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DETERMINATION OF OPTICAL CONSTANTS OF THERMALLY EVAPORATED CdS_xSe_{1-x} THIN FILMS USING ONLY TRANSMISSION SPECTRA

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A procedure to calculate the optical constants and thickness of thin films, using only data from the transmission spectra, has been employed in the case of cadmium sulfo-selenide films prepared by thermal evaporation. Using this technique, the calculated thickness was found to an accuracy ranging between 1.0 and 3.0% compared with other methods. The refractive index and the absorption coefficient, as a function of composition (i.e. value of x) have been derived using this technique that proved to be very accurate. CdS_xSe_{1-x} films have a direct energy gap for films of various composition, and the values of the energy gap were found to increase when increasing the content of sulphur (x).

1. Introduction

It is known that the deviation from stoichiometry of II-VI binary compounds influences strongly their photoelectrical properties. The semiconductors CdS and CdSe are highly sensitive to light and other radiation. Both CdS and CdSe display peculiar features of photoconductivity which are common to the two substances [1].

Cadmium sulfo-selenides are solid solutions od CdS and CdSe. They appear very promising for various practical applications. To a great extent, these expectations are based on the possibility of controllable changing of important parameters (lattice constants, band gaps, etc.). The band gap of CdS_xSe_{1-x} crystal changes continously with the composition (x) within the energy range corresponding to the visible wavelengths [2].

A number of workers [2-8] studied the physical properties of CdS_xSe_{1-x} crystals. The electrical and optical properties as well as the structure of CdS_xSe_{1-x} thin films and the effect of heat treatment on these properties were reported [9].

In the present paper, the transmission spectra of thin CdS_xSe_{1-x} films with $0 < x < 1$ were investigated. Main aim of this work is to determine the thickness of the films from the interference fringes of the transmission spectrum as well as the refractive index and the absorption coefficient using transmission spectra only.

2. Experimental

Thin films of CdS_xSe_{1-x} of different composition were prepared by the thermal evaporation method of the mixture of separately ground and weighed amounts of pure CdS and CdSe, under vacuum of about 10^{-8} Pa. To get high quality and uniform CdS_xSe_{1-x} thin films, the substrate holder was rotated during the deposition process with a speed of about 240 rev/min.

The chemical composition of the prepared CdS_xSe_{1-x} thin films was determined using atomic absorption GBC 980 and Perkin Elmer (model 1100) spectrophotometers. The thickness of the films was determined using multiple-beam Fizeau fringe method [9]. Transmission measurements were performed with an accuracy of 3% in the spectral range from 400 to 2000 nm using UV, VIS, NIR Shimatzu type 3100 spectrophotometer.

3. Results and discussion

Figure 1 shows the experimetal transmission spectra measured at 300 K of all samples investigated in this work. All spectra reveal very pronounced interference effects for photon energies below the fundamental absorption edge. Such behaviour of the spectra is evidence of the thickness uniformity of the films. Otherwise, the interference fringes would have been destroyed, resulting in smooth transmission curves. However, some features of the spectra indicate that the uniformity of the films must be discussed more carefully.

3.1. Determination of the refractive index n

The extrema of the transmission spectra were used to calculate the refractive index n. The envelopes connecting the interference maxima and minima (full lines in Fig. 2, shown as a representative example of CdS_xSe_{1-x} thin films) are considered to be continuous functions of the wavelength λ. Therefore, for each maximum of the transmission curves, T_M, a corresponding minimum, T_m, may be determined at the same λ, and vice versa.

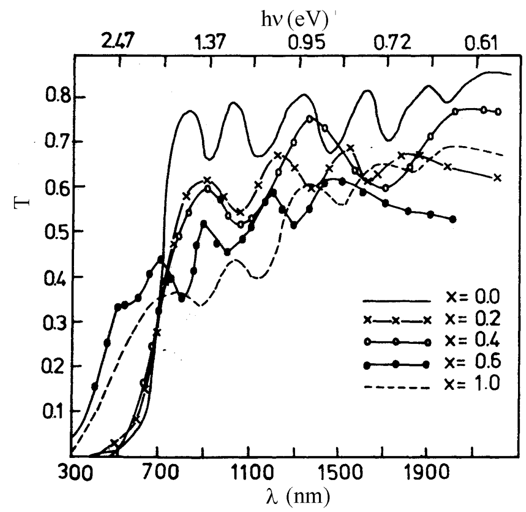

Fig. 1. Transmission spectra of CdS_xSe_{1-x} *thin films of different composition (x = 0, 0.2, 0.4, 0.6 and 1).*

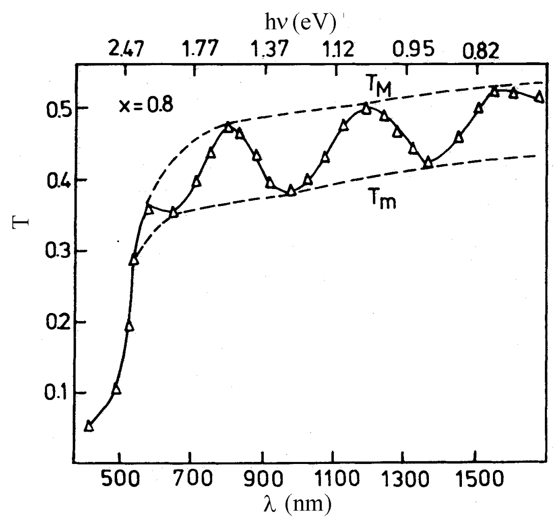

Fig. 2. Transmission spectra of $CdS_{0.8}Se_{0.2}$ $CdS_{0.8}Se_{0.2}$ *thin films.*

From the work of Swanepoel [10], the following equations describing the envelopes were used to calculate the refractive index *n* of the films:

$$n_1 = \sqrt{N + \sqrt{N^2 - n_2^2}}\,, \tag{1}$$

$$N = 2n_2 \frac{T_M + T_m}{T_M T_m} + \frac{n_2^2 + 1}{2} \, , \tag{2}$$

where T_M and T_m are the transmission maximum and minimum, respectively, on the envelope at a certain wavelength, and n_2 (1.517 in our case) is the refractive index of the substrate. Figure 3 represents the derived values of the refractive index n_1 as a function of composition x (x = 0, 0.2, 0.4, 0.6, 0.8 and 1), for the six measured films. These values were found to be in good agreement with the values published in Ref. 9. They show the increase of n_1 with the composition x.

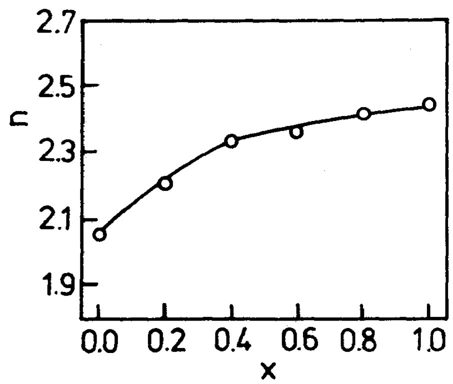

Fig. 3. Refractive index n of CdS_xSe_{1-x} *thin films vs. composition x.*

3.2. Determination of the film thickness d

The thickness of the prepared films has been determined using three different techniques.

1) It has been calculated from the transmission curves of Figs. 1 and 2 using the relation

$$d = \frac{\lambda_1 \lambda_2}{2(n_1' \lambda_1 - n_1'' \lambda_2)} \, , \tag{3}$$

where n_1' and n_1'' are the refractive indices at two adjacent maxima (or minima) corresponding to the wavelengths λ_1 and λ_2.

2) A simple graphical method was employed using the basic equation for the interference fringes

$$2nd = m\lambda, \tag{4}$$

where m is an integer for maxima and half-integer for minima. Equation (4) can be written as

$$\frac{I}{2} = 2d \frac{n}{\lambda} - m, \qquad I = 0, 1, 2, 3, \ldots . \tag{5}$$

Plotting of $I/2$ versus n/λ, one obtains a straight line with the slope $2d$ and a cut-off on the ordinate equal to $-m$. Figure 4 shows this plot for the six samples with different compositions x. From this figure, the thickness d and the integer m can be calculated.

3) The multiple-beam Fizeau fringes method [11] has been used to determine the film thickness, only for the sake of comparison.

Table 1 summarises the results of the determination of thickness using the three methods mentioned. From the inspection of the data, it was found that the values of d for thin CdS_xSe_{1-x} films determined by the different methods are in very close agreement. The results differ by less than 3%.

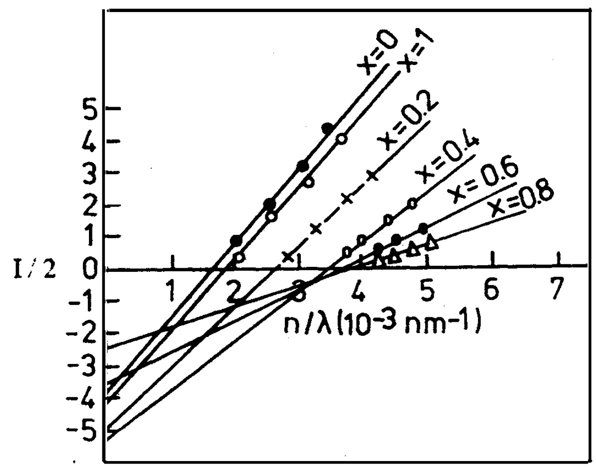

Fig. 4. Plot of I/2 vs. n/λ for the CdS_xSe_{1-x} thin films of different composition x.

TABLE 1. Results of determination of thickness of thin films of CdS_xSe_{1-x} using the three different methods.

Sample technique	Composition x					
	$x=0$	$x=0.2$	$x=0.4$	$x=0.6$	$x=0.8$	$x=1$
Transmission	1167.73	838.55	738.70	469.53	331.82	1146.18
Graphical	1166.96	833.33	740.05	470.23	329.51	1140.52
Interferometric	1170.95	840.33	745.35	474.27	333.98	1150.23

3.3. *Determination of the absorption coefficient* α

Knowing the values of the refractive index $n(\lambda)$ and the thickness d, the absorption koefficient $\alpha(\lambda)$ can be calculated using the formula [10]

$$X = e^{-\alpha(\lambda)d}, \tag{6}$$

where X is the absorbance for a system and is given in terms of the interference-free transmission T by [10]

$$X = P + \frac{\sqrt{P^2 + 2QT(1 - X_2X_3)}}{Q}. \quad (7)$$

T is the geometric mean of T_M and T_m,

$$T = \sqrt{T_M T_m}\,, \quad (8)$$

and

$$P = (X_1 - 1)(X_2 - 1)(X_3 - 1),$$

$$Q = 2T(X_1X_2 + X_1X_3 - 2X_1X_2X_3),$$

$$X_1 = \frac{1 - n_1}{1 + n_1},$$

$$X_2 = \frac{n_1 - n_2}{n_1 + n_2},$$

$$X_3 = \frac{n_2 - 1}{n_2 + 1}.$$

The absorption coefficient α, as calculated using these equations, for the six samples of different composition, as a function of photon energy $h\nu$, is shown in Fig. 5.

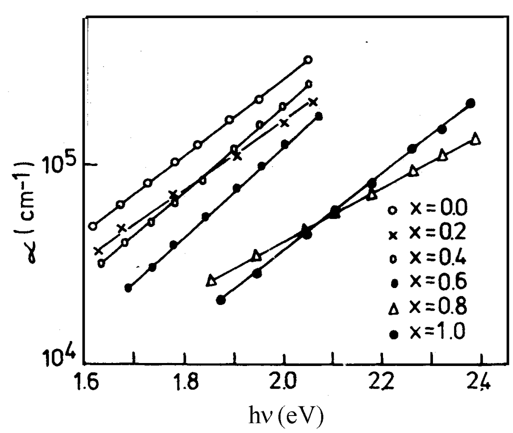

Fig. 5. Absorption coefficient α *as a function of photon energy for* CdS_xSe_{1-x} *thin films of different composition* x.

Plots of $(\alpha h\nu)^2$ versus photon energy $h\nu$ indicate the existence of the direct transition. The intercepts of lines showing $(\alpha h\nu)^2$ versus $h\nu$, shown in Fig. 6, extrapolated to $h\nu = 0$, are taken as the values of the direct optical energy gap. The direct-transition energy gap, E_g, for CdS_xSe_{1-x} thin films for different x values is shown in Fig. 7. From this figure, it is clear that the energy gap increases with increasing composition x. This is probably due to the increase of the depth of donor levels associated with sulphur vacancies [12].

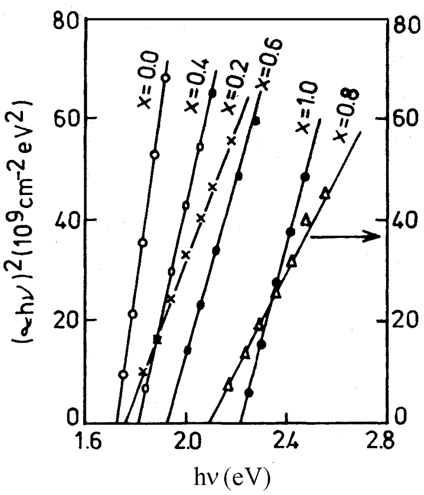

Fig. 6. Plot of $(\alpha h\nu)^2$ *vs. photon energy* $h\nu$ *for* CdS_xSe_{1-x} *thin films of different composition x.*

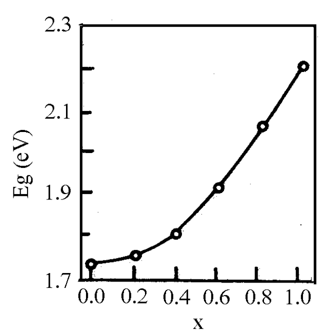

Fig. 7. Energy gap against composition for CdS_xSe_{1-x} *thin films.*

4. Concluding remarks

This work presents the result of the transmission measurements of thin CdS_xSe_{1-x} films. Key results of this work are summarized as follows:

(a) The refractive index *n* vs. the composition *x* is reported for the first time for CdS_xSe_{1-x} films.
(b) The refractive index *n* increases when increasing the composition *x*.
(c) The absorption coefficient revealed the direct transition for all films of different composition *x*.
(d) The direct energy gap increases with increasing composition *x*.
(e) The determination of film thickness of films of various composition has proved to be useful, easy and accurate in the case of our CdS_xSe_{1-x} evaporated films.

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ODREĐIVANJE OPTIČKIH KONSTANTI VAKUUMSKI NAPARENIH TANKIH SLOJEVA CdS_xSe_{1-x} MJERENJEM TRANSMISIJSKIH SPEKTARA

Primijenili smo račun za određivanje optičkih konstanti tankih slojeva kadmij sulfoselenida, na osnovi samih transmisijskih spektara. Na taj smo način postigli točnost određivanja debljine slojeva od 1.0 do 3.0%. Tim smo postupkom izveli vrijednosti indeksa loma i apsorpcijskog koeficijenta za niz vrijednosti *x*, i te su vrijednosti vrlo točne. Tanki slojevi CdS_xSe_{1-x} imaju izravan energijski procijep, a našlo se da veličina procijepa raste s povećanjem sadržaja sumpora.