of the main angle Φ and ellipticity tgψ measured for different areas of the sample in comparison with the calculated ones. The theoretical curve was calculated using the parameters presented in Table, marks on the curve indicate the film thickness in nanometers.

Point out the fact that the obtained values of the refraction index are considerably smaller than the refraction index of monocrystalline cadmium telluride (~ 3 in the given spectral range).

3.2. The multiangular ellipsometric method

During calculation of multiangular measurements under measured on each incident light angle two ellipsometric parameters cosΔ and tgψ, we can determine two unknown parameters of a reflective system. In our case, we have to determine three unknowns: the refraction index and index of absorption of the film as well as its thickness. That's why, the certain calculation procedure was used. Treating the multiangular ellipsometric measurements could give the additional to the mono-angular information about the investigated system, in particular, about film homogeneity along the thickness.

The refraction index n_2 and index of absorption κ_2 of the film were calculated for each angle of incidence by using the thickness value d_2 representation in the limits of expected due to the automated program [2] that was changed a little with the purpose that iteration would be taking place only when searching the optical constants of the absorptive film. If the represented thickness differs from the true than obtained values of optical parameters of the film would be changed with the angle of incidence. Conversely values would be unchangeable (in the range of certain statistic dispersion) independent from the angle of incidence only in that case when the model of the investigated system coincides with that accepted at data calculation and accepted thickness value coincide with the true one.

In Fig. 3, presented are the curves for the wavelength 579 nm that illustrates this method on the example of peripherical and central areas of investigated sample. Calculation of optical parameters of the film was carried out for several thickness values both larger and smaller than the value that was obtained in the previous method of the main angle (see Table).

The wide dispersion of optical constant values of the film in the peripherical area of the sample attracts attention (Fig. 3a). This fact is not strange because the

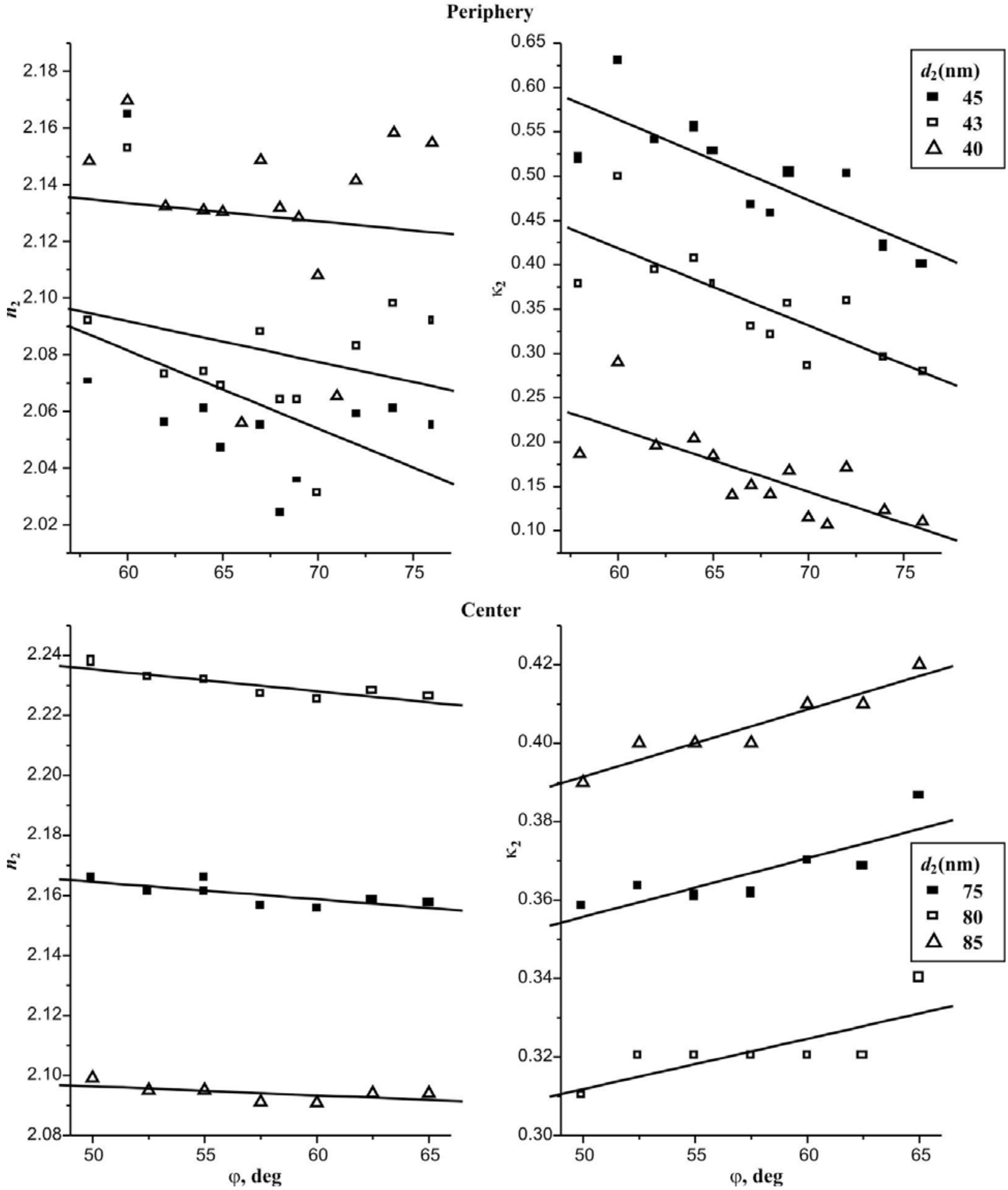

Fig. 3. Values of the refraction index n_2 and index of absorption κ_2 (λ = 579 nm) at the periphery and in the central areas of the film calculated from the ellipsometric data for different angles of incidence φ when choosing the different thicknesses d_2 (nm).

thickness in this area is the smallest as it can be seen from Fig. 2. In this case, experimental points find their place in that area of diagram of measured values where curves of invariable values of optical constants lie near to each other, that is why even small errors in measurements of ellipsometric parameters results in essentially larger mistakes, when determining the film optical parameters.

The linear interpolation of the data, which was carried out by mathematical means of the graphic editor, shows that in the peripherical area of the sample (Fig. 3a) both values of the refraction index n_2 and index of absorption κ_2 of the film decrease in the interval of incident light angles ~9°. Besides, the decrease in the refraction index reaches $\Delta n_2 = -(0.01\ldots0.06)$, while that of absorption index is $\Delta\kappa_2 = -0.15$, which is sufficiently greater than the statistic dispersion of corresponding values with respect to the interpolation curves.

Using the wavelength 435 nm, we obtained similar results: calculated values of the refraction index increase approximately by 0.05, and values of absorption index stay practically unchanged within the limits of the statistic dispersion ±0.03.

We may note that choosing the film thickness cannot eliminate the angular dependence of the calculated values of the film optical constants in its peripherical area, they stay approximately similar at the thickness variation within the range of ±5 nm and even wider.

The angular dependence of optical constants for the central area of the sample is considerably smaller (Fig. 3b). According to the main angle data, the film thickness in this area is close to 80 nm (see Fig. 2 and Table); multiangular measurements show that some angular dependence of calculated values of optical constants that couldn't be removed by thickness variation within the range of ±5 nm is observed, but this dependence is much smaller than that for the peripherical area.

The obtained data testify that the film parameter values that would stay invariable in a wide area of incident light angles were not found for this object.

Similar results were also obtained on other (intermediate) areas of the investigated structure. In some cases, the thickness variation within the range of values that are presented in Table can straighten angular dependences, for instance for the refraction index, but at that same time the angular dependence of the absorption index remains unchanged.

4. Discussion of results

The main peculiarity of the obtained results is that the values of the refraction and absorption indexes of the film depend on the experimental conditions such as the angle of sounding light incidence on the investigated structure. The following questions appear: defects of the applied procedure to determine film parameters can serve as the cause of this residual angular dependence; it is also possible that the angular dependence is the consequence of an incorrect choice of the model for experimental data calculation.

With the aim to check up these assumptions, the model calculations were carried out; its aim was to define what angular dependence of optical constants appears as a result of the incorrect choice of the film thickness when calculating the optical constants by using the method described earlier.

4.1. The model calculations

Using given parameters of the reflective system that are close to those that are observed in our measurements ellipsometric parameters $\cos\Delta$ and $\mathrm{tg}\psi$ were calculated in the same range of incident light angles as in the experiment. Then, using the calculated values of ellipsometric parameters, n_2 and κ_2 were obtained using the thickness value changing by ±5 nm relatively to the true value close to the experimental data.

Results of model calculations for the homogeneous film with the thickness $d_2 = 40$ (a) and 80 nm (b) and optical constants close to optical parameters of the investigated film on its peripherical and central areas are presented in Fig. 4.

It is seen that the choice of wrong thickness values that differ from the true value results in the angular dependences of optical constants. Thus, the thickness underestimation leads to the decreased refraction index (curves for 38 nm) and its overestimation results in the increased refraction index with increasing the angle of incidence (curves for 45 nm). Only in that case when we calculate n_2 and κ_2 for the true thickness value $d_2 = 40$ nm, the obtained values of optical constants wouldn't depend on the incident light angle (except the case when other wrong solution for optical parameters exists; look at the p. 4.2).

Analogues results were obtained for the film thickness 80 nm with optical constants close to optical parameters of the central area of the investigated object (Fig. 4b).

This situation is similar to the previous case of the thin film: when reducing the thickness relatively to its true value by 5 nm (down to 75 nm) the calculated refraction index decreases, and with growing the thickness by the same value up to 85 nm the refraction index decreases with increasing the incident light angle and stays invariable only in that case when we chose the true thickness value (80 nm) to calculate n_2 and κ_2.

Situation with the angular dependence of the absorption index κ_2 is somewhat ambiguous, it could be practically constant and independent from the incident light angle (Fig. 4a) or it could have the same inclination by the value and this fact to some extent depends on the choice of the thickness (λ = 435 nm).

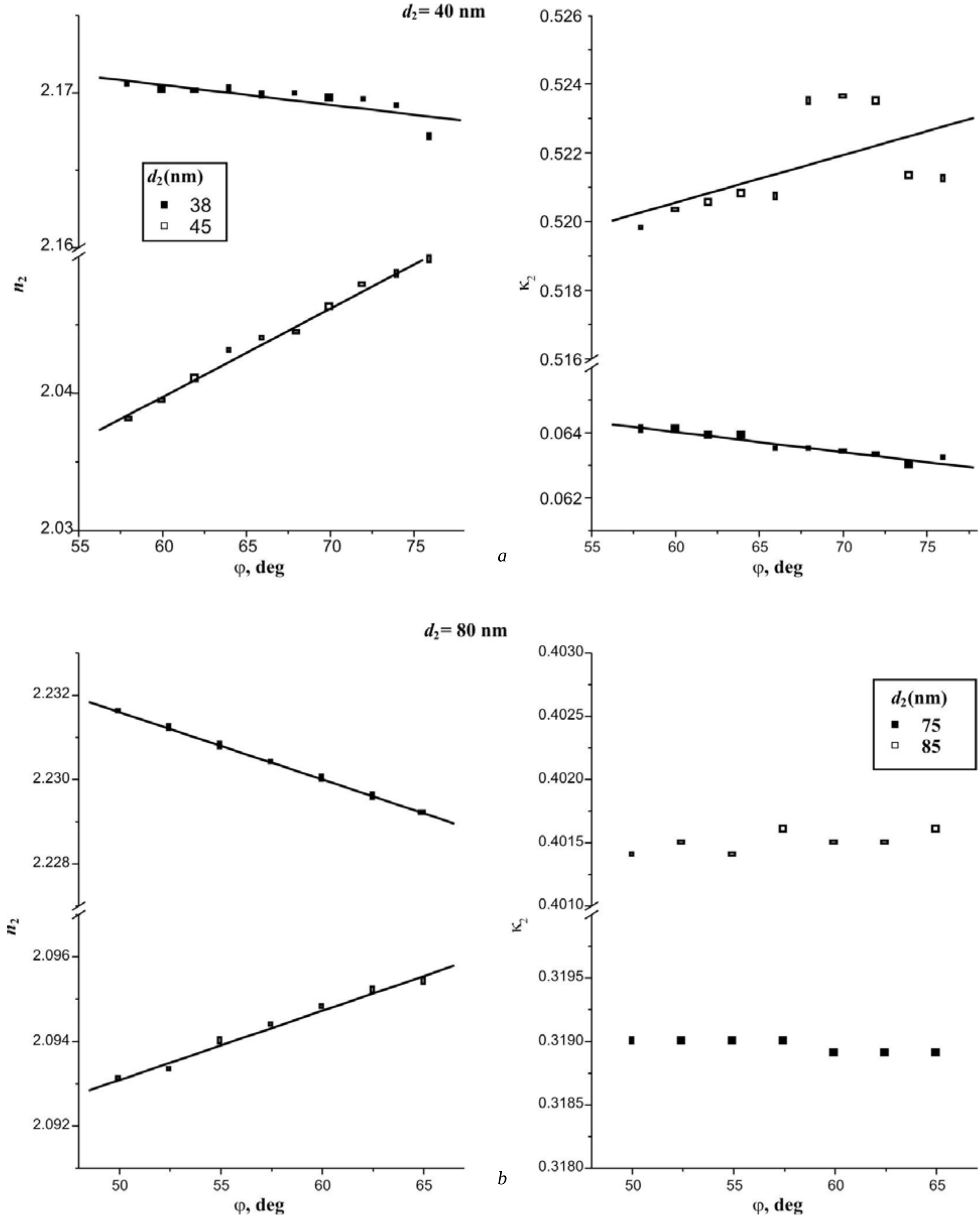

Fig. 4. Refraction index n_2 and index of absorption κ_2 (λ = 579 nm) calculated for different angles of incidence φ when choosing different values of the film thickness both larger and smaller than the true one. True values of hypotetic film parameters: $n_2 = 2.13$, $\kappa_2 = 0.18$, $d_2 = 40$ nm (a); $n_2 = 2.16$, $\kappa_2 = 0.365$, $d_2 = 80$ nm (b).

In the case of model experiment, we have to pay attention to two circumstances:

1. When the thickness mistake is 5 nm variation of the refraction index within the range of angles ~10° is 0.001…0.005, which is less than for angular dependences observed by us on the presented structure $\Delta n = 0.005$ (centre), 0.01 (periphery).
2. The incorrect choice of the thickness considerably influence on the absolute values of optical constants increasing or decreasing them by several tenths.

Our model calculations have shown that the definite method of multiangular ellipsometric data analysis permits to determinate three unknown parameters of the film finding such thickness that values of optical constants would be the same at all angles. However, the error of initial ellipsometric measurements has to be rather small for us to obtain optical parameters with an error of some thousandths.

In our case, the experimental angular dependences of optical constants considerably exceed those appearing from calculations performed in the model of homogeneous film. It is evident that the reflective system model (homogeneous layer on the homogeneous substrate) chosen in data calculations doesn't correspond to the true one; in reality, the surface film could be inhomogeneous with optical parameters varying along the depth.

The investigated film in the central area is the most close to the homogeneous; it has the smallest angular changes of optical constants that approximate to the experiment error. In this case, the film could be characterized by some equivalent parameters such as optical constants and the thickness that by their physical intension corresponds to such homogeneous film that replaces presented inhomogeneous film by action on it light wave reflected from it. Obviously, such parameters so much better describe the system when the ellipsometric function (dependence of ellipsometric parameters from the angle of incidence) calculated using experimental data is as much as nearer to the experimental points.

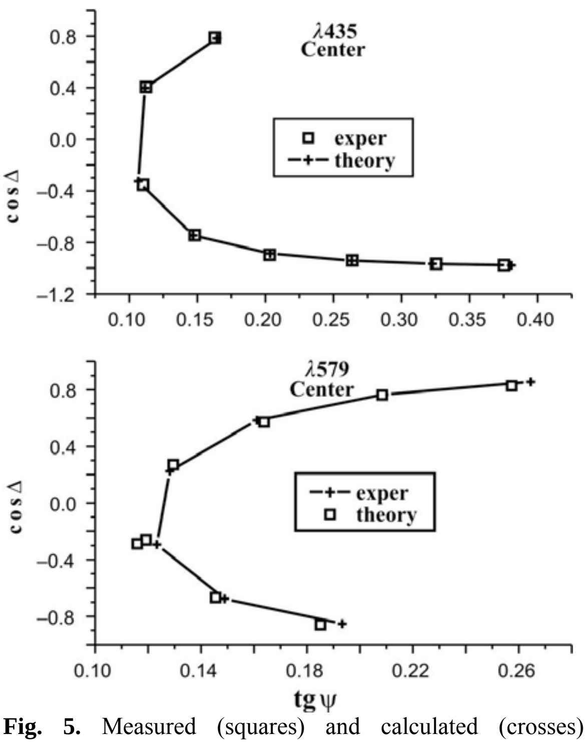

Fig. 5. Measured (squares) and calculated (crosses) ellipsometric parameters cosΔ and tgψ for various angles of incidence (ciphers near reference points) for the central area of the film with the thickness $d_2 = 80$ nm. Parameters of the theoretical curves: λ579 – $n_2 = 2.16$, $\kappa_2 = 0.366$; λ435 – $-n_2 = 2.37$, $\kappa_2 = 0.34$.

We founded equivalent parameters of the investigated film in its central area by averaging values of optical parameters over all the angles of incidence and on several thicknesses in measures of the most probable once. Then, using the averaged optical constants of the film ellipsometric function and its values mean square deviation from the measured ones in the given angle interval were calculated for every accepted thickness. It was discovered that the smallest deviation from each other for theoretical and experimental curves corresponds to the thickness 80 nm, that's why it was this value that we considered to be the most probable thickness value in the central area. Juxtaposition of the calculated ellipsometric function with the experimental one is shown in Fig. 5. It's seen that a good coordination of curves, particularly at the wavelength 435 nm, is observed. The theoretical curve deviation from the experimental one is situated in the interval of ellipsometric parameter calculation error.

4.2. The problem of solution multiplicity

When treating the multiangular ellipsometric measurements, we came across with the problem of solution multiplicity. So, in the case of large thickness (the central area of the investigated film), every angle of incidence is corresponded with two solutions, two couple of values of film optical constants always appeared. For instance, at the wavelength 579 nm and the film thickness 80 nm such couples are as follows: 1) $n_2 = 2.16$, $\kappa_2 = 0.36$ and 2) $n_2 = 2.3$, $\kappa_2 = 0.16$.

The first solution is generic for all the areas of the investigated system; it describes the dispersion of experimental points on the diagram for the main angle ellipticity (Fig. 2) and for this argument we consider this decision to be true.

The second solution is wrong; we don't take it into account because the values of optical parameters of the film on different areas of the same sample are different for it. Optical constants of the second solution much greater depend on the angle of incidence than the optical constants of the first solution, and any choice of the thickness can't eliminate this angular dependence. Besides, the second set of optical parameters can't describe the dispersion of the experimental points obtained at light reflection from different areas of the same sample.

Maybe in the measurements error interval not only for two but for a larger number of solutions can appear; at least we haven't find papers devoted to the expert mathematical analyses of ellipsometric function on the topic of multiplicity of its solutions. However, existing of multivariate solutions at ellipsometric data calculation on the base of ellipsometric equation became understandable coming from the general considerations that are based on the evidence representation of the ellipsometric function using the rectangular diagrams (look at Fig. 2), which contain real ψ and imaginary Δ parts of ellipsometric function or other corresponding characteristics of reflected light (Φ and tgψ).

In the case of the one-layer reflective system, the ellipsometric function on such diagram is represented by the set of curves each of them is corresponded by the constant values of optical parameters of the film and along which the thickness is increasing. Curves of the one-layer unabsorbing system begin from the certain point that presents a free from the film substrate and pass through, covering during the period the certain array of the ellipsometric parameter values, having no intersections with each other.

Model calculations testify that in the case of absorptive film, as we have, curves of constant values of optical parameters can get across with each other and thus several curves, each of which is characterized by its own couple of optical constants, can pass through each point on the diagram of ellipsometric parameters.

So, availability of several solutions for a given couple of measured ellipsometric parameters represents properties of the ellipsometric equation, and we have to be very careful in calculations while screening wrong solutions.

5. Conclusions

Optical parameters, namely, the refraction index, index of absorption and also the film thickness on each area were determined by the position of experimental points on the diagram of measured values (couples of ellipsometric parameter values) that belongs to areas with different thicknesses.

It was discovered that the film thickness increases from 43 nm on the periphery to 80 nm in the centre, and the refraction index of the film is considerably smaller than the refraction index of the monocrystalline cadmium telluride; that could be explained by the friable structure of the film or roughness of the film surface.

Also, it was discovered that values of film optical parameters insignificantly but depends on the experimental conditions such as the angle of incidence of the sounding light on the investigated structure, being larger at the periphery and smaller in the central areas of the sample.

The assumption that this residual angle dependence is caused by the inhomogeneity of optical parameters of the film along its thickness or roughness of the film surface was considered.

The obtained values of film parameters rather well describe the ellipsometric function that was measured in the central areas of the sample.

Our model calculations as well as experiments testified that one more wrong solution according to the optical parameters of the film that could be easy distinguished from the true ones by using the strong angular dependence of calculated values often appears when treating the multiangular ellipsometric measurements.

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