

Energy band gaps and optical absorption properties of the CdZnS and CdZnS:PEO thin films prepared by chemical bath deposition

M. A. Hussein^a, K. A. Mohammed^{b,*}, R. A. Talib^c

^aPhysics, Physics in materials, Ministry of Education, Baghdad, Iraq

^bDepartment of Medical Physics, Hilla University College, Babylon, Iraq

^cPolymer research center, University of Basrah, Basra, Iraq

The optical characteristics of (CdZnS) and (CdZnS:PEO) nanofilms made by the chemical bath deposition technique were examined in the current paper. The films displayed an typical transmission of 65-90% ranging between 500-900 nm. Transmission touched the 90% for wavelength of 600 nm and above. The bandgap energy of CdZnS film was 3eV and was found to be increased to 3.1 eV after using poly ethylen oxide (PEO). All of these results show that PEO can make CdZnS film better. The better transmission of the prepared films also shows that the method described is good for making CdZnS thin films for solar cells.

(Received January 13, 2022; Accepted May 5, 2022)

Keywords: CdZnS, Thin films, Optical properties, CBD

1. Introduction

Because of their widespread application in the construction of photovoltaic and solar cells and optoelectronics equipment, Chalcogenide II-VI semiconductors have caught the attentions of researchers and scientists [1,2]. When it comes to II-VI semiconductor materials, zinc and cadmium chalcogenides are the most important members since they exhibit direct energy gaps of 3.6 and 2.42 eV when measured at room temperature. [3].

CdS is a semiconductor and colored in yellow, working in commerce as a yellow dye, in acid solution, it dissolves readily, but not in water; it is also thermally stable and chemically stable [4]. Single crystals, thin films, nanoparticles, and nanowires have all been produced from CdS. Cubic and hexagonal phases of CdS can be distinguished by their crystalline structures [5]. The use of a dopant may contribute to enhance the electrical and optical properties of the CdS used for this particular application. One of the most investigated and doped elements is zinc (Zn), which can be found in a variety of Cd_{1-x}Zn_xS combinations with varying compositions [6]. Due to its high optical transmittance and smaller ionic radius than Cd ($r_{Zn^{2+}} < r_{Cd^{2+}} = 0.074$ nm), Zn is considered to be more significant than the other dopants in semiconductors [7]. Depending on the concentration, the energy gap of the Cd_xZn_{1-x}S II-VI semiconductor varies between 2.42 eV for CdS and 3.70 eV for ZnS [8,9]. It has been widely reported that Cadmium Zinc Sulfide (CdZnS) nanoparticles, which are produced with an acceptable Cd:Zn ratio, are capable of forming large band gap semiconductors for the construction of heterojunction thin films solar cell [10,11].

With the purpose of create CdZnS thin film, a variety of thin-film deposition procedures such as "vacuum evaporation, spray pyrolysis, dip method, electrodeposition, chemical bath deposition (CBD), and SILAR" have been utilized, among others [12-16]. CBD is largely regarded as the preferred approach for synthesizing CdZnS thin films among the several deposition processes available. The approach is basically the simplest and most inexpensive method for producing a stable, uniform, and adherent hard film in the absence of a vacuum environment [17].

Polymer-based nanocomposite materials have recently piqued researchers' interest due to their ease of manufacture. Polymer nanocomposites can be regarded an optical environment because of low-dimensional nanomaterials. So, the nanocomposites may deliberated homogeneous optical environment under certain condition. It is believed that these conditions are

Corresponding author: kahtan444@gmail.com

<https://doi.org/10.15251/CL.2022.195.329>

associated to the inner structure of polymer nanocomposites, as well as their monodispersity and uniform dispersion. This means that the optical properties of polymer nanocomposites, nanoparticles generated inside the polymer matrix, and pure nanomaterials are distinct from one another, with the nanoparticle concentration and their sizes playing a significant role in this distinction [18]. So, According to our knowledge the use of PEO as a matrix for preparing CdZnS:PEO nanocomposite thin films done for the first time and study their optical properties. In the present work, tailoring the optical properties of CdZnS thin film by using PEO as a capping agent .

2. Experimental work

The CdZnS film deposition process was based on our work published in ref [19]

CdZnS:PEO nanocomposite thin film was prepared in the same method and steps in [19] where 20 ml of 1% PEO added to zinc and cadmium precursors.

3. Results and discussions

It was discovered that the CdZnS films produced by this process were smooth, homogeneous in thickness, adherent, pinhole free, and bright yellow in color. Figure 1 depicts a FESEM micrograph of a CdZnS nanocrystalline thin film that has been freshly produced. In the photos, the CdZnS is arranged in a nanowalls structure, which represents the formation of the compound.

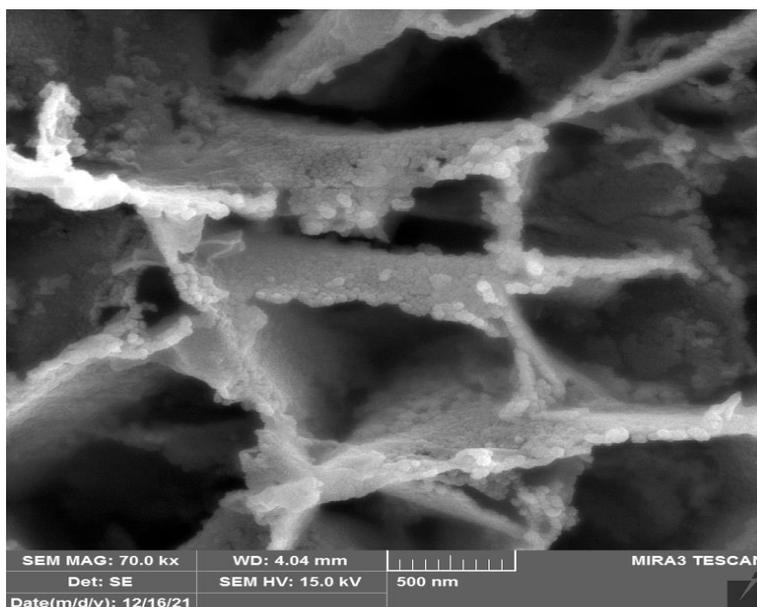


Fig. 1. FESEM images of CdZnS thin film.

The XRD pattern of CdZnS thin film was revealed in figure 2. Hexagonal-shaped XRD patterns of CdZnS ternary thin films are caused by scattering from "(002), (110) and (112)". The observed diffractions patterns are matching with the data of the typical JCPDS cards, which is as follow: 49-1302 [15]. It can be seen from the XRD pattern that the (002) reflections is most intense in the phase of hexagonal, which shows a general tendency for the caxis of the CdZnS nanocrystallites to be preferred perpendicular to the thin film surface in general. XRD analysis of the films revealed that they are constituted of fine crystallies or nano crystallites, as shown by the low intensity peaks detected in the pattern [16]. The peak at about $2\theta = 27^\circ$ and peak 44° fit to structure of wurtzite and approve the creation of CdZnS crystals, owning desired orientations along the (002) and (110) planes respectively. The peaks observed at 27° and at 44° corresponded

to the structure of wurtzite for CdZnS [18,3]. Table 1 demonstrates parameters collected from XRD of CdZnS film.

Table 1. the parameters collected from XRD for CdZnS thin film.

Pos. [$^{\circ}2\text{Th.}$]	Planes	Height [cts]	FWHM Left [$^{\circ}2\text{Th.}$]	d-spacing [\AA]
27.2384	002	336.07	0.7872	3.27407
44.8252	110	69.36	1.1808	2.02200
52.7901	112	40.08	1.1808	1.73417

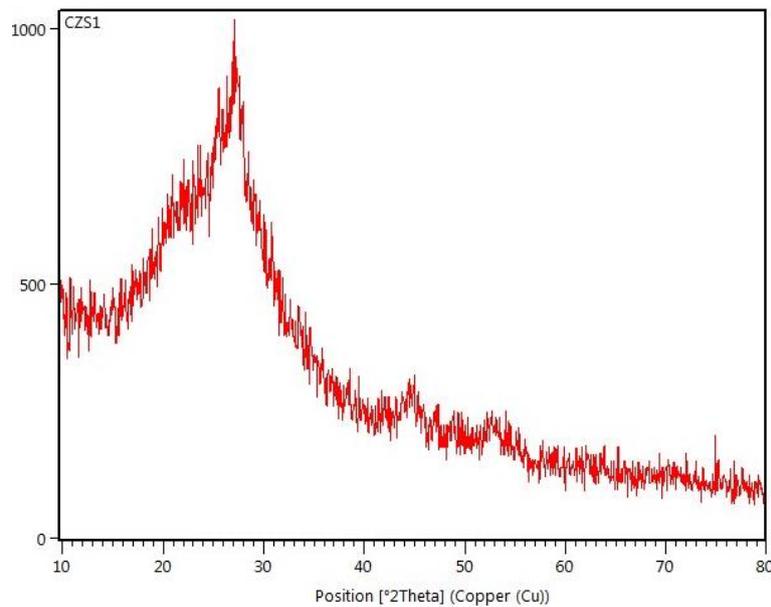


Fig. 2. XRD patterns of CdZnS film.

The optical properties of the CdZnS and CdZnS/PEO nanocomposite have been examined by determining the transmission and absorption spectra of prepared samples by UV–VIS spectrophotometer. All of the samples were tested at room temperature in the range of 300–1000 nm in wavelength. Fig. 3 designates the optical absorption spectrum of CdZnS and spectrum CdZnS:PEO thin films. Because of the quantum confinement effect on CdZnS band gap, the absorption edge of PEO as a capping agent is obviously blue shifted.

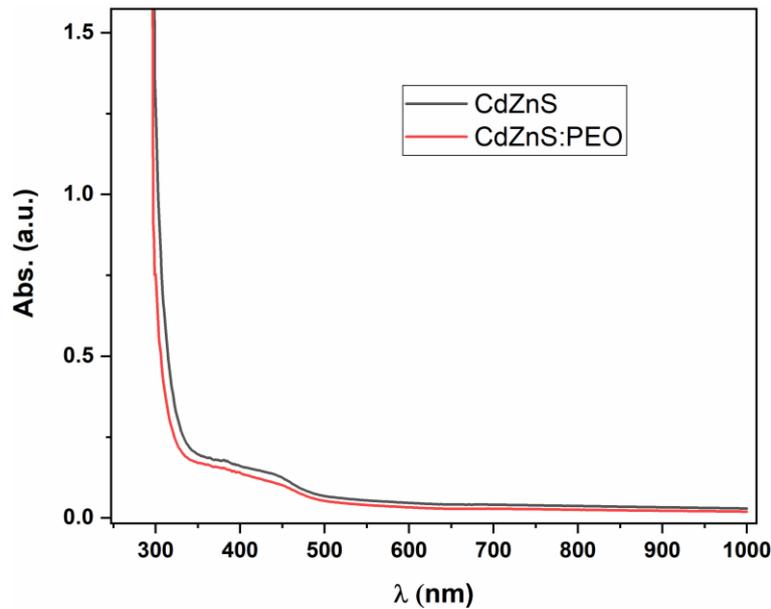


Fig. 3. UV-VIS absorption spectrum for CdZnS and CdZnS:PEO films.

The spectra of transmission for both CdZnS and CdZnS:PEO films were showed in Figure 3. It has been established that the transmission fluctuates between 65 and 90 percent in the visible area of the optical spectrum, which is between 350 and 900 nm in wavelength. PEO, used as a stabilizing agent in the process, increases the transparency of thin films, demonstrating the feasibility of using thin films as buffer layers in solar cells.

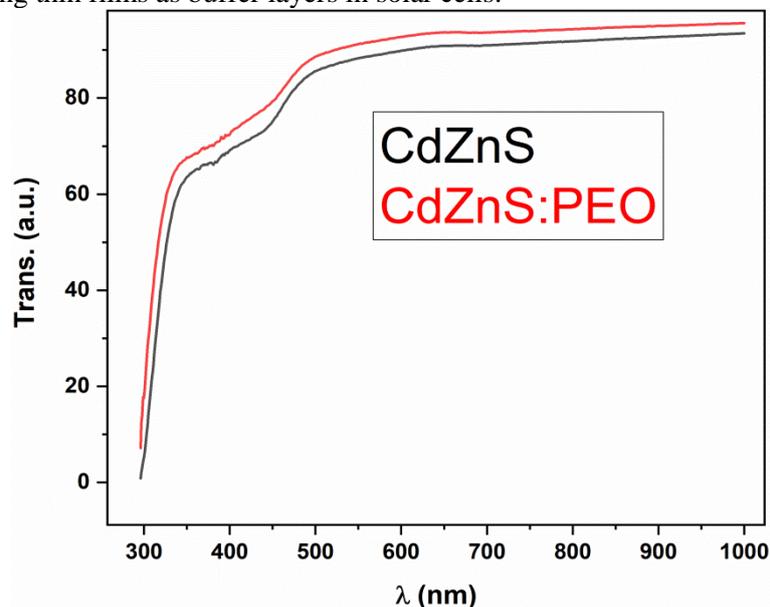


Fig. 4. UV-Visible transmission spectrum of CdZnS and CdZnS:PEO films.

Tauc's relation has been used to compute the optical energy gap (E_g) of CdZnS and CdZnS:PEO nanocrystalline films, and the results were promising. The creation of CdZnS compound was confirmed by an increase in the energy band gap when compared to the bandgap of CdS compound. As shown in figure 5, the band gaps energies for CdZnS and CdZnS:PEO nanocrystalline films were determined to be 3 eV and 3.1 eV, respectively, for the two materials. The band gap increased with the use of PEO [20]. It is possible that the natures of those

energy gaps variation makes it suited for use as a window material in the manufacturing of solar cell windows. As shown in fig. 6, the indirect band gap energies for CdZnS and CdZnS:PEO nanocrystalline films were found to be 2.2 eV and 2.3 eV, respectively, for the two materials.

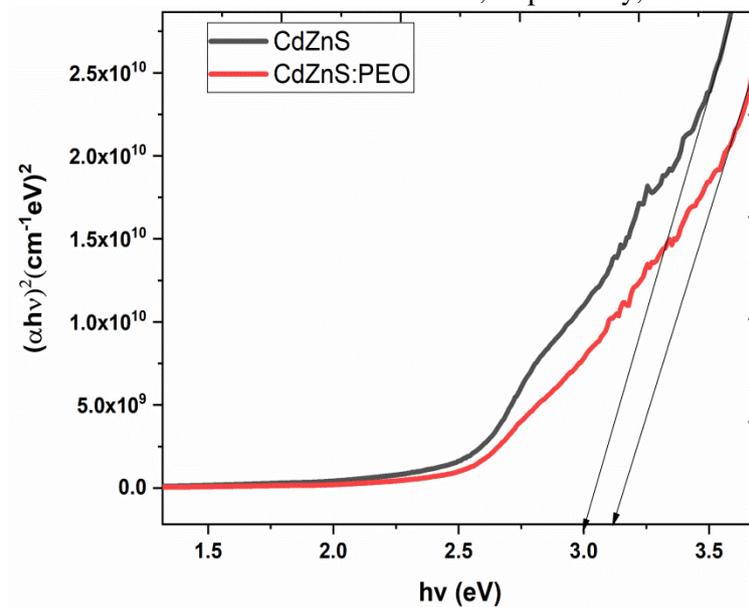


Fig. 5. the direct optical bandgap of CdZnS and CdZnS:PEO films.

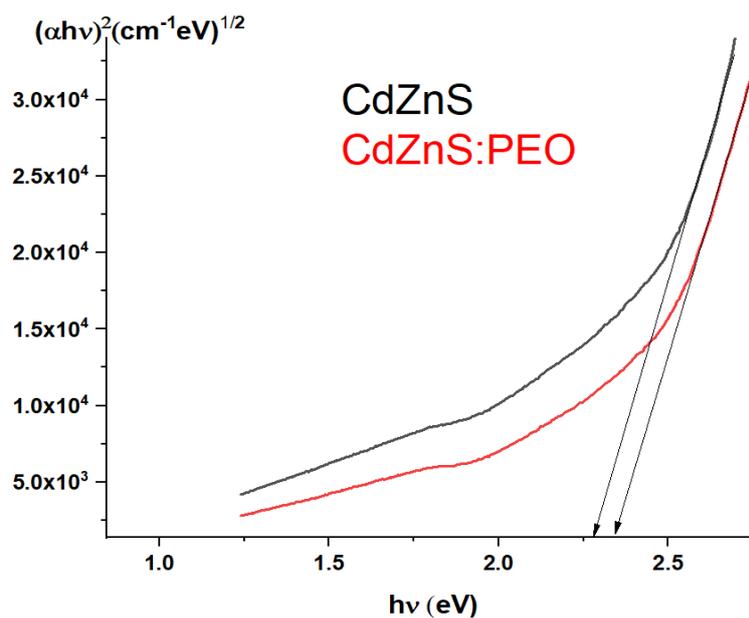


Fig. 6. indirect optical band gap of CdZnS and CdZnS:PEO films.

4. Conclusions

The CBD approach, which is simple and low-cost, has been used to create CdZnS thin films with a large surface area and high transmission. Transparent yellow CdZnS film were confirmed by X-ray diffraction. the effect of PEO presence for achieving greater transmission of the films for solar cell window applications. The films revealed an average transmission of 65-90% in 500-900 nm range. Transmittance reached in between 90% for wavelength of 600 nm and above. The direct Optical band gap increased from 3 eV to 3.1 eV in the presence of PEO. This

confirms the impact of PEO on CdZnS film in all of its findings. Moreover, the increased transparency of the films provides further evidence that the preparation approach reported here is acceptable for the depositing of CdZnS nanostructures for solar cell applications.

References

- [1] Ahilfi, D. N., Alkabbi, A. S., Mohammed, K. A., & Ziadanc, K. M. (2020, November). Fabrication and Characterization of polyaniline/CdSe Device for Applications in Nano Structured Solar Cells. In IOP Conference Series: Materials Science and Engineering (Vol. 928, No. 7, p. 072069). IOP Publishing; <https://doi.org/10.1088/1757-899X/928/7/072069>
- [2] Mohammeda, K. A., Hadib, M. M., Al-Kabbic, A. S., & Ziadanc, K. M. (2021). Effect of substrate type on the parameters of CdSe-TSC Schottky diode. Chalcogenide Letters, 18(7), 421-427.
- [3] Horoz, S., Akyol, M., Ekicibil, A., & Sahin, Ö. (2017). Structural, optical and magnetic properties of CdZnS and Ni: CdZnS nanoparticles. Journal of Materials Science: Materials in Electronics, 28(23), 18193-18199; <https://doi.org/10.1007/s10854-017-7765-x>
- [4] Baron, A. S., Mohammed, K. A., & Abood, M. M. (2021). The role of Ag layer in the optical properties of CdS thin film. Chalcogenide Letters, 18(10), 585-588.
- [5] Erturk, K., Isik, M., Terlemezoglu, M., & Gasanly, N. M. (2021). Optical and structural characteristics of electrodeposited Cd 1-xZnxS nanostructured thin films. Optical Materials, 114, 110966; <https://doi.org/10.1016/j.optmat.2021.110966>
- [6] Azizi, S., Dizaji, H. R., & Ehsani, M. H. (2016). Structural and optical properties of Cd1-xZnxS (x= 0, 0.4, 0.8 and 1) thin films prepared using the precursor obtained from microwave irradiation processes. Optik, 127(18), 7104-7114; <https://doi.org/10.1016/j.ijleo.2016.05.030>
- [7] Bairy, R., Jayarama, A., Kulkarni, S. D., Murari, M. S., & Vijeth, H. (2021). Improved nonlinear optical absorption mechanism and susceptibility ($\chi(3)$) of CdS nanostructured thin films: Role of zinc doping. Materials Science in Semiconductor Processing, 121, 105400; <https://doi.org/10.1016/j.mssp.2020.105400>
- [8] R.S. Mane, C.D. Lokhande, Review Chemical deposition method for metal chalcogenide thin, Materials Chemistry and Physics 65 (2000) pp 1-31; [https://doi.org/10.1016/S0254-0584\(00\)00217-0](https://doi.org/10.1016/S0254-0584(00)00217-0)
- [9] D. Xia, T. Caijuan, T. Rongzhe, L. Wei, F. Lianghuan, Zhang Jingquan, Wu Lili, and Lei Zhi, "Structural and optical properties of Cd_{0.8}Zn_{0.2}S thin films," Journal of Semiconductors, 32 (2) (2011) pp 022003(1-4); <https://doi.org/10.1088/1674-4926/32/2/022003>
- [10] . S.Y. Kim, D.S. Kim, B.T. Ahn, H.B. Im, J. Mater. Sci. 4, 178 (1993); <https://doi.org/10.1007/BF00180470>
- [11] K.W. Mitchell, A.L. Fahrenbruch, R.H. Bube, J. Appl. Phys. 48, 4365 (1977); <https://doi.org/10.1063/1.323429>
- [12]. Burton LC, Hench TL (1976) Zn_x Cd_{1-x}S films for use in heterojunction solar cells. Appl Phys Letters 29: 612-614; <https://doi.org/10.1063/1.89162>
- [13]. Yamaguchi T, Yamamoto Y, Tanaka T, Demizu Y, Yoshida A (1996) (Cd,Zn)S thin films prepared by chemical bath deposition for photovoltaic devices. Thin Solid Films 281-282, 375-378; [https://doi.org/10.1016/0040-6090\(96\)08624-5](https://doi.org/10.1016/0040-6090(96)08624-5)
- [14]. Zhou J, Wu X, Teeter G, To B, Yan Y, et al. (2004) CBD-Cd_{1-x}Zn_x S thin films and their application in CdTe solar cells. Basic Solid State Phys 241: 775-778; <https://doi.org/10.1002/pssb.200304218>
- [15]. Gaewdang N, Gaewdang T (2005) Investigations on chemically deposited Cd_{1-x}Zn_x S thin films with low Zn content. Mater Letters 59: 3577-3584; <https://doi.org/10.1016/j.matlet.2005.06.031>
- [16] . Valkonen MP, Kannianen T, Lindroos S, Leskela M, Rauhala E (1997) Growth of ZnS, CdS and multilayer ZnS/CdS thin films by SILAR technique. Appl Surf Science 115: 386-392; [https://doi.org/10.1016/S0169-4332\(97\)00008-1](https://doi.org/10.1016/S0169-4332(97)00008-1)

- [17] Akhanda, S., Matin, R., Bashar, M., Kowsar, A., & Rahaman, M. (2017). Experimental Study on Structural, Optical and Electrical Properties of Chemical Bath Deposited CdZnS Thin Films. *J Fundam Renewable Energy Appl* 7: 222. doi: 10.4172/20904541.1000222 Volume 7 Issue 1 Page 2 of 3 *J Fundam Renewable Energy Appl*, an open access journal ISSN: 2090-4541 Figure 1: XRD images of CdZnS thin films. Figure.
- [18] Muradov, M. B., Gahramanli, L. R., Balayeva, O. O., Nasibov, I. N., Eyvazova, G. M., Amiraslanov, I. R., & Aghamaliyev, Z. A. (2020). Formation mechanism of $Cd_xZn_{1-x}S/PVA$ nanocomposites by SILAR method. *Results in Physics*, 18, 103280; <https://doi.org/10.1016/j.rinp.2020.103280>
- [19] Hadi M. M. and Mohammed K. A. (2022). Investigation of the role of annealing time in the optical, structural and morphological properties of ternary CdZnS thin films prepared by chemical bath deposition. *Chalcogenide Letters*, 19(4), 277 – 283.
- [20] Chavhan, S., & Sharma, R. P. (2005). Growth, structural and optical transport properties of nanocrystal $Zn_{1-x}Cd_xS$ thin films deposited by solution growth technique (SGT) for photosensor applications. *Journal of physics and chemistry of solids*, 66(10), 1721-1726; <https://doi.org/10.1016/j.jpcs.2005.07.009>