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Study of CdSe thin films using the spectroscopic ellipsometry method

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In this research, we investigated the optical properties of CdSe thin films on glass substrates using spectroscopic ellipsometry. The samples were analysed using an M-2000 rotation compensator spectroscopic ellipsometer at room temperature, covering a photon energy range of 1.5-7.0 eV. We used an appropriate dispersion model to obtain the spectral dispersion of the optical constants. We calculated the thickness, dielectric permittivity (real and imaginary parts), refraction, and extinction coefficients of the thin layers. The results showed high transparency that varied with the size of the CdSe thin films. Additionally, we determined the bandgap width for samples with thicknesses of 350 nm and 400 nm, which were produced using the chemical deposition method.

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1. Introduction

The compound CdSe belongs to the II-VI group of complex semiconductors. It is widely used in fundamental research and various technological applications due to its wide absorption spectrum across the visible spectrum. There is a known technology for increasing the width of the forbidden zone in thin layers of this compound, but a comprehensive optical analysis validating this technology has not been proposed. The physical properties of cadmium selenide are directly affected by its size and shape, making nanostructures of this compound useful in solar cells, lasers, and light-emitting diodes. In recent years, significant progress has been made in the research of CdS and CdSe nanostructures. The study of the structure and optical parameters of thin layers of these materials has further increased interest in them [2-4].

There are several research methods for studying the optical properties of thin films, with Spectroscopic Ellipsometry being one of the most prominent. Ellipsometry is recognized globally as an ideal technique for investigating the physical parameters of thin films and is widely employed in optoelectronics [5-7]. This method is particularly powerful because it allows for precisely determining the state of the light signal using four Stokes parameters. As the world standard for studying solid, liquid, and gaseous environments, ellipsometry provides a highly accurate means of determining these Stokes parameters [8-10]. Consequently, results obtained through ellipsometry spectroscopy comprehensively cover experimental optical studies [11-14].

A key characteristic derived from ellipsometry investigations is the dielectric function of the system. The dielectric function serves as a unique "dielectric fingerprint," determined within the frequency range corresponding to the electronic transitions and vibrational excitations of the

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molecules and atoms in the sample. Understanding the optical properties of thin layers, especially as they vary with the thickness of multilayer structures, is of great importance.

Unlike standard methods that measure light based on emission and absorption, ellipsometry measures the polarization state of light rather than its intensity. This distinction enables ellipsometry to determine optical parameters with greater accuracy. Another significant advantage of this method is its ability to analyze individual components of complex systems over a wide spectral range.

The technique of ellipsometry measurements relies on analyzing the changes in polarization parameters Ψ and Δ after a linearly polarized light beam reflects off the surface of a sample. These changes are expressed through two variables, Ψ and Δ, which describe the phase shift and the ratio of the amplitudes of the components parallel (p) and perpendicular (s) to the plane of incidence of the light's electric field. These quantities are represented as the ratio of the Fresnel coefficients r_p and r_s for p- and s-polarized light, respectively:

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

The results of ellipsometric measurements on a bulk material with a defect-free surface can be directly converted into the material's optical constants: the refractive index n and the extinction coefficient k:

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

In practical applications, the previously mentioned possibilities are seldom encountered, as real materials typically have surface defects, oxides, and other imperfections [15-17]. In such cases, an optical model that describes the optical parameters of the system is constructed and compared with experimental results.

The optical properties of CdSe thin films have not been fully studied, despite extensive research into their physical properties. In this study, we obtained 350 nm and 400 nm thick cadmium selenide thin films and analyzed their optical parameters using Spectroscopic Ellipsometry.

2. Experimental

CdSe thin films were deposited onto glass substrates using a standard chemical deposition method [18-20]. The optical properties of these thin films were analyzed using a spin-compensated Spectroscopic Ellipsometer (M-2000DI, J.A. Woollam Co., Inc.) over a photon energy range of 1.5–7 eV, at room temperature, with incidence angles varying from 55° to 70°. An optimal incidence angle of 65° was used for the analyses. A three-layer optical model was employed to interpret the experimental results across the entire photon energy range. The constructed model for the thin film system is depicted in Figure 1.

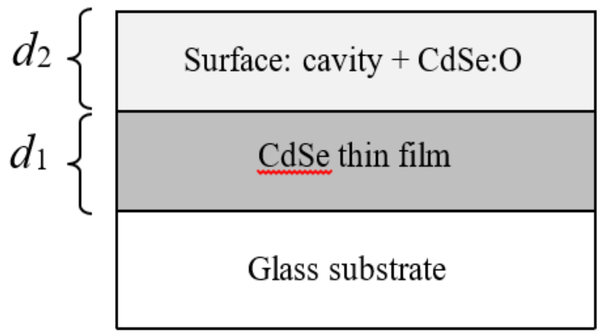

Fig. 1. The optical model used in the analysis.

The optical model, depicted in Figure 1, comprises three distinct layers: a glass substrate, a CdSe thin layer, and a CdSe:O+ void layer situated on the surface of the thin layer. The optical properties of the CdSe thin film were simulated using appropriate Gaussian and PsemiTri dispersion models, while the optical properties of the surface layer were acquired using the Bruggeman Effective Medium Approximation (BEMA) applied to the CdSe:O and cavity mixture [21]. The surface roughness is determined based on the established model. Using linear regression analysis (XRA), the following parameters were determined: d – thickness of CdSe thin layers, ε_1 and ε_2 – real and imaginary part of the dielectric function of CdSe layers, n – refractive index, and k – extinction coefficient.

3. Result and discussion

The thicknesses of the CdSe thin films were determined by fitting the experimental results to a model designed for two different layered structure samples. It was found that the thicknesses of the thin layers obtained through the chemical deposition method were 350 nm and 400 nm. The optical constants of these thin films were calculated using the Gaussian and PsemiTri oscillators as part of the oscillator model. Throughout the calculations, the root mean square error fluctuated around 1, indicating that the optical model accurately describes the experimental parameters. The dielectric functions of CdSe thin films with different thicknesses obtained from the analysis are illustrated in Figure 2.

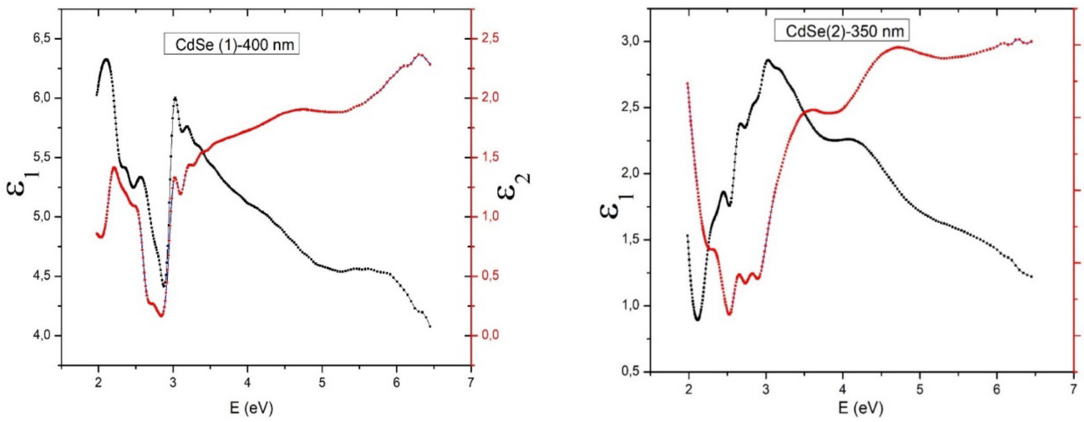

Fig. 2. The real and imaginary parts of the dielectric function of 350 nm and 400 nm thick CdSe thin films.

A comparison of the imaginary parts of the dielectric function is shown in Figure 3 for CdSe thin films with thicknesses of 350 nm and 400 nm. In Figure 3, it is evident that the energy transitions of CdSe thin films correspond to the CdSe crystal, but the width of the forbidden zone shifts to shorter wavelengths as the film thickness decreases. The studies revealed that the width of the forbidden zone in a CdSe crystal is 1.7 eV, while in a thin layer of CdSe with a thickness of d = 350 nm, Eg = 2.2 eV and Eg = 1.9 eV in a thin layer with a thickness of d = 350 nm.

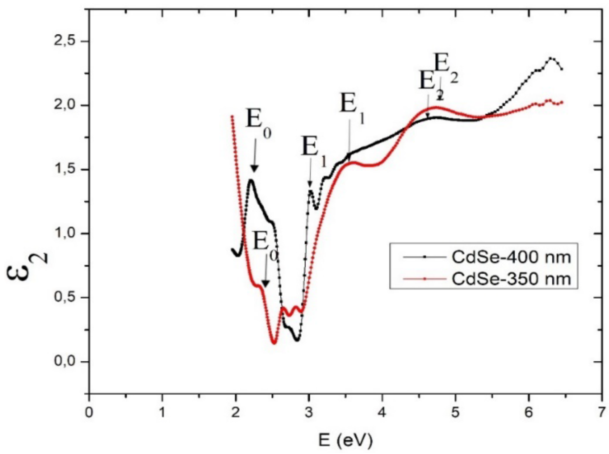

Fig. 3. Comparison of the imaginary parts of the dielectric functions of 350 nm and 400 nm thick CdSe thin films.

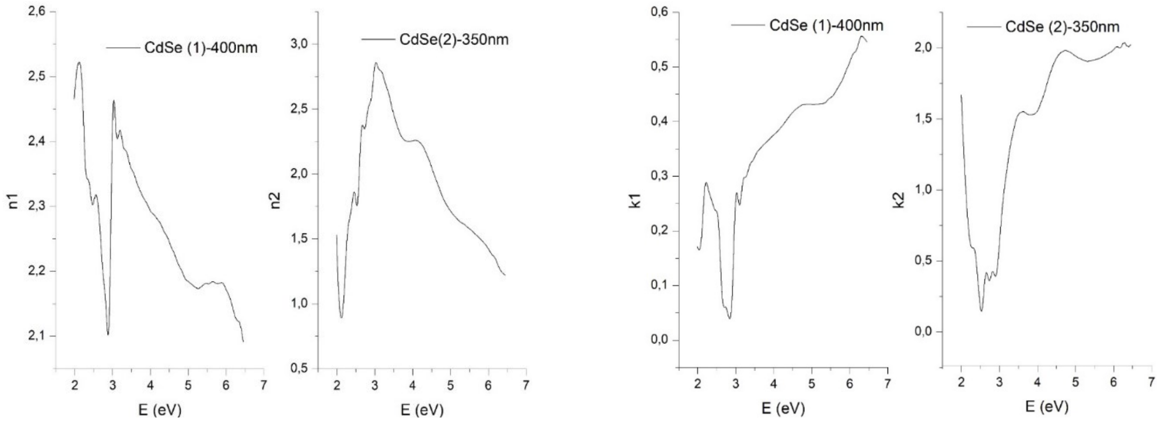

Fig. 4. Refractive and extension coefficients of CdSe thin films at 350 and 400 nm thickness.

Based on the results of studies conducted using the spectroscopic ellipsometry method, the extension and refraction coefficients of 350 nm and 400 nm thick CdSe thin layers were calculated (see Figure 4). The extension and refraction coefficients of CdSe thin films were determined in the energy interval of 1.5-7 eV. According to the results, the refractive index of a thin film with a thickness of d = 400 nm is 2.3-2.8 eV, and a CdSe thin film with a thickness of d = 350 nm varies in the range of 2.1-2.9 eV, corresponding to the range of the refractive index of the CdSe crystal (2.5-2.65 eV). The research revealed that, like the CdSe crystal, which has high transparency in the visible region and the ability to absorb ultraviolet rays, the studied thin layers of different thicknesses also exhibit these properties. The study of the change in optical constants of CdSe thin films using modern methodology expands their potential applications in various optical devices.

4. Conclusion

In this study, we examined CdSe thin films created on glass substrates using the chemical deposition method and analyzed them using spectroscopic ellipsometry. We used a dispersion model to calculate the optical constants and determine the thickness, dielectric permittivity (real and imaginary part), refraction, and extension coefficients of the thin layers. We found that the width of the forbidden zone in the 350 nm and 400 nm thick cadmium selenide thin films corresponds to Eg = 1.9 eV and Eg = 2.2 eV. The widening of the forbidden zone is attributed to the phase formation process within the thin layers. Additionally, we observed that as the thickness of the thin layers increased, the width of the forbidden zone adapted to the CdSe crystal due to the phase formation process.

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