

## Thickness variation on some physical properties of CdS: MgO films

W. H. Albanda<sup>a</sup>, M. H.Saeed<sup>a</sup>, M. Z. Abdullah<sup>b</sup>, M. H. Al-Timimi<sup>c,\*</sup>

<sup>a</sup>Science Department - College of Basic Education, Mustansiriyah University, Iraq

<sup>b</sup>Materials Research Directorate, Ministry of Science and Technology, Iraq

<sup>c</sup>Department of Physics, College of Science, University of Diyala, Iraq

In this study, CdS: MgO films were synthesized using the chemical spray pyrolysis method, varying the film thickness. X-ray diffraction (XRD) analysis confirmed the polycrystalline nature of the films, with an observed increase in average crystallite size corresponding to thicker films, and The films' surface morphology indicates an absence of crystal defects such as holes and voids . The investigation of energy gap and optical parameters revealed a dependency on film thickness, with the energy gap shifting from 2.412 eV for a thickness of 150 nm to 2.354 eV for a thickness of 750 nm. Hall effect measurements demonstrated an augmentation in carrier concentration with increasing film thickness. The findings suggest a substantial influence of thickness on the physical properties of CdS: MgO thin films. Notably, thicker films exhibit characteristics that make them promising candidates for application as absorber layers in solar cells. This research provides valuable insights into tailoring the properties of these films for optimal performance in solar energy conversion devices, emphasizing the importance of controlling thickness in achieving desired electronic and optical characteristics.

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### 1. Introduction

The thickness of cadmium sulfide (CdS) and magnesium oxide (MgO) films prepared by chemical spraying can affect their optical and electrical properties, which in turn can impact their performance in various applications, for MgO and CdS films prepared by chemical spraying, their thickness can influence their performance in solar cell applications [1,2,3]. The thickness of the absorber layer (which is typically made of CdS) is critical for optimizing the efficiency of the cell. Thicker absorber layers can absorb more light, but can also increase the resistance of the cell and decrease its efficiency. Therefore, finding the optimal thickness for the absorber layer is crucial for achieving good efficiency in solar cells [4,5,6]. cadmium sulfide (CdS) films mixed with metal oxides can have various effects on their properties, depending on the specific metal oxide used and the method of inlaying. One potential effect is on the optical properties of the film, For example, mixing CdS films with metal oxides such as (ZnO) or (TiO<sub>2</sub>) can increase their transparency and reduce their light absorbance, due to the higher refractive index of these metal oxides compared to CdS [7,8], This can be beneficial in applications such as photovoltaic cells or photoelectrochemical cells, where higher transparency can increase the efficiency of light harvesting. The method of inlaying can also affect the properties of the CdS film, for example, mixing CdS films with metal oxides using a physical vapor deposition (PVD) method can result in a different crystal structure and morphology compared to inlaying using a chemical method such as spin-coating or dip-coating[9,10]. The doping of CdS films with metal oxides can have various effects on their properties, including improving their transparency, conductivity, and resistance

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\* Corresponding author: muhammadtimimi@yahoo.com  
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[11,12], The specific effects depend on the metal oxide used and the method of mixing and can be tailored to the specific application [13]. This research described investigated the effect of film thickness on the structural, optical, and electrical properties of cadmium sulfide (CdS) films mixed with magnesium oxide (MgO) prepared by chemical spray pyrolysis.

## 2. Experimental details

To deposit CdS: MgO films by spray pyrolysis, the following experimental details could be followed:

a-Materials: Cadmium acetate, Thiourea, Magnesium acetate, Deionized water, Methanol, Glass substrate, Spray pyrolysis system.

b- Procedure: Clean the glass substrate with acetone and ethanol, and dry it with nitrogen gas. Prepare the precursor solutions by dissolving Cd(CH<sub>3</sub>COO)<sub>2</sub>, CH<sub>4</sub>N<sub>2</sub>S, and Mg(CH<sub>3</sub>COO)<sub>2</sub> in deionized water separately to obtain 0.1 M solutions. Mix the Cd(CH<sub>3</sub>COO)<sub>2</sub> solution and the CH<sub>4</sub>N<sub>2</sub>S solution in a 1:1 molar ratio, and add the Mg(CH<sub>3</sub>COO)<sub>2</sub> solution dropwise to obtain a final CdS: MgO. Using air (carrier gas), pressure (1.5 bar), flow rate (4 m/s), and distance between the nozzle and the substrate (32 cm), the spray time was (12 s), and the interval spray time was (2 min). Heat the spray pyrolysis system to a temperature of 673 K. Spray the solution onto a glass substrate with different spray durations to obtain CdS: MgO thin films with different thicknesses, Anneal the films in the air at 673 K for 1 hour to improve the crystallinity and stability of the films. Shimadzu XRD-6000 powder diffractometer was used to distinguish the crystal structure type of films, Shimadzu UV-Probe Japan was used to record the transmittance spectra, and Hall effect measurement was used to determine the electrical properties.

## 3. Results and discussion

The crystalline structure of CdS :MgO films was determined using a Shimadzu XRD-6000 powder diffractometer to distinguish the crystal structure type of synthesized nanostructure. Figure 1 presents the X-ray diffraction of CdS: MgO films in the range of (20° to 80°) at different thicknesses (150, 350, 550, and 750 nm). The XRD pattern at a thickness (150 nm) proved the formation of hexagonal CdS nanostructure, space group (P63mc no.18), (a=b= 4.1409 °Å and c= 6.7198 °Å), ( $\alpha=\beta= 90^\circ$  and  $\gamma= 120^\circ$ ), which well agreed with the standard data (ICDD 00-041-1049) [14], at the characteristic peaks ( $2\theta= 24.8^\circ, 26.5^\circ, 28.18^\circ, 36.62^\circ, 43.68^\circ, 47.84^\circ, 51.82^\circ, 52.79^\circ, 66.77^\circ, \text{ and } 77.85^\circ$ ) of the planes (100) (002) (101) (102) (110) (103) (112) (201) (203) and (105) respectively. Other peaks located at ( $2\theta = 3.86^\circ, 42.82^\circ$  and  $62.16^\circ$ ) of the planes (111) (200) and (220) respectively, which referred to the formation of cubic MgO nanostructure, space group (Fm-3m no.225), (a=b= c= 4.22 °Å), ( $\alpha=\beta=\gamma= 90^\circ$ ), corresponded to the standard data (ICDD 01-074-1225) [15], The X-ray diffraction results show that all the prepared CdS: MgO films possessed a polycrystalline nature and random orientations. This can be attributed to the heat treatment temperature (over 400 °C) of the chemical spray pyrolysis method and the heat exposure time [16], where if the temperature of the substrate is above 420 °C, this leads to degrades the structure to randomly oriented structures [17], The crystalline size of prepared CdS: MgO nanostructure at different thicknesses (150, 350, 550, and 750 nm) was calculated using Scherrer's equation to be (27.84, 28.11, 29.02, and 32.08 nm) respectively. Observed that the crystal size of CdS: MgO becomes higher with increasing the film's thickness, due to the particles amount of the precursor solutes increasing with increasing the deposition period, leading to large electrostatic interactions between the particles, thus increasing the crystal size [18].

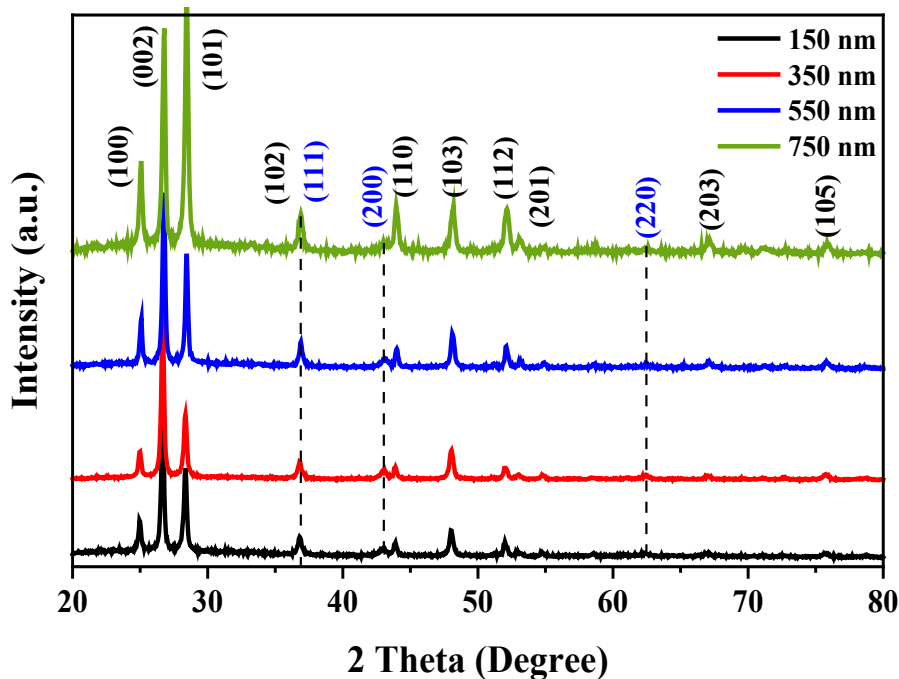


Fig. 1. XRD for CdS: MgO films.

FE-SEM can provide important insights into the surface and structural properties of CdS: MgO thin films. Analyzing films of different thicknesses allows us to investigate how the film's thickness influences the surface morphology and It offers comprehensive details regarding the material's composition, topography, and surface morphology. A high-resolution, magnification surface imager (FE-SEM) was used to study the surface morphology of CdS: MgO films. We observe that the surface structures of the generated films extensively agglomerate dense quasi-spherical nanoparticles, and highlight the films' voids, asymmetrical shapes, and irregular particle sizes. This is consistent with the research conducted by GÜZELÇIMEN, Feyza, et al. and ALAGARASAN, Devarajan, et al. [19, 20] , as shown in Figure (2).

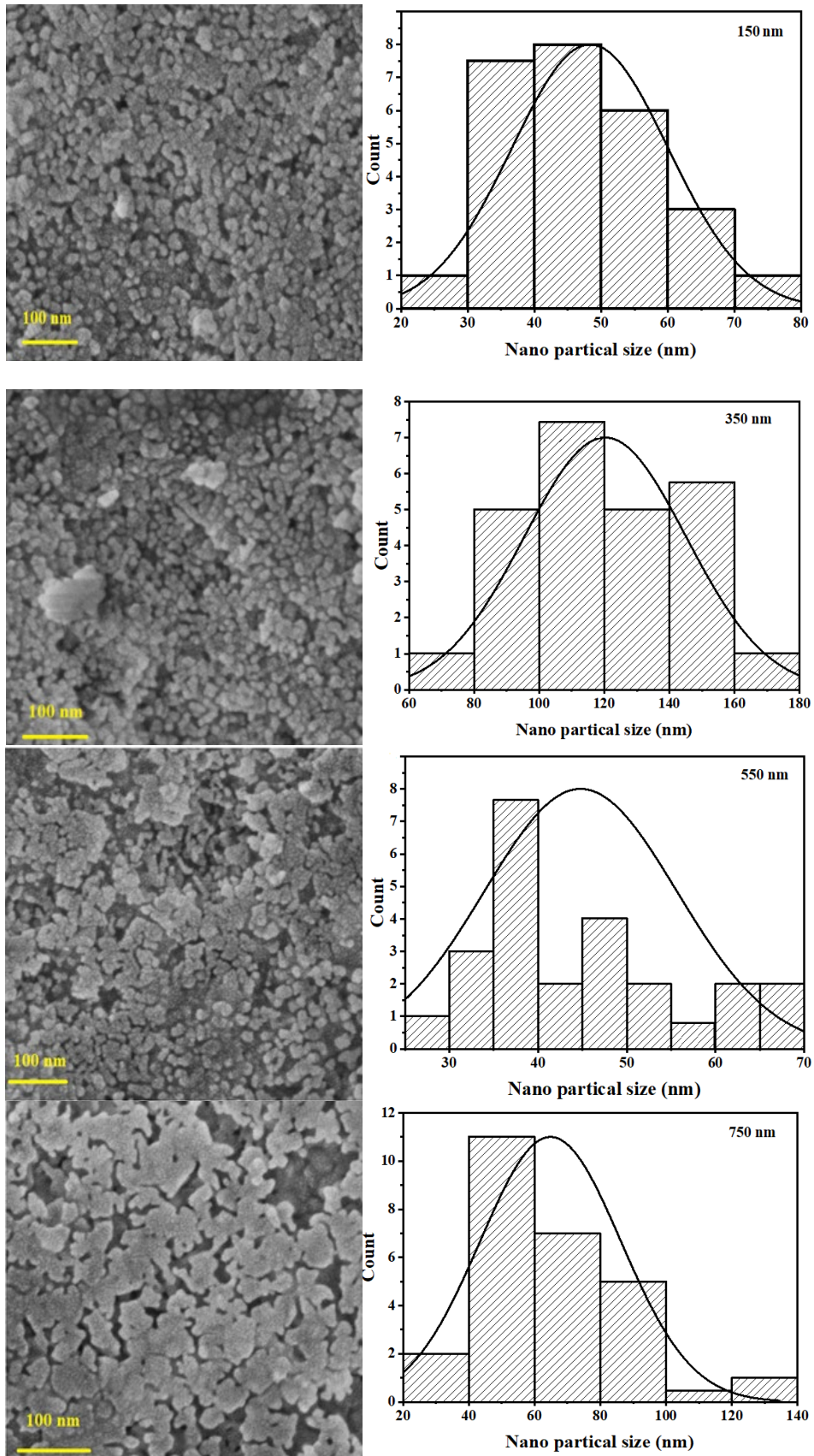


Fig. 2. FE:SEM for CdS: MgO films.

Fig.2 shows the transmittance spectrum of CdS: MgO films at different thicknesses (150, 350, 550, and 750 nm), the CdS: MgO films show a decrease in the transmittance with increasing thickness of films, and a redshift in the absorption edge of the spectra, which is due to the increase in the absorption path length and the scattering of photons by the film, and photons have enough energy in this region to excite electrons from the valence band to the conduction band. As a result, photons are absorbed by the thin film material, which is a characteristic feature of semiconducting materials [21, 22], This decrease in transmittance is due to the absorption of photons by the CdS: MgO films [23], which results in the promotion of electrons from the valence band to the conduction band, The energy required for this process is determined by the bandgap energy of the CdS: MgO films, which can be estimated from the absorption edge of the transmittance spectra [24,25]. This is supported by researchers Alqahtani and Liu [26,27]. Fig. 2 shows the reflectance spectra of CdS: MgO films show a gradual increase in reflectance with increasing wavelength, This increase in reflectance is due to the interference of light waves reflected from the top and bottom surfaces of the thin film, which results in constructive interference at certain wavelengths and destructive interference at others [28,29], the reflectance spectra of CdS: MgO thin films can also provide information about the electronic and structural properties of the films. the presence of defects, impurities, or surface roughness can lead to changes in the reflectance spectra and affect the overall optical properties of the thin films [30].

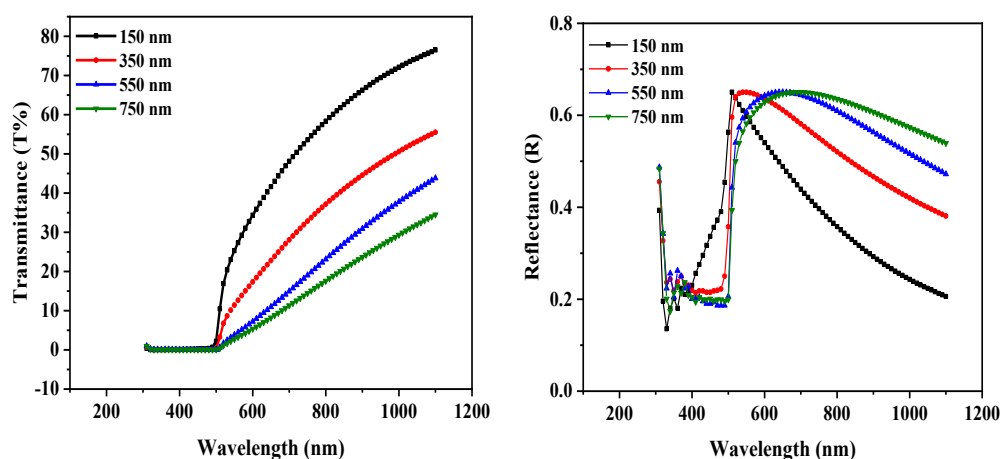


Fig. 3. Transmittance and reflectance for CdS: MgO films.

The absorption coefficient ( $\alpha$ ) calculate by [31]:

$$\alpha = 2.303A/t \quad (1)$$

When the absorption coefficient is very large ( $>104 \text{ cm}^{-1}$ ), it indicates that the allowed direct electronic transitions occur [31]. The energy gap was calculated by equation [32]:

$$(\alpha h\nu) = A(h\nu - E_g)^r \quad (2)$$

For CdS: MgO films the bandgap energy can be modified by changing the thickness of the film, When the film thickness decreases, the energy levels become quantized and discrete, increasing the bandgap energy in the range of (2.412-2.354) eV [31], This is supported by researchers Akaltun and Essahlaoui [34,35] as shown in fig. 3.

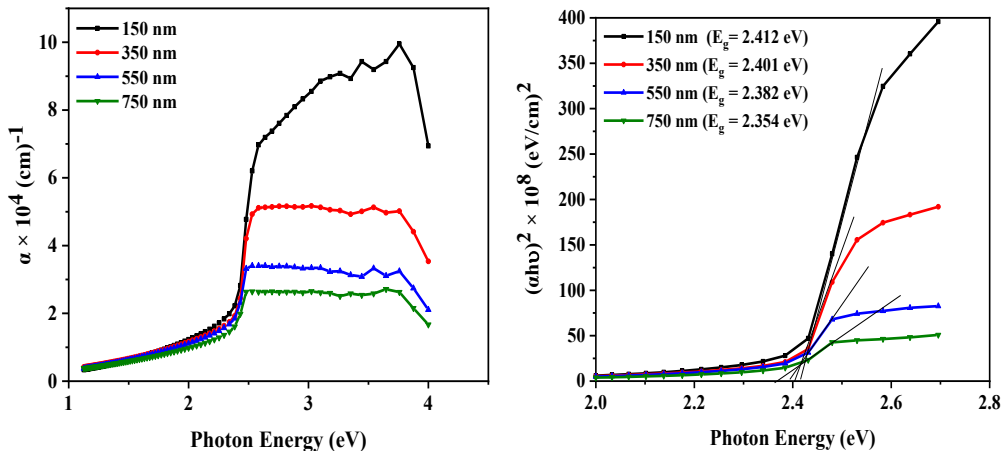


Fig. 3. Absorption coefficient and energy gap for CdS: MgO films.

The refractive index and extinction coefficient ( $k_0$ ) calculate by eq.(3.4) [36,37]:

$$n_o = \left[ \left( \frac{1+R}{1-R} \right)^2 - (K_o^2 + 1) \right]^{1/2} + \frac{1+R}{1-R} \tag{3}$$

$$k_o = \frac{\alpha\lambda}{4\pi} \tag{4}$$

For CdS: MgO films, the refractive index can change significantly as the thickness of the film is varied, This is because the refractive index of CdS: MgO is dependent on the electronic and optical properties of the material, which can vary with the thickness of the film [38], the refractive index of CdS: MgO thin films is a complex function of many different factors, including the thickness of the film, Understanding the relationship between the thickness of the film and the refractive index is important for many applications, such as optical coatings, solar cells, and other optoelectronic devices[39].

The extinction coefficient (also known as the absorption coefficient) for thin films is known to be affected by the thickness of the film. The extinction coefficient is a measure of how much light is absorbed by a material [40]. For thin films, the thickness of the film can affect the extinction coefficient by the thickness of the film increases, the amount of light absorbed by the material also increases. This is because a thicker film allows more light to penetrate and interact with the material, resulting in a greater amount of absorption [41,42], as shown in Fig. 3. Table 1. Shows the optical Properties of CdS: MgO films (150, 350, 550, and 750 nm).

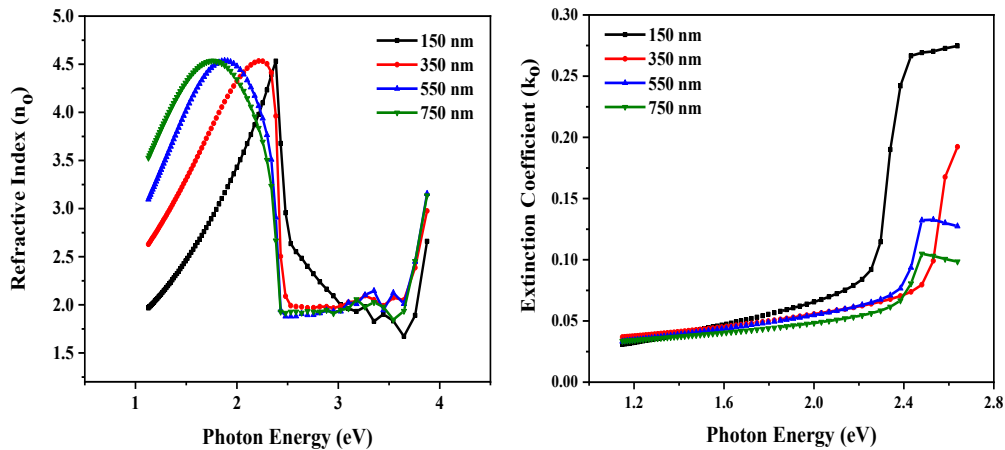


Fig. 4. Refractive index and extinction coefficient for CdS: MgO films.



Table 1. Optical properties of CdS: MgO films.

Thickness (nm)	E <sub>g</sub> (eV)	( $\alpha \times 10^4 \text{ cm}^{-1}$ ) Maximum	(n <sub>o</sub> ) Maximum	(k <sub>o</sub> ) Maximum
150	2.412	9.919	4.517	0.274
350	2.401	5.129	4.544	0.191
550	2.382	3.302	4.535	0.134
750	2.354	2.695	4.534	0.104

The Hall coefficient is the ratio of the transverse electric field to the applied magnetic field. the thickness of the film can have a significant impact on the Hall coefficient [43,44], This is because the thickness of the film can affect the carrier concentration and mobility of the charge carriers within the film, As the thickness of the film decreases, the carrier concentration may also decrease due to the reduced volume of the material. Additionally, the surface-to-volume ratio of the film may increase, which can lead to increased scattering of the charge carriers at the surface, thereby decreasing the mobility of the carriers, and this can lead to a decrease in the Hall coefficient [45], as shown in Table 2.

Table 2. Hall coefficient and electrical parameters of CdS: MgO films.

Thickness (nm)	Concentration (cm) <sup>-3</sup>	Hall Coefficient Rh(m <sup>2</sup> /C)	Conductivity (Ω.cm) <sup>-1</sup>	Resistivity (Ω.cm)	Mobility (cm <sup>2</sup> /v.s)
150	2.584x10 <sup>6</sup>	2.416x10 <sup>7</sup>	1.035x10 <sup>-5</sup>	9.662x10 <sup>4</sup>	2.500x10 <sup>2</sup>
350	4.325x10 <sup>7</sup>	-2.886x10 <sup>6</sup>	5.337x10 <sup>-7</sup>	1.874x10 <sup>7</sup>	1.540x10 <sup>1</sup>
550	4.953x10 <sup>6</sup>	-3.781x10 <sup>7</sup>	1.309x10 <sup>-5</sup>	7.638x10 <sup>4</sup>	4.950x10 <sup>2</sup>
750	1.228x10 <sup>7</sup>	-2.034x10 <sup>7</sup>	3.369x10 <sup>-6</sup>	2.968x10 <sup>5</sup>	6.852x10 <sup>1</sup>

#### 4. Conclusions

The article explores the relationship between the thickness of CdS: MgO thin films and their structural, optical, and electrical properties by using a chemical spray pyrolysis technique to deposit films. The study found that the crystal size of CdS: MgO becomes higher with increasing the film's thickness, the optical transmittance of the films decreased with the increase in the thickness ranging from (150, 350, 550, and 750 nm), and the bandgap energy of the films decreased with the increase in the thickness, as it was (2.412 eV) for the thickness (150 nm) and (2.354 eV) for the thickness (750 nm), the study suggests that the thickness of CdS: MgO thin films has a significant impact on their physical properties, which could have important implications for their use in solar cells and optoelectronic device applications.

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