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# COMPARATIVE OPTICAL CHARACTERIZATION OF CDSE AND CDS THIN FILMS BY SPECTROSCOPIC ELLIPSOMETRY FOR PHOTOVOLTAIC APPLICATIONS

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**Abstract.** In this study, the optical properties of CdSe and CdS thin films synthesized on glass substrates were systematically investigated using the Spectroscopic Ellipsometry (SE) method. The samples were measured at room temperature using an M-2000 rotating compensator Spectroscopic Ellipsometer within the photon energy range of 1.5-7 eV. Based on appropriate dispersion models, the spectral dispersion of optical constants was obtained, and the film thickness, real and imaginary parts of the dielectric function, as well as the refractive index and extinction coefficient, were determined with high accuracy. The analysis showed that both CdSe and CdS thin films exhibit high transparency depending on thickness and possess favorable optical properties for use in solar cells. Furthermore, the band gap energy was found to be approximately 1.7 eV for CdSe and about 2.4 eV for CdS. These results indicate that CdS, with its wider band gap, is more suitable as a transparent window layer, while CdSe, with a narrower band gap, is better suited as an absorber layer. Thus, Spectroscopic Ellipsometry proves to be a powerful and effective research method for the comparative analysis and optimization of photovoltaic materials.

**Keywords**: CdSe, CdS thin films, Spectroscopic Ellipsometry, optical constants, band gap, photovoltaic materials.

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## 1 Introduction

CdSe and CdS materials, which belong to the II–VI group of semiconductors, have great significance both in fundamental scientific research and in photovoltaic and optoelectronic applications (Green, 2006; Shim et all, 2011; Kitano et al., 2013). CdSe possesses a high light absorption capability and exhibits activity across a wide range of the visible spectrum, making it ideal for use in the light-absorbing layer together with CdS (Li et al., 2021). CdS, on the other hand, is commonly used as a window layer and complements the light absorption spectrum of CdSe due to its relatively wide band gap (Chu et al., 1991). Moreover, the nanoscale dimensions and morphology of both materials directly influence their optical and electrical properties, which determine their applicability in solar cells, lasers, and light-emitting diodes (Liu et al., 2017;

Nakajima et al., 2015; Khalilova et al., 2015).

In recent years, significant progress has been achieved in studying the optical and structural properties of CdSe and CdS thin films (Fujiwara, 2007; Azzam & Bashara, 1987; Bayramov *et al.*, 2019). These investigations provide an important database for better understanding the performance of these materials in photovoltaic devices and for assessing their application potential.

Several techniques are available for measuring the optical properties of thin films, one of the most powerful being Spectroscopic Ellipsometry (SE) (Gamzayeva et al., 2019; Adachi, 2005; Bayramov et al., 2019; Guseynov et al., 2019). The SE method demonstrates effectiveness not only for solid and bulk materials but also for solutions (Ahmadova & Jabarov, 2022, 2023; Aliyeva et al., 2023; Mehdiyev et al., 2023). Through this technique, parameters such as film thickness, refractive index, extinction coefficient, and the real and imaginary components of the dielectric function can be determined with high precision and in a non-destructive manner. One of the major advantages of SE is that it measures the polarization state of light rather than its intensity, allowing the detailed analysis of each layer in complex multilayer systems across a wide spectral range (Paduschek et al., 1995; Ibrahimova et al., 2024).

Ellipsometric measurements are based on the change in the $\Psi$ and $\Delta$ parameters resulting from the reflection of light from the sample surface:

$$\rho = \frac{r_p}{r_s} = tan\Psi e^{i\Delta} \tag{1}$$

here, $r_p$ and $r_s$ are the Fresnel reflection coefficients for the p and s polarized components, respectively. For homogeneous and defect-free materials, these parameters are used to calculate the optical constants the refractive index (n) and the extinction coefficient (k):

$$e = \varepsilon_1 + i\varepsilon_2 = \tilde{n} = \ (n+ik)^2 = sin\Phi\left[1 + tan(\Phi)^2 \cdot \left(\frac{1-\rho}{1+\rho}\right)^2\right] \tag{2}$$

In reality, various surface defects and oxides may exist, and in such cases, an appropriate optical model is constructed and fitted to the experimental data (Fujiwara & Kondo, 2005; Gasymov et al., 2015; Nassar et al., 2015).

In this work, CdSe and CdS thin films with thicknesses ranging from 80 to 200 nm were fabricated, and their optical parameters were comparatively investigated using the spectroscopic ellipsometry (SE) method. The obtained results provide a clearer understanding for evaluating the photovoltaic application potential of these materials.

## 2 Experimental Section

In this study, CdS and CdSe thin films were synthesized on glass substrates using the standard Chemical Bath Deposition (CBD) method (Ahmadova, 2020, 2021; Mamedov et al., 2017; Nurubeyli & Ahmadova, 2021; Alekperov et al., 2015). Prior to deposition, the substrates were sequentially cleaned in an ultrasonic bath with acetone, ethanol, and distilled water, followed by drying under a nitrogen flow. For the preparation of CdS films, cadmium acetate (Cd(CH3COO)2) and thiourea (NH2CSNH2) were used as precursors, while cadmium acetate and sodium selenosulfate (Na2SeSO3) were employed for CdSe film deposition. The temperature of the chemical solutions was maintained within the range of 70-80 °C, and continuous stirring was applied to ensure homogeneous growth. The deposition time was selected between 40 and 60 minutes, resulting in thin films with thicknesses ranging from 80 to 200 nm. After deposition, the samples were rinsed with distilled water and annealed in air at 200-300 °C for 1 hour to improve crystallinity.

The optical constants of the thin films were determined using a rotating compensator spectroscopic ellipsometer (M-2000DI, J.A. Woollam Co., Inc.). Measurements were carried out at room temperature in the photon energy range of 1.5-7 eV and at incident angles between 55° and 65°, with 65° chosen as the optimal angle of incidence. For modeling the experimental data, a three-layer optical model was applied. This model consisted of a glass substrate, a CdS (or CdSe) thin film, and a surface layer composed of a CdS:O (or CdSe:O) and void mixture.

The real ($\varepsilon 1$) and imaginary ($\varepsilon 2$) parts of the dielectric function, as well as the refractive index ($n$) and extinction coefficient ($k$) of CdS and CdSe thin films, were determined using Gaussian and Psemi-Tauc-Lorentz dispersion models, respectively. The optical constants of the surface layer were obtained using the Bruggeman Effective Medium Approximation (BEMA) method (Ciambriello et al., 2022). The film thickness ($d$) and surface roughness were calculated based on linear regression analysis.

## 3 Results and Discussion

The optical constants of CdS and CdSe thin films were investigated using the Spectroscopic Ellipsometry (SE) technique. Measurements were performed in the photon energy range of 1.5-7 eV and at incidence angles between 50° and 65°, with 5° intervals. The $\Psi$ and $\Delta$ spectra for CdS and CdSe, presented in Figure 1, demonstrate that the experimental data were fitted with high accuracy.

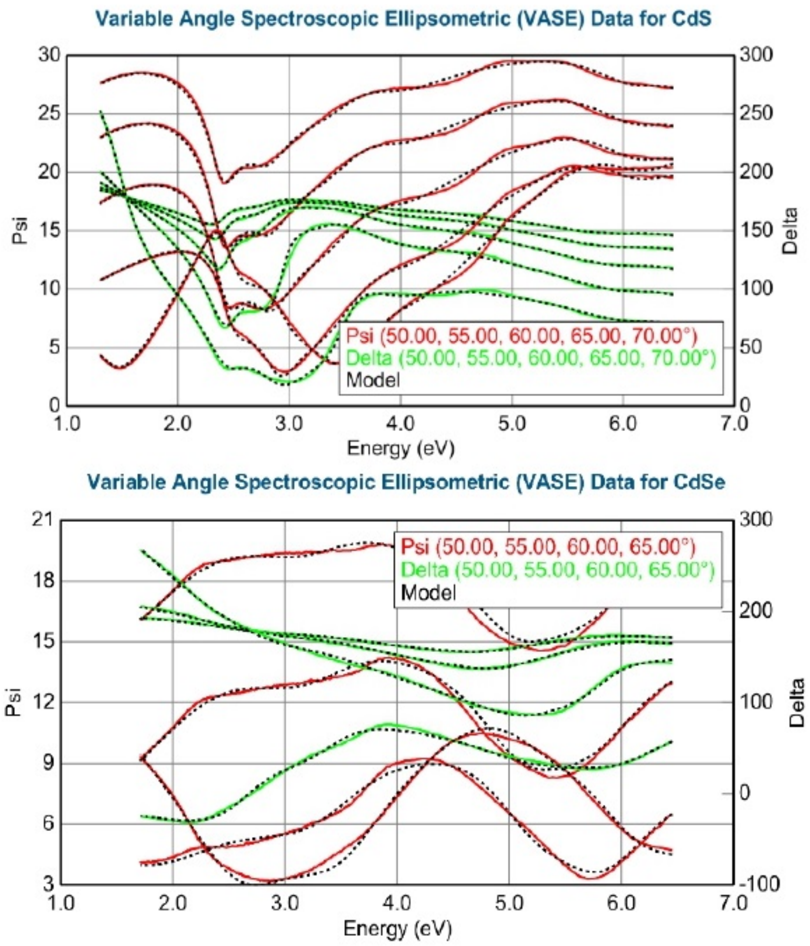


**Figure 1:** $\Psi$ and $\Delta$ spectra for CdS and CdSe, where theoretical and experimental results are in agreement.

A three-layer optical model was employed for the analysis, consisting of a glass substrate, a main thin film layer (CdS or CdSe), and a surface layer composed of a CdS:O (CdSe:O) and void mixture. The excellent agreement between the experimental and theoretical curves (fitting error $< 2\%$) confirms the reliability of the applied Gaussian and Psemi-Tauc-Lorentz dispersion models. This also verifies the effectiveness of ellipsometry as a powerful method for precise determination of the optical constants of thin films. Furthermore, the results indicate that the real surface morphology, including the presence of a thin oxide/void layer, was accurately considered in the optical model.

The most significant outcome of the study is the high accuracy observed between the experimental ellipsometry spectra and the theoretical modeling results. During the fitting of the $\Psi$ and $\Delta$ spectra, the mean squared error was minimal, confirming the correct application of the chosen dispersion models (Gaussian and Psemi-Tauc-Lorentz) as well as the Bruggeman Effective Medium Approximation (BEMA).

This agreement indicates that the selected optical model not only explains the experimental results but also accurately represents the actual physical and chemical structure of the thin films. Based on the optical model, the film thicknesses were determined to be olaraq $d_{CdS}$= 200 nm and $d_{CdSe}$= 350 nm. Moreover, the optical constants ($n$, $k$, $\varepsilon 1$, $\varepsilon 2$) were determined with high precision.

From the modeling of the ellipsometry results, the real ($\varepsilon 1$) and imaginary ($\varepsilon 2$) parts of the dielectric function of the CdS and CdSe thin films were obtained (Figure 2). The $\varepsilon 1$ function reflects the dispersion properties of the material, while $\varepsilon 2$ corresponds to the absorption processes. For CdS, the maximum value of $\varepsilon 1$ was observed around 4.5, whereas for CdSe it reached approximately 6.2. The $\varepsilon 1$ function indicates the dispersion characteristics of the materials and shows a decreasing trend at higher photon energies. In contrast, $\varepsilon 2$ exhibits maxima at the primary optical transitions, with the peaks for CdSe being associated with strong electronic transitions of the Cd–Se bonds.

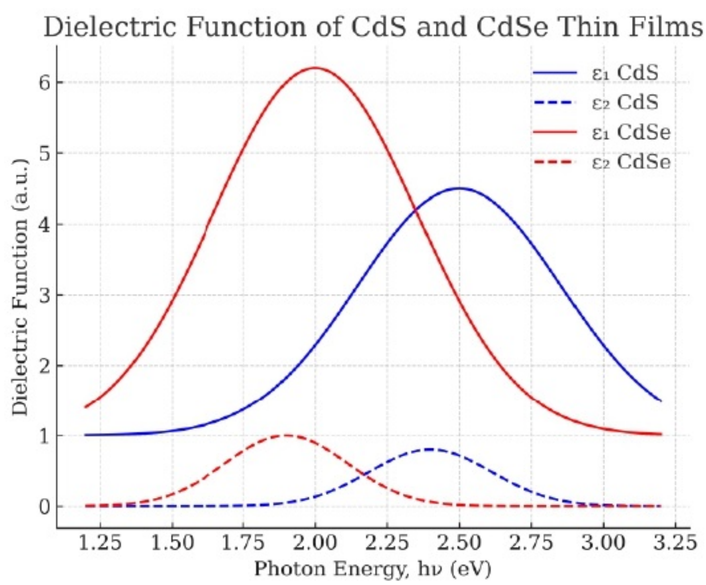


**Figure 2:** Photon energy dependence of the real ($\varepsilon_1$) and imaginary ($\varepsilon_2$) parts of the dielectric function for CdS and CdSe thin films.

The refractive index (n) and extinction coefficient (k) varied within the ranges of 2.2-2.6 and 0.1-1.5, respectively (Figure 3). In the visible spectrum, the CdS films exhibited higher transparency, whereas the CdSe films demonstrated stronger light absorption.

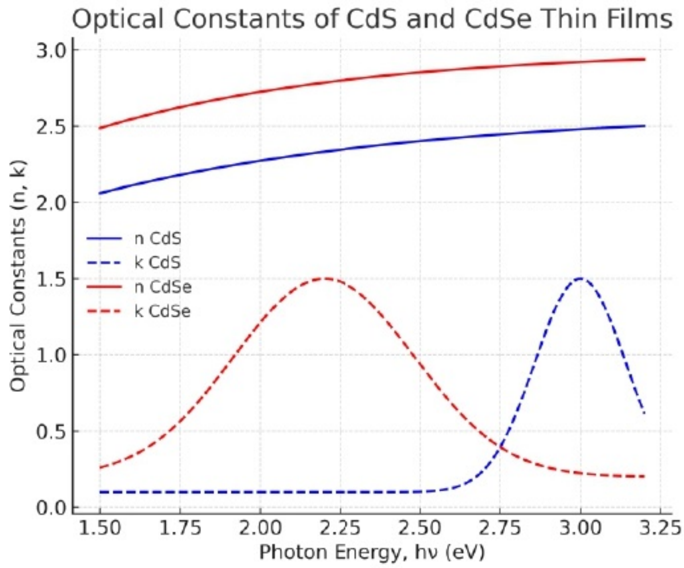


**Figure 3:** Refractive index (n) and extinction coefficient (k) of CdSe and CdS thin films (thickness 350–200 nm).

As shown in Figure 3, the $n(E)$ curves for both materials exhibit a typical dispersion behavior with increasing photon energy. For CdS, the refractive index values range from 2.2 to 2.6 within the visible spectrum, whereas for CdSe, they lie between 2.6 and 3. These results are in good agreement with literature data. Furthermore, it can be seen from the figure that CdS films exhibit significant absorption only at higher photon energies, while CdSe films show strong absorption over a large portion of the visible spectrum. This difference enables their respective use in optoelectronic devices as a “window layer” (CdS) and an “absorbing layer” (CdSe).

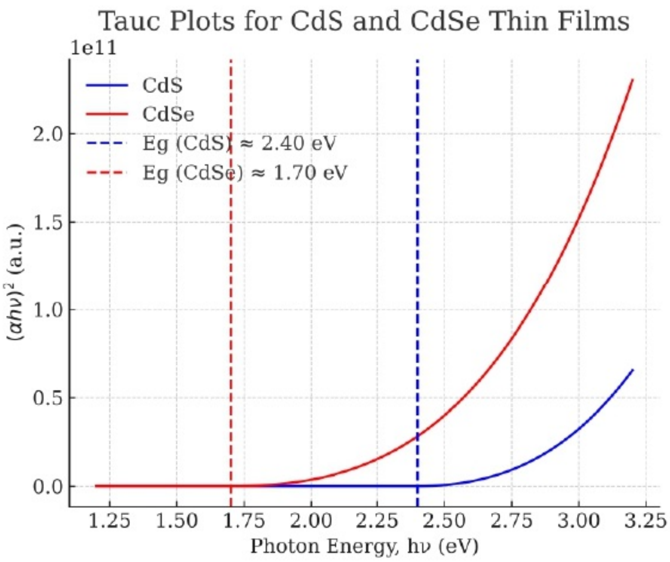


**Figure 4:** $(\alpha h\nu)^2$ versus $h\nu$ plots of CdS and CdSe thin films (Tauc method).

The optical band gaps of the CdS and CdSe thin films were determined using the Tauc method (Figure 4). Based on Tauc extrapolation, the optical band gap energies were found to be approximately 2.4 eV for CdS and 1.7 eV for CdSe. These values are consistent with previously reported data for thin films obtained via the CBD method and confirm the suitability of these films for photovoltaic applications.

Such precise modeling of the optical properties of CdS and CdSe thin films further demonstrates their potential for photovoltaic and optoelectronic applications. CdS, with its wide energy gap and high transparency, is ideally suited as a window layer, while CdSe, with its narrow energy gap and strong absorption, is ideally suited as a light-absorbing layer. The agreement between the obtained results, both theoretically and experimentally, further strengthens the prospects for the use of these films in technological applications.

## 4 Conclusions

In this work, CdS and CdSe thin films were synthesized on glass substrates by chemical vapor deposition (CBD) and their optical properties were studied by spectroscopic ellipsometry in the photon energy range of 1.5-7.0 eV. During the analysis, a glass/CdS(CdSe)/surface roughness ternary optical model was used and the surface layer was described by the Bruggeman effective medium approach. The obtained results showed that: the refractive index (n) and absorption (k) exhibited semiconducting properties depending on the photon energy. The values of n for CdS varied in the visible range from 2.2-2.6, and for CdSe in the range from 2.6-3. The real and imaginary parts of the dielectric function ($\varepsilon 1$, $\varepsilon 2$) were fitted to the model with high accuracy, especially the maximum of $\varepsilon 2$ corresponded to strong optical transitions. The optical bandgaps were ˜2.4 eV for CdS and ˜1.7 eV for CdSe according to Tauc analysis, which indicates their application as window layers and absorber layers, respectively. The application of dispersion models (Gaussian and Psemi-Tauc-Lorentz) provided a high-precision agreement between the experimental and theoretical results (fitting error $<2\%$). This confirms that ellipsometry is a powerful method for the accurate determination of the optical constants of thin films. The surface roughness was estimated in the range of 3–5 nm as a result of the thickness modeling, which indicates the homogeneity of the thin films obtained by the CBD method. In general, the conducted studies show that CdS and CdSe thin films obtained by the CBD method give stable and reproducible results in terms of optical constants. CdS layers are promising as transparent window materials, while CdSe layers are promising as absorber layers for solar cells and other optoelectronic devices due to their high absorption capacity.

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