

# Influence of the thickness on optical properties of cadmium sulfide thin films

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## EXPERIMENTAL DETAILS

Cadmium sulfide thin films with different thickness were deposited on quartz substrates by the method of high-frequency magnetron sputtering using a VUP-5M vacuum station (Selmi, Ukraine). Commercial target of 99.99 % purity was used for deposition. The target-substrate distance was equal to 60 mm. The start and end of the sputtering process were controlled by means of a movable shutter. The phase analysis and crystal structure refinement was examined with X-ray diffraction data (XRD) obtained on DRON-2.0M diffractometer at room temperature with the  $K\alpha$  radiation ( $\lambda = 1.936087 \text{ \AA}$ ) of Fe. The spectral dependence of optical transmittance and reflection of the obtained samples were measured in the visible and near infrared regions (300-1500 nm) at room temperature using the spectrometer Shimadzu UV-3600.

## RESULTS AND DISCUSSION

Crystal structure of CdSe thin films has been determined from XRD. Cadmium sulfide thin film crystallizes in hexagonal structure (structure type - ZnO, space group  $P6_3mc$  (No. 186)). No additional peaks (by X-ray analysis) belonging to other phases can be detected, which indicates the formation of a pure single phase of CdSe.

Fig. 1 shows the transmission spectrum of the CdSe thin films-substrate combinations. The transmission coefficient strongly depends on the film structure, which is determined by the preparation methods, film thickness and deposition conditions. The transmission spectra of the thin films exhibit periodic peaks and minimums associated with interference effects, indicating the high structural perfection of thin films. A very rough surface will destroy the interference due to multiple reflections.

To determine the thickness of the films under investigation, we can use the following equation:

$$d = \frac{M \cdot \lambda_1 \cdot \lambda_2}{2 \cdot (n(\lambda_1) \cdot \lambda_2 - n(\lambda_2) \cdot \lambda_1)} \quad 1$$

where,  $\lambda_1$  and  $\lambda_2$  are the wavelengths corresponding to the neighboring extreme points in the transmission spectrum and  $M=1$  for two neighboring extrema of one type (max-max, min-min) and  $M=0.5$  for two neighboring extrema of opposite types (max-min, min-max). The thickness of the CdSe thin films are listed in Table 1.

To estimate the absorption band edge energy of the films the first derivative of the optical transmittance can be used. Position of the characteristic highest first peak of  $dT/d\lambda$  corresponds to the optical band gap energy. The optical bandgap  $E_g$  has been determined also from the spectrum of the absorption coefficient  $\alpha(h\nu)$ . For this purpose the known Tauc relation for the direct optical transition between valence and conduction bands has been used. This values are listed in Table 1.

The optical properties of a thin film (refractive index  $n(\lambda)$ , absorption coefficient  $\alpha(\lambda)$ , extinction coefficient  $k(\lambda)$ , dielectric functions  $\epsilon(\lambda)$  and thickness  $d$ ) can be easily evaluated from a transmission spectrum with interference effects using the envelope method. The envelope curves  $T_{\max}(\lambda)$  and  $T_{\min}(\lambda)$  can be obtained by means of parabolic extrapolation of experimentally determined points that coincide with the location of interference maxima and minima (see Fig. 1).

Refractive index  $n(\lambda)$  of the CdSe thin films can be calculated using the following equation:

$$n = \sqrt{N + (N^2 - n_s^2)^{1/2}}, \quad N = 2 \cdot n_s \cdot \frac{T_{\max} - T_{\min}}{T_{\max} \cdot T_{\min}} + \frac{2 \cdot n_s^2 + 1}{2}, \quad n_s = \frac{1}{T_s} + \sqrt{\frac{1}{T_s^2} - 1} \quad 2$$

where  $n_s$  is the refractive index of the substrate,  $T_s$  is the transmittance of the substrate in the transparent zone. For the quartz substrate  $n_s = 1.513$ .

The calculated refractive index  $n$  of the thin film studied decreases with increasing wavelength  $\lambda$ . Here, the dispersion  $n(\lambda)$  is normal and may be well approximated by the single oscillator model (proposed by Wemple and Di Domenico). Result of analysis are listed in Table 2.

Absorption coefficient  $\alpha(\lambda)$  for CdSe thin films can be calculated using the following equation:

$$\alpha(\lambda) = \frac{1}{d} \ln \left\{ \frac{[n-1] \cdot [n-n_s] \cdot \left[ \left( \frac{T_{\max}}{T_{\min}} \right)^{1/2} + 1 \right]}{[n+1] \cdot [n+n_s] \cdot \left[ \left( \frac{T_{\max}}{T_{\min}} \right)^{1/2} - 1 \right]} \right\} \quad 3$$

It is known that the real and imaginary parts,  $\epsilon_1$  and  $\epsilon_2$  (see Fig. 2), of the complex dielectric permittivity  $\epsilon = \epsilon_1 + i\epsilon_2$ , are related to the refractive index  $n$  and extinction coefficient  $k$  by the Eqs. (4),

$$\epsilon_1 = n^2 - k^2, \quad \epsilon_2 = 2 \cdot n \cdot k \quad 4$$

For the values of  $n$  much greater than  $k$ , the value  $\epsilon_1$  is approximately equal to  $n^2$  and the dependence of  $\epsilon_1(\lambda)$  can be fitted using the relation valid for the free electrons light absorption,

$$\epsilon_1 = n^2 = \epsilon_\infty - \left( \frac{e^2}{\pi \cdot c^2} \right) \cdot \left( \frac{N_c}{m^*} \right) \cdot \lambda^2 \quad 5$$

where,  $c$  is the speed of light,  $m^*$  is the effective mass of the carrier,  $N_c$  is the carrier density,  $e$  is the electronic charge, and  $\epsilon_\infty$  is the high-frequency dielectric constant. To obtain the high frequency dielectric constant  $\epsilon_\infty$  we plot a graph  $n^2$  as a function of  $\lambda^2$  and extrapolated the linear part of the curve to  $\lambda^2 = 0$  (see Table 3).

**Table 1** – Optical parameters of CdSe thin films.  $E_u$  - Urbach energy,  $T(R)_{\text{int}}$  - integral transmittance (reflection).

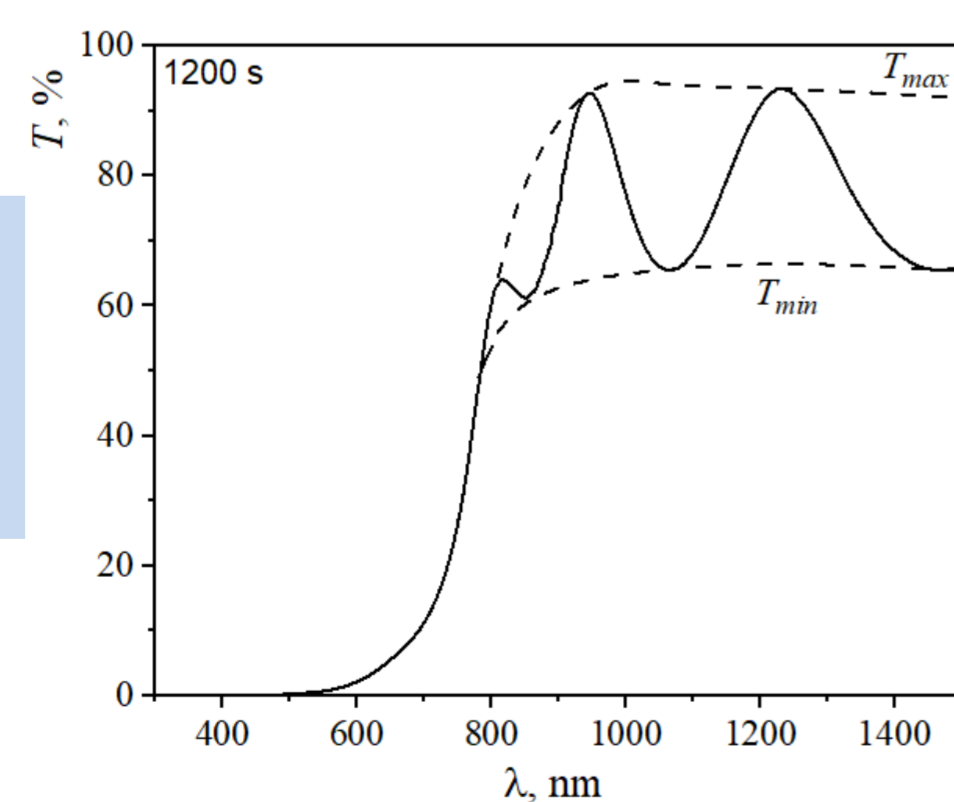
Sample	$d, \mu\text{m}$	$t, \text{s}$	$T_{\text{int}}, \%$	$R_{\text{int}}, \%$	$E_g, \text{eV}$	$E_g(dT/d\lambda), \text{eV}$	$E_u, \text{eV}$
CdSe-1200 s	0.73	1200	47.398	18.73	1.573	1.618	0.98
CdSe-720 s	0.4	720	45.306	31.287	1.621	1.662	0.45
CdSe-540 s	0.242	540	52.717	25.796	1.61	1.664	0.16
CdSe-360 s	0.133	360	55.359	26.234	2.016	–	–
CdSe-180 s	0.016	180	52.719	26.545	2.324	–	–

**Table 2** – Single oscillator parameters of CdSe thin films.

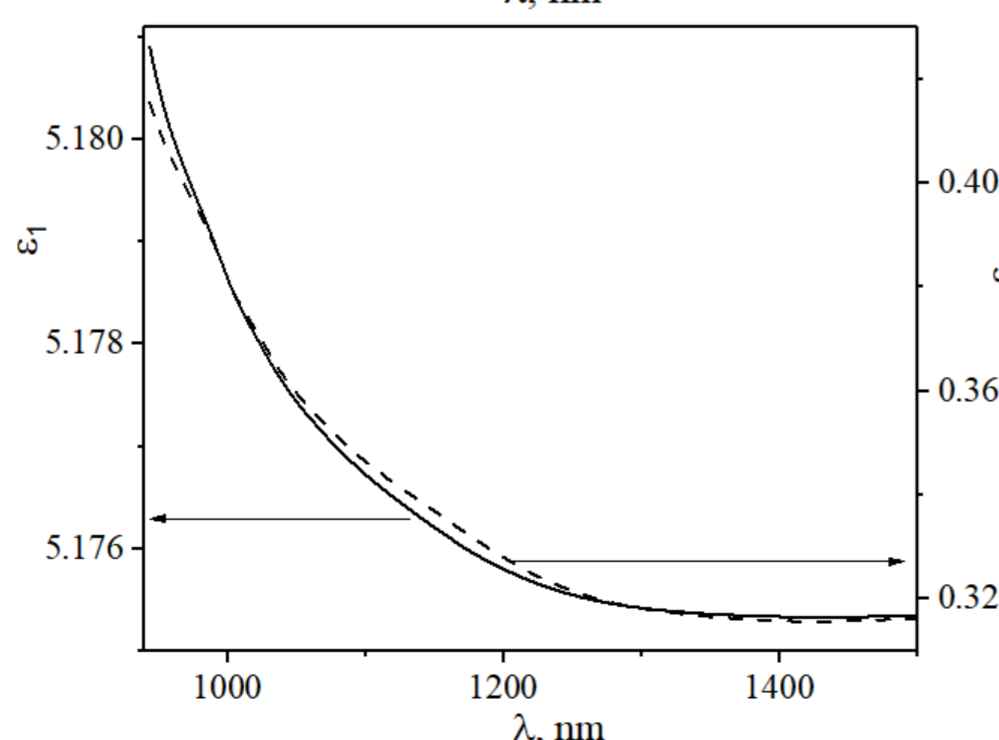
Sample	$E_0, \text{eV}$	$E_d, \text{eV}$	$n_0$	$M_1$	$M_3, \text{eV}^{-2}$	$f, \text{eV}^2$	$\lambda_0, \text{nm}$	$S_0, \text{nm}^{-2}$	$\beta, \text{eV}$
CdSe-1200 s	7.25	30.11	2.27	4.15	0.08	218.3	54.07	$1.4 \cdot 10^{-3}$	0.47
CdSe-720 s	7.03	29.21	2.27	4.16	0.08	205.35	55.96	$1.3 \cdot 10^{-3}$	0.46
CdSe-540 s	6.82	28.21	2.27	4.14	0.09	192.4	57.51	$1.3 \cdot 10^{-3}$	0.44

**Table 3** – Optoelectronic constants of CdSe thin films obtained from analysis of optical dielectric functions.

Sample	$\epsilon_\infty$	$(N_c/m^*), \text{kg}^{-1} \text{m}^{-3}$	Charge carrier density ( $N_c$ ), $\text{m}^{-3}$
CdSe-1200 s	5.16	$2.54 \cdot 10^{45}$	$3.01 \cdot 10^{14}$
CdSe-720 s	5.18	$2.23 \cdot 10^{45}$	$2.64 \cdot 10^{14}$
CdSe-540 s	5.16	$4.78 \cdot 10^{46}$	$5.66 \cdot 10^{15}$



**Fig. 1.** Transmission spectra of CdSe thin film-substrate combination (convert curves for interference maxima -  $T_{\max}$  and minima -  $T_{\min}$ ).



**Fig. 2.** Real ( $\epsilon_1$ ) and imaginary ( $\epsilon_2$ ) parts of dielectric functions depending on on wavelength of CdSe (720 s) thin film