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Vasyl Stefanyk Precarpathian
National University

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H.A. Ilchuk, A.I. Kashuba, R.Yu. Petrus, I.V. Semkiv, N.A. Ukrainets

Simulation the spectral dependence of the transmittance for semiconductor thin films

Lviv Polytechnic National University, Lviv, Ukraine, e-mail: AndriyKashuba07@gmail.com

The spectral dependence of the transmittance as a function of the film thickness, the refractive index of the substrate, bandgap and the Cauchy parameters (α and β) of the semiconductor material were determined from condition of interference extremes. The absorption coefficient was simulated for the structure – thin film/substrate. Cadmium chalcogenides (CdTe, CdSe, and CdS) deposited on quartz substrates were selected as model samples. Experimental behavior of substrate transmittance was used to determine its refractive index. The theoretical results are compared with the experimental data and shows good agreement.

Keywords: thin films, bandgap, optical functions, transmission, reflectance.

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Introduction

In designing modern materials for optoelectronics and optoelectronic device, it is important to know the refractive index as a function of wavelength to predict photoelectric behavior of a device. One of the most informative optical functions is the transmittance. The spectral behavior of all optical functions is possible to calculated using Swanepoel's method [1-6]. The complexity of theoretical calculations is due to the contribution of multiple light reflections from the boundaries of the medium/film, film/substrate and substrate/medium.

Some results of the theoretical calculation of the transmittance spectral behavior are present in Ref. [7, 8]. However, these works are given theoretical modeling of the transmission spectral behavior only in the transparency region and don't include reflection from all boundaries of the environment section.

Theoretical calculations of the spectral dependence of the transmittance in the absorption and transparency regions with taking into account all boundaries of the environment section are present. Thin films of cadmium chalcogenides (CdX, X = S, Se, and Te) are used as model samples. They are actively used as materials for obtaining solar cells. Thin films of cadmium chalcogenides (CdX, X = S, Se and Te) representative of $A^{II}B^{VI}$ crystal group and shows semiconductor behavior. As substrate we were used quartz with quality of "КВ".

I. Methods of calculation

For the theoretical modeling of the spectral dependence of the transmittance it should be noted that its behavior is different in the field of transparency and absorption region. Taking into accounts that refractive index is a dependent from wavelength and is a complex quantity.

The structure of thin film/substrate is shown in Fig. 1. Where d and n are the thickness and refractive index of the thin film, respectively. The refractive index of the environment is taken as $n_0 = 1$. R_1 – the intensity of the reflected light at the boundary medium/film, R_2 – the intensity of the reflected light at the boundary film/substrate and R_{12} – the intensity of the reflected light at the boundary substrate/medium. The substrate has a thickness several times larger than d, and the refractive index n_s, determined from relation (1).

$$n_S = \frac{1}{T_S} + \sqrt{\frac{1}{T_S^2} - 1}, \qquad (1)$$

where T_s is the transmittance of the substrate in the transparent zone.

The refractive index n_s of a substrate cannot be constant in the all optical range. Therefore, we use the first approximation: we consider the refractive index of substrate don't dependence from optical wavelength (400 - 2500 nm).

The including of scattering process due to defects, impurities, or structural inhomogeneities is difficult because it needed all information about the study material. The intensity of light propagating in the forward direction is attenuated by the scattering event and it can be quantified in a way equivalent to absorption. The intensity has an exponential dependence on path length d analogous to Beer's law: $I(z) = I_0 e^{-S \cdot d}$, where S is the scattering coefficient. When the scattering center is smaller than the wavelength of light this phenomenon is called Rayleigh scattering and the scattering coefficient S varies with the inverse fourth power of the wavelength: $S(\lambda) \propto \frac{1}{\lambda^4}$.

By measuring light attenuation we cannot tell the difference between absorption and scattering and the total attenuation is $\alpha_{tot} = \alpha + S$. However, the scattering contribution is generally much weaker than the absorption and can be neglected so that $\alpha_{tot} = \alpha$ [9]. That is, in the first approximation, we do not consider the scattering of light on the crystalline structure of the film, the boundaries of the section or the substrate.

The basis of the theoretical calculation is the condition of interference extremes. The model of the thin films on a thick quartz substrate is shown in Fig. 1. The transmission could be expressed as [7, 8]:

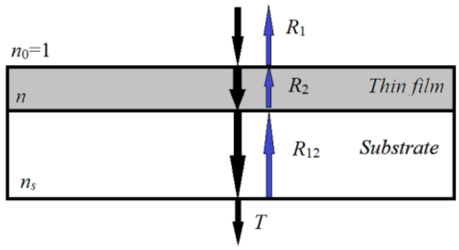


Fig. 1. Model of the thin films on a thick glass substrate.

$$T_1(\lambda) = T_0(\lambda) - 2\sqrt{R_1 R_2 R_{12}} \cdot \cos(\varphi(\lambda)), \qquad (2)$$

where:

$$\varphi(\lambda) = \frac{2n(\lambda)d}{\lambda} \cdot 2\pi + \pi$$

$$R_1 = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2},\ R_2 = \frac{(n_s - n)^2}{(n_s + n)^2},\ R_{12} = \frac{(1-n_s)^2}{(1+n_s)^2}.$$

$T_0(\lambda)$ is considered to be the term of transmission with no interference effect and will be described as: $T_0(\lambda) = (1 - R_1)e^{-\alpha(\lambda) \cdot d}$, where $\alpha(\lambda)$ – absorption coefficient, d – thickness of thin films.

Thus, the dependence of the thin film transmittance coefficient was obtained as a function of the refractive index and the thickness of thin films. Refractive index is associated with the absorption and extinction coefficients ($\alpha(\lambda) = 8nc(\pi/\lambda)^2$ and $k = (2\pi n)/\lambda$ [9]).

Therefore, using the formula (2) it is possible to modeling the transmission coefficient of a thin film in the transparency region. The only unknown function is the spectral behavior of the refractive index.

But, taking into account the results reported in [10-12], where was found that the spectral behavior of the refractive index describes the Cauchy dependence (α and β). Other functional dependencies showed less convergence compared to the Cauchy function. Using the Cauchy parameters we can obtain the dependence of the transmittance coefficient on the wavelength and the thickness of the film.

For obtained the spectrum envelopes T_{max} i T_{min} can be used Eq. (2). In the first case T_{max} it is assumed that $\cos(\varphi(\lambda)) = -1$, in the other case T_{min} – $\cos(\varphi(\lambda)) = 1$.

$$T_{\max}(\lambda) = T_0(\lambda) + 2\sqrt{R_1 R_2 R_{12}},$$

$$T_{\min}(\lambda) = T_0(\lambda) - 2\sqrt{R_1 R_2 R_{12}},$$

One of the optical parameters material is the bandgap. Which is allows the separation region of optical transparency and fundamental absorption. The absorption coefficient can be expressed as a ratio [4, 5] for absorption region:

$$\alpha(\lambda) = \frac{1}{d} \ln\left\{ \frac{[1 - R_1(\lambda)] \cdot [1 - R_2(\lambda)] \cdot [1 - R_{12}(\lambda)]}{T_2(\lambda)} \right\}, \qquad (3)$$

The spectral dependence of the transmittance coefficient in the absorption region is described by:

$$T_2(\lambda) = (1 - R_1(\lambda)) \cdot (1 - R_2(\lambda)) \cdot (1 - R_{12}(\lambda)) \cdot e^{-\alpha \cdot d} \qquad (4)$$

Using relations (2) and (4), we can establish the spectral dependence of the transmittance coefficient.

$$T(\lambda) = \begin{cases} T_0(\lambda) - 2\sqrt{R_1 R_2} \cdot \cos(\varphi(\lambda)),\ \lambda > \lambda_{E_g} \\ (1 - R_1(\lambda)) \cdot (1 - R_2(\lambda)) \cdot (1 - R_{12}(\lambda)) \cdot e^{-\alpha \cdot d},\ \lambda < \lambda_{E_g} \end{cases} \qquad (5)$$

where λ_{Eg} –wavelength corresponding to the bandgap (~1239,77/E_g).

II. Results and Discussion

The approximations used for theoretical modeling of spectral dependence of the transmittance coefficient are listed in Table 1. Quartz (quality "KB") is used as substrate material. The experimental behavior transmission spectrum of substrate is given in Fig. 2. The refractive index of the substrate can be determined using the relation (1). In the first approximation of the theoretical modeling of the spectral dependence of the transmittance we used the average value of the refractive

Table 1

Basic parameters of cadmium chalcogenides thin films used for theoretical calculation of the transmittance (n_s = 1,534; $c = 3 \cdot 10^6$ м/с)

Sample	λ_{Eg}, nm	α	β, μm²	d, μm
CdTe	886	2.46	0.28	1.39
CdSe	738	2.129	0.257	1.875
CdS	519	2.23772	0.017881	0.38

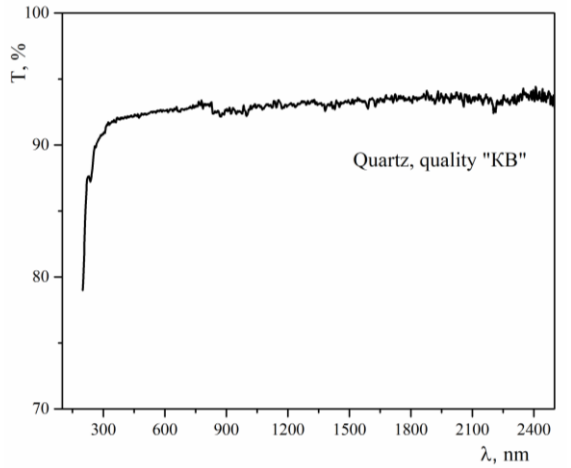
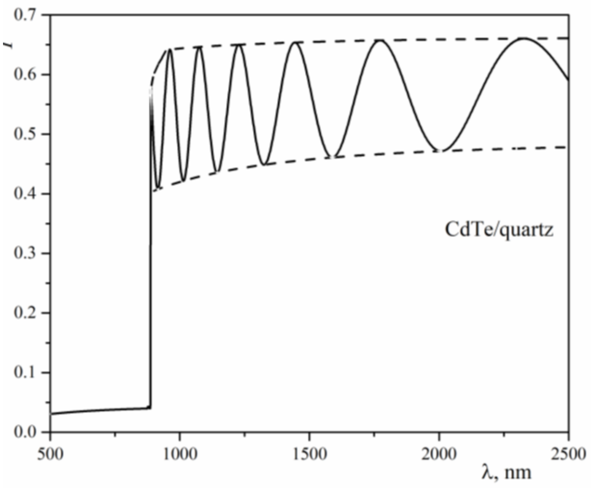


Fig. 2. Transmission spectra of the quartz substrate Quality – KB.

Table 2

Theoretical and experimental data of transmission spectra of CdS thin films [12]

λ, nm		700	800	1100	1200	1300	1400
T_{teor}	CdS	78.35	81.48	72.26	76.85	81.06	83.73
T_{exp}	CdS [12]	76.42	83.94	77.11	77.58	81.36	86.12



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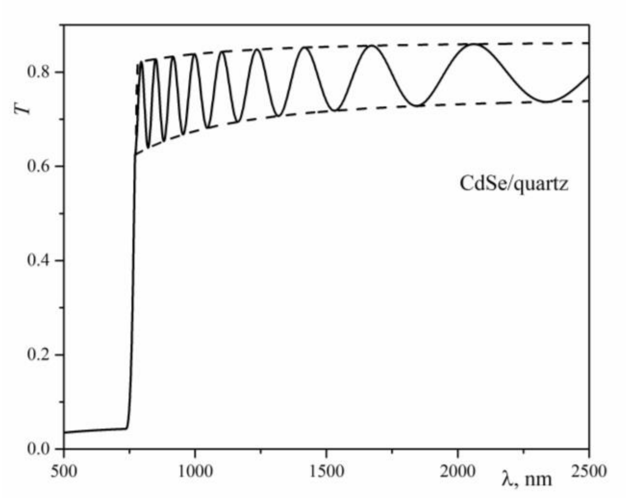

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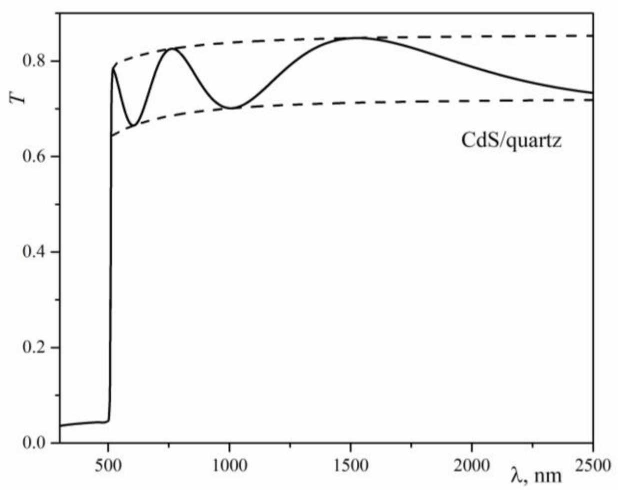

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Fig. 3. Simulation of transmission spectra of cadmium chalcogenides (1 – CdTe/quartz, 2 – CdSe/quartz, 3 – CdS/quartz).

index of the substrate.

From the obtained dependence (see Fig. 3), we can see a good correlation of the transmission coefficient with the experimental data [12-14]. A comparison of theoretical results with experimental data for the CdTe and CdSe thin films is excellent. Because, in Ref. [13, 14] as the substrate used glass (in our case – quartz).

Table 2 given compares the theoretically calculated transmittance with the experimental results for CdS [12]. In Ref. [12] are present the transmission spectrum for similar condition used in our theoretical calculations. A small difference between theoretical and experimental results is due to the use of approximations which are listed above.

Therefore, the presented method of calculating the spectral behavior of transmittance coefficient based on the value of the bandgap, the Cauchy coefficients and the thickness of thin film are shows good correlation.

Conclusion

The theoretical calculations of the spectral behavior of the transmittance coefficient are given, taking into account the reflection from the boundaries of the section. For the first time, the contribution of the substrate to the transmittance is taken into account. The spectral behavior of the transmittance is determined by the bandgap, thin film thickness, substrate material, and the Cauchy parameters (α and β) set for the reflectance of the semiconductor compounds under study. Also, using this technique, the modeling of spectrum envelopes was performed (T_{max} i T_{min}). Theoretical and experimental values are in good agreement.

Petrus R.Yu. – Ph.D., Leading Researcher at the Department of General Physics;
Ilchuk H.A. – Sc.D., Profesor at the Department of General Physics;
Kashuba A.I. – Ph.D., Senior Research at the Department of General Physics;
Semkiv I.V. – Ph.D., Senior Research at the Department of General Physics;
Ukrainets N.A. – Ph.D., Docent at the Department of General Physics.

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Г.А. Ільчук, А.І. Кашуба, Р.Ю. Петрусь, І.В. Семків, Н.А. Українець

Моделювання спектральної залежності коефіцієнта пропускання напівпровідникових тонких плівок

Національний університет, Львів, Україна, e-mail: AndriyKashuba07@gmail.com

Використовуючи умову інтерференційних екстремумів визначено спектральну залежність коефіцієнта пропускання, як функцію товщини плівки, показника заломлення підкладки, ширини забороненої зони та параметрів Коші (α і β) напівпровідникових тонких плівок. Проведено моделювання коефіцієнта пропускання для структури – тонка плівка/підкладка. В якості модельних зразків обрано халькогеніди кадмію (CdTe, CdSe та CdS) осаджені на кварцові підкладки. Коефіцієнт пропускання підкладки встановлено експериментально для визначення його показника заломлення. Проводиться порівняння теоретичних результатів із експериментальними даними та вказується на хорошу збіжність.

Ключові слова: тонкі плівки, ширина забороненої зони, оптичні функції, пропускання, коефіцієнт відбивання.