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Thermally Evaporated CdTe Films with Various Thicknesses for Optoelectronics Applications

Hanan Salim Hadi[1] **Khalid Haneen Abass[2]**

1College of Education for Pure Sciences, University of Babylon, hanansalim757@gmail.com , Babil, Hilla, Iraq
2College of Education for Pure Sciences, University of Babylon, pure.khalid.haneen@uobabylon.edu.iq , Babil, Hilla, Iraq

***Corresponding author email** pure.khalid.haneen@uobabylon.edu.iq

اغشية تيلورايد الكادميوم ذات الاسماك المختلفة المحضرة بواسطة التبخير الحراري للتطبيقات الالكترونات الضوئية

خالد حنين عباس[2] **حنان سالم هادي*[1]**

كلية التربية للعلوم الصرفة، جامعة بابل، hanansalim757@gmail.com ، بابل، حله، العراق

كلية التربية للعلوم الصرفة، جامعة بابل، pure.khalid.haneen@uobabylon.edu.iq، بابل، حله، العراق

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ABSTRACT

Background:

There are numerous optoelectronic uses for semiconductor thin films II-VI. One such substance that has proven effective is cadmium telluride (CdTe).

Materials and Methods:

CdTe thin films were created by thermally vaporizing the material under a high vacuum and depositing them on glass substrates with different thicknesses (72, 80, and 88 nm) by using thermal evaporation technique.

Results:

According to the results of the XRD test, the thermally evaporated CdTe films are polycrystalline and have a cubic structure. From (AFM) is used to evaluate the morphology of the film demonstrating the good homogenous surface. From (UV) incresed of thickness of the material resulted in a concurrent increase in absorbance and a decrease in transmittance. The values of the direct energy gap calculated from the Tauc relation decreased from (3.60) to (3.42) eV with increased thickness. The surface energy loss function (SELF) and volume energy loss function (VELF) incresed when thickness incresed. The structural tests and energy gap values refer to fine particle size and the surface of the prepared films and can be candidates for optoelectronic applications.

Conclusions:

The X-ray diffraction (XRD) analysis revealed that the CdTe films exhibited a polycrystalline nature, characterized by a cubic crystal structure. A noticeable enhancement in the crystal structure was noticed as the thickness increased. The clear result of the scanning electronic microscopy is that homogeneously distributed crystal grain morphology was observed. The inference of SEM is consistent with the result of the XRD measurement.

Keywords: CdTe, Vacuum deposition, Morphology, Crystallite size.

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INTRODUCTION

Within the present framework, thin-film technology emerges as a highly auspicious subject for the investigation of energy-efficient optoelectronics and renewable energy. From the perspective of device manufacturing, the technique offers a wide range of uses [1]. Cadmium telluride is a compound made of two elements-cadmium and tellurium [2]. It is commonly used as an II-VI semiconductor material in photovoltaic cells, which convert sunlight into electricity [3]. Cadmium telluride is a crucial material in the solar energy industry due to its high efficiency, low cost, and stability [4]. It is worth noting, however, that cadmium telluride is a toxic substance and must be handled with care during production and disposal to prevent harm to both humans and the environment [5].

The bandgap of cadmium telluride is around 1.4 electron volts (eV), which makes it suitable for absorbing solar radiation and converting it into electricity efficiently [6]. The high absorption coefficient (10^4 cm^{-1}) of the material in the visible and near IR region of the solar spectrum [7]. Furthermore, cadmium telluride is known for its high photoconductivity, meaning that it can conduct electricity when exposed to light. Cadmium telluride has a crystalline structure and is typically dark brown or black [8]. CdTe thin films are used in solar cells, LEDs, infrared photodetectors, and other optoelectronic devices. CdTe films can be deposited on glass, FTO, ITO, and others [9-11].

Due to its physical properties, thermal evaporation is a popular thin film production method. This method makes homogeneous CdTe films on many substrates easy to make. The method also yields high deposition and low contamination. Production is cheaper than high-end physical methods [12]. The objective of this study is to investigate the impact of deposition thickness on the structural and optical characteristics of CdTe thin films fabricated using thermal evaporation. We studied it with very small thicknesses, noting that these thicknesses have very small crystal sizes. They were studied in a nanoscale way, so we expect to obtain quantum dots. This work examined the link between deposition thickness and XRD, AFM, SEM, optical bandgap energy, extinction coefficients, and refractive index. The study also examined VELF and SELF in connection to tiny particle size.

EXPERIMENTAL

2.1 Purification of Cadmium Tellurium Nanofilms

The experimental setup utilized for the deposition of CdTe nanofilms on a glass substrate involved the utilization of a thermal evaporation system, namely the (Edward C-306 model). The chamber of this system was modified to achieve a very high vacuum condition. This configuration is seen in Figure 1. The molybdenum boat was fabricated using (99.9% pure CdTe powder) as source materials. The chamber underwent a process of evacuation, resulting in a pressure level of (10^{-7}) mbar. The spatial separation between the source and the substrate was estimated to be roughly (15 cm).

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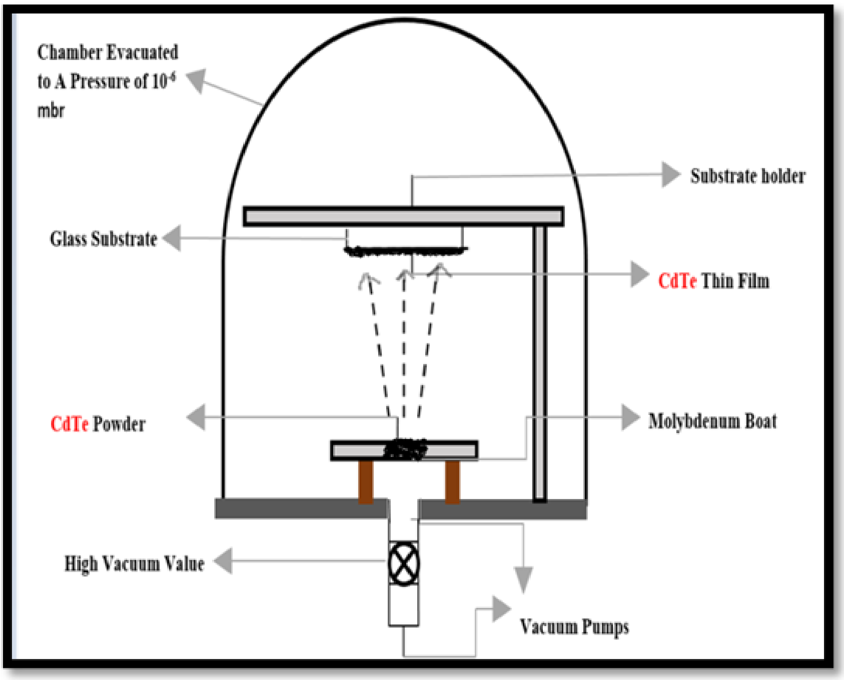

Fig 1. The schematic diagram of the thermal evaporation setup [12].

2.2 Descriptions

During the processing step, Cadmium Tellurium (CdTe) undergoes several thickness variations. The glass substrate was subjected to a cleaning procedure involving the use of distilled water and ethanol to effectively remove any surface contaminants. Following this, the substrate was allowed to completely dry. Following this, the substrate was securely attached to a substrate support. The sample was placed onto a Molybdenum boat using a thermal evaporation device, namely the Edward C-306 model. The determination of film thickness was conducted using two distinct methods: optical thin-film measuring utilizing the Lambda Limf-10) instrument, and the weight approach. The measurements acquired were (65, 72, and 80 nanometers. The investigation of the optical characteristics of the CdTe thin films was conducted using a (Shimadzu UV-1650 PC UV-Visible spectrophotometer) manufactured by Phillips in Japan. The transmission spectra of the thin films were measured in the wavelength range spanning from (200 to 1100 nm). The structure of the films was examined through the utilization of a SHIMADZU X-ray diffractometer system (XRD-6000) that was equipped with a Cukα source generating radiation with a wavelength of (λ = 1.5406 Å). The investigation of surface roughness was carried out with an Atomic Force Microscopy (AFM) device known as the (Aa3000 SPM).

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RESULTS AND DISCUSSION

The X-ray diffraction (XRD) patterns of as-deposited CdTe films with thicknesses of (72, 80, and 88 nm) were seen in Figures (2-4). These films were thermally evaporated. The X-ray diffraction pattern of as-deposited CdTe thin films exhibits diffraction peaks at (2θ) positions, as depicted in Figures (2-4). These peaks correspond to a well-indexed film thickness and indicate a prominent orientation along the (111) crystal plane. Additionally, there is an unidentified peak at 2θ less than 10o, which can be attributed to the presence of an extremely thin coating on the substrate. This thin coating hinders the X-ray resolution, preventing the penetration of the substrate and resulting in grazing of the sample. The angle exhibits a rightward shift, suggesting a diminutive crystallite dimension. The CdTe films, which were deposited using thermal evaporation, exhibited a polycrystalline structure characterized by a cubic phase.

The X-ray diffraction (XRD) patterns were employed to determine the size of the crystallite, along with other microstructural parameters. The determination of the crystallite size (D) was conducted using the Scherrer formula. The equation is formulated in the subsequent fashion [13]:

$$D = \frac{k\lambda}{cos\theta} \qquad (1)$$

In the given context, k represents a constant with a specific value of (0.9) λ denotes the wavelength of the X-ray, B represents the full width at half maximum (FWHM) peak intensity, and θ signifies Bragg's diffraction angle. The crystallite size determined using calculations, as presented in Table 1.

The comprehension of the correlation between the size of crystallites and the thickness of CdTe thin films holds significance in the context of enhancing the performance of photovoltaic solar cells constructed from this material. It has been found that the degree of crystallinity in thin films exhibits an upward trend as the film thickness increases [14].

The observed widening of diffraction peaks indicates the presence of nanocrystals, providing confirmation that the CdTe thin films were really generated within the nanocrystalline size range. The data in Table 1 demonstrates that when the film thickness grows from (72 to 88 nm), the crystallite size exhibits a range of (4.1484 to 10.1268 nm).

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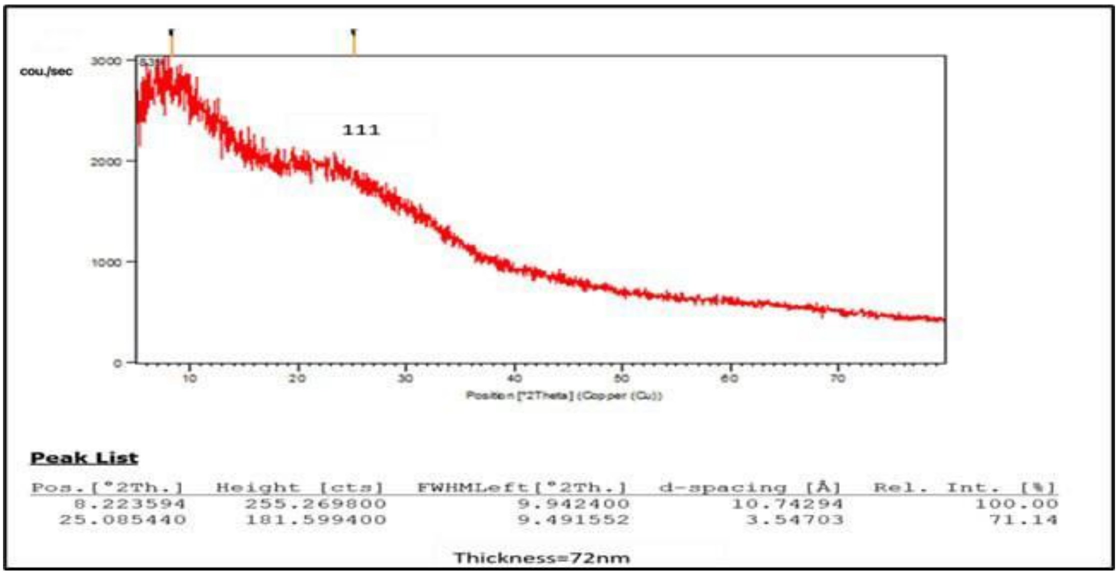

Fig 2. X-ray diffraction patterns of CdTe thin films with a thickness of 72 nm.

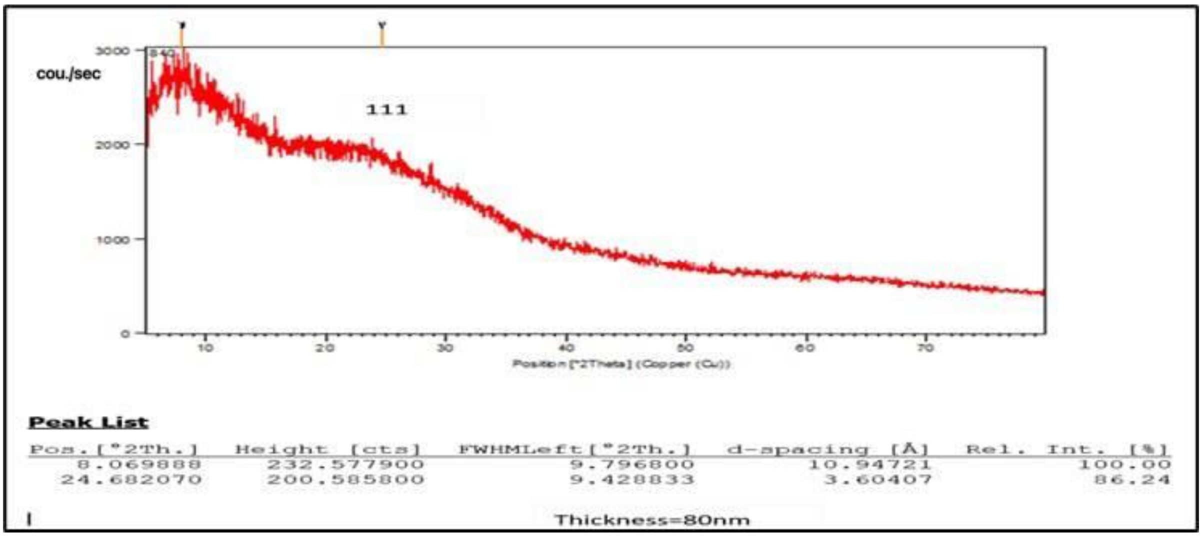

Fig 3. X-ray diffraction patterns of CdTe thin films with a thickness of 80 nm.

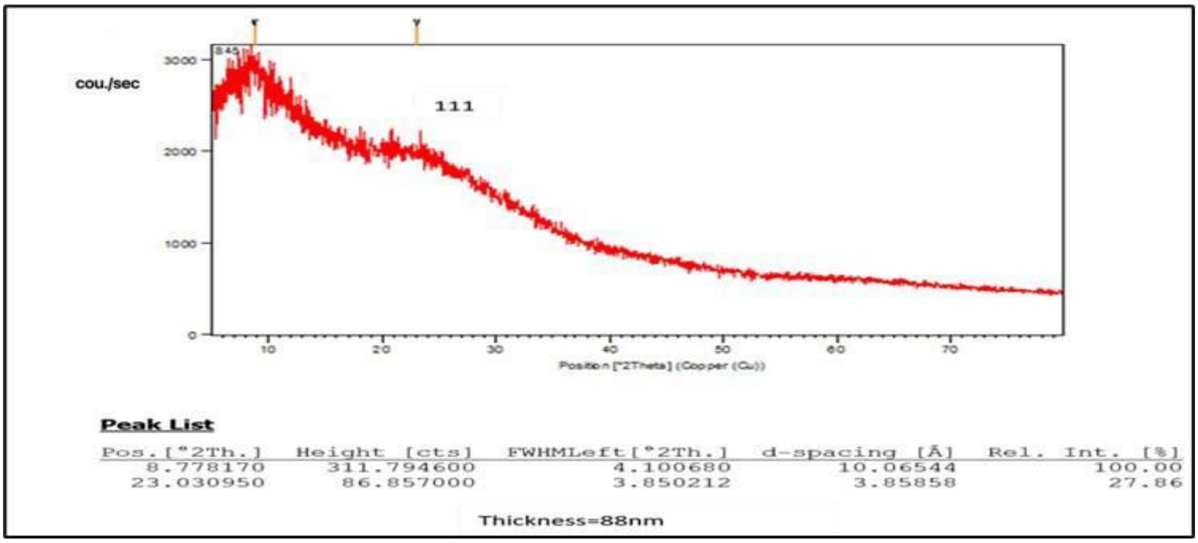

Fig 4. X-ray diffraction patterns of CdTe thin films with a thickness of 88 nm.

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Table 1. The values of crystallite size for CdTe thin films

Thickness (nm)	peak position (2θ°)	FWHM (2θ°)	D (nm)	The average crystallite size (nm)
72	25.085	9.4915	8.57863	4.1484
	8.223	9.9424	8.01498	
80	24.6821	9.4288	8.62899	4.19058
	8.069	9.7968	8.13332	
88	23.031	3.8502	21.0675	10.1268
	8.778	4.1006	19.4399	

3.1.2 Scanning Electronic Microscopy (SEM)

Scanning Electron Microscopy (SEM) is a powerful tool in the study of materials, providing high-resolution images and detailed information about the sample's surface [15] Scanning Electron Microscopy (SEM) analysis of CdTe thin film is an essential technique employed in material science to characterize the morphology and structure of materials.[16]

Fig. 5 (parts a, b, and c) displays the SEM images of CdTe films with various thicknesses. Due to aggregation and agglomeration of the grains, it can be noticed from images that grains deposited at lower thicknesses are smaller in size than those of greater thicknesses. It was possible to see the morphology of the uniformly scattered crystal grains. Due to the coalescence of atoms and molecules on the substrate surface, the films' improved crystallinity increases with film thickness. This conclusion is congruent with the XRD measurement's findings.

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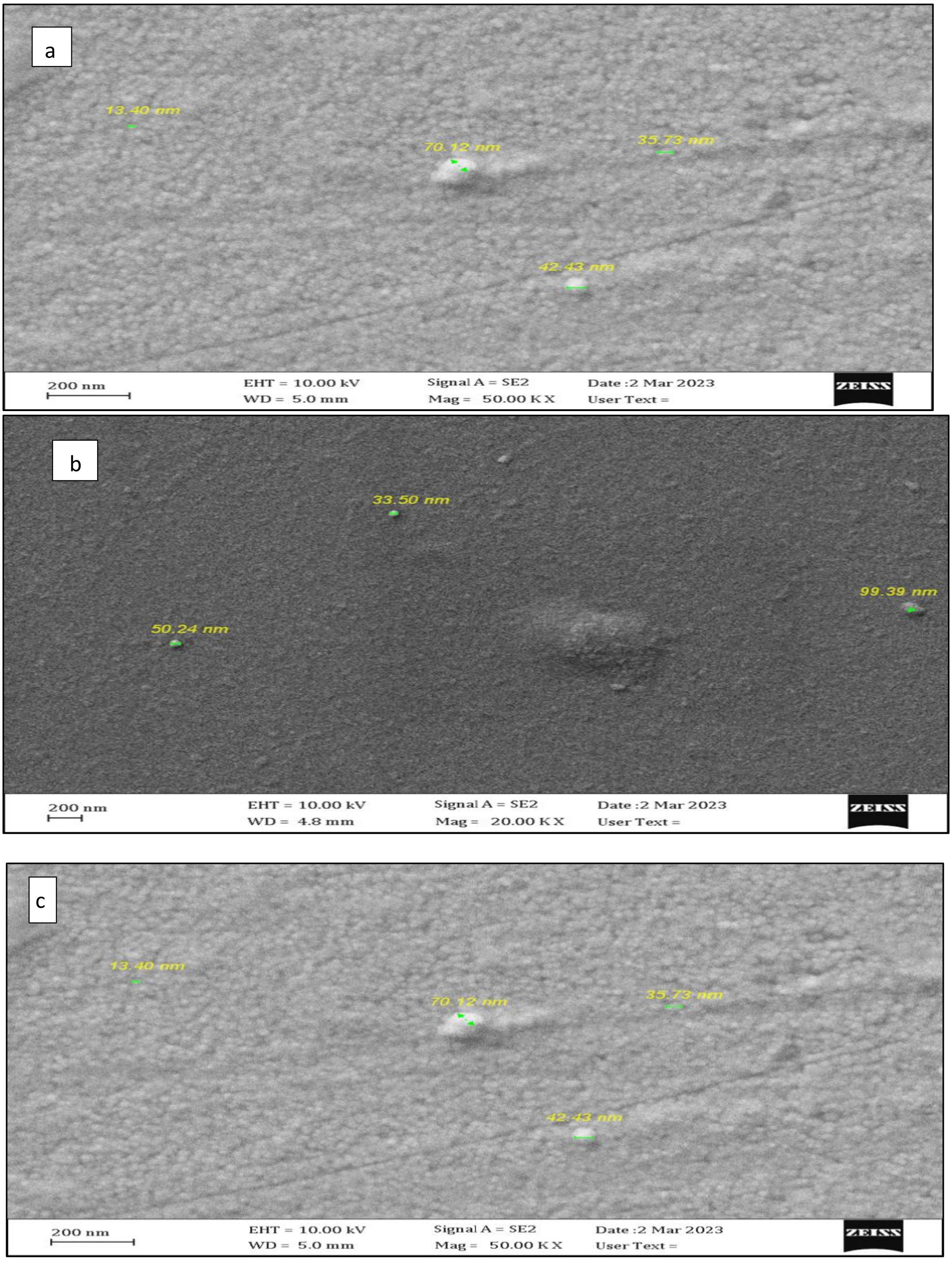

Fig 1. The SEM images of CdTe films with different thicknesses a) 65, (b) 72 nm, and (c) 88 nm.

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3.2.2 Atomic Force Microscopy (AFM)

Atomic Force Microscopy (AFM) is a form of scanning probe microscopy that use a diminutive probe to meticulously traverse the surface of a substance, thereby generating a comprehensive three-dimensional representation of its surface topography [17]. Atomic Force Microscopy (AFM) has been employed as a valuable tool for investigating the nanoscale surface topography and characteristics of Cadmium Telluride (CdTe) [18]. Figures 6-8 display the Atomic Force Microscopy (AFM) pictures of CdTe thin films with varying thicknesses, which were fabricated using the thermal evaporation approach. Every picture in the dataset includes images represented in two-dimensional (2D) and three-dimensional (3D) formats, as well as histograms depicting grain distribution and height distribution. The atomic force microscopy (AFM) pictures of the CdTe thin film exhibit a notable degree of surface homogeneity, as evidenced by the uniform distribution of crystalline granules. This homogeneity is further supported by the convergence of the roughness and root mean square (RMS) values, as presented in Table 2. The presence of white regions in the photos suggests the presence of stacked crystalline granules, implying that neighboring granules likely aggregate to create larger clusters. Hence, the surface shape of a thin film is significantly influenced by the extent of aggregation. The data presented in the figures indicates that the films exhibit a high level of homogeneity, as evidenced by the low values of roughness average (ranging from 0.425 to 0.244 nm) and root mean square (ranging from 0.549 to 0.312 nm). The surface roughness and root mean square (RMS) values exhibited a decrease as the thickness rose. The decreases can be attributed to the increment in grain-size particles of the thin film, resulting in a smoother surface. Recent research on thin films has yielded interesting findings regarding the relationship between film thickness and surface roughness (in the range of the critical thickness). In particular, it has been observed that as the thickness of the film increases, both the roughness and root mean square (RMS) value decrease [19]. This relationship is illustrated in Table (2), which shows a decrease in the RMS surface roughness value as the thickness of a CdTe thin film increases. This finding is consistent with other studies that report a similar trend between thin film thickness and surface roughness [20]. The ten-point height refers to the homogeneity of the film surface. The low values of the ten-point height indicated a smooth surface without cracks and pinholes. The values were decreased from 3.68 nm to 2.62 with increasing film thickness as listed in Table 2.

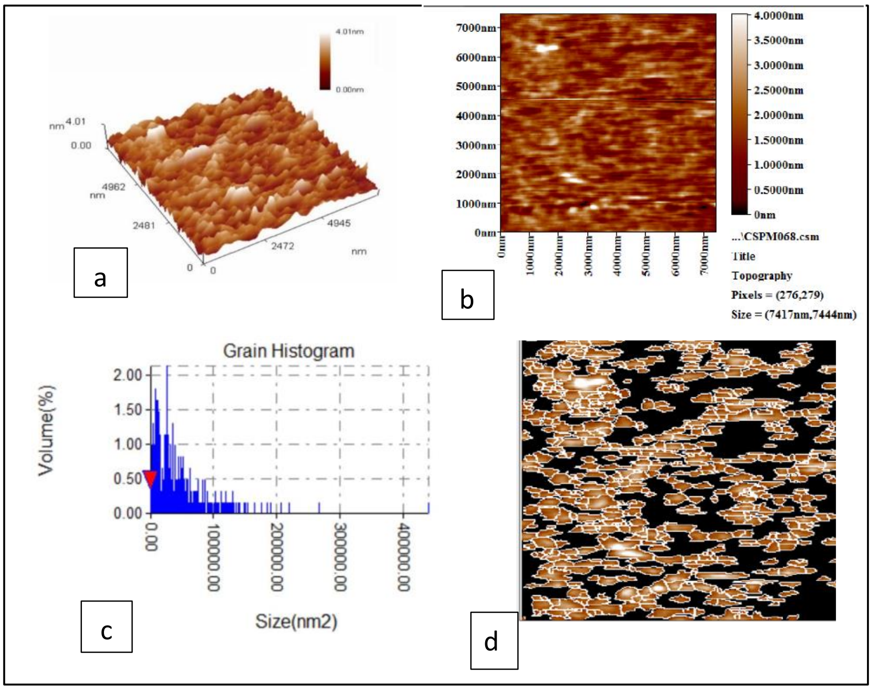

Fig 6. AFM images of CdTe thin films at thickness 72 nm of a) 2D, b) 3D, c) Histogram grain, and d) Height distribution

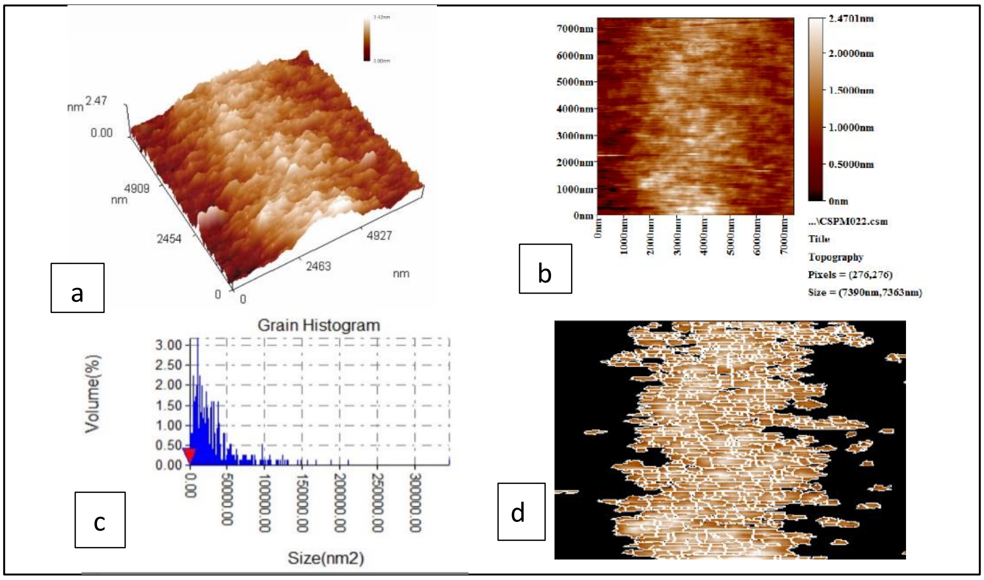

Fig 7. AFM images of CdTe thin films at a thickness of 80 nm of a) 2D, b) 3D, c) Histogram grain, and d) Height distribution.

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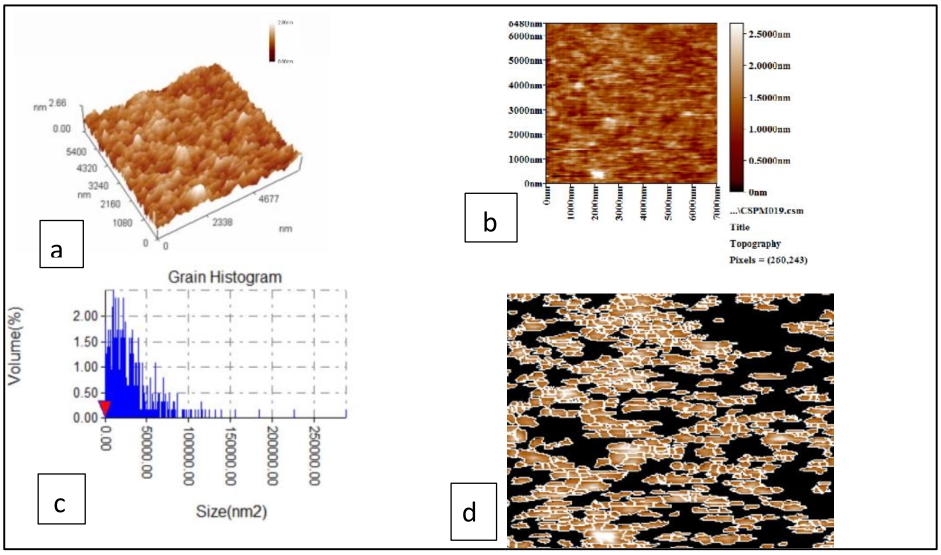

Fig 8. AFM images of CdTe thin films at thickness 88 nm of a) 2D, b) 3D, c) Histogram grain, and d) Height distribution.

Table 1. CdTe thin film thickness morphology.

Thickness (nm)	Roughness average (Sa) (nm)	Root mean square (Sq) (nm)	Ten point height (Sz) (nm)	Average diameter (nm)
72	0.425	0.549	3.68	231.5
80	0.369	0.451	2.38	200.1
88	0.244	0.312	2.62	198.2

3.2.3 Optical properties

CdTe films have received considerable attention due to their unique optical properties CdTe films that make them attractive for various optoelectronic device applications [21]. The behavior of electrons and the existence of imperfections in the films largely dictate the optical characteristics of the films. The thickness of the films can affect their optical properties due to the impact of crystal structure on the mobility of electrons. The spectra of optical absorbance were measured within the wavelength range between (200 to 1100 nm) .

Numerous factors, including the method of fabrication, the conditions of production, surface morphology, varying thicknesses, contact with the environment, etc., affect a material's optical properties. We investigated how the thickness of CdTe thin films affected their optical characteristics using a UV-Vis-NIR spectrophotometer. By examining the absorbance spectrum, one may determine the effect of CdTe thin film thickness on optical energy gaps (Eg), transmittance spectra, extinction coefficient (ko), real and imaginary dielectric constant (εr, εi) by evaluating absorbance range. The volume energy loss function (VELF) and surface

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energy loss function (SELF) was an important factor in the nanofilms to study the behavior of the very fine particles on the surface and the ability of these particles the interaction because of the free dangling bonds .

From Fig 9, it can be observed that the transmittance reduced with raising thickness in the CdTe films. It is important to take into account the transmittance of CdTe thin films when they are utilized in solar cells and optical devices. The thickness of CdTe thin films plays a critical role in determining their transmittance. Typically, the transmittance of thicker films is lower since they absorb more light. This results in a decrease in the overall amount of light that is transmitted through the film. One outcome that has been obtained is consistent with the discoveries made by scholars [22-24].

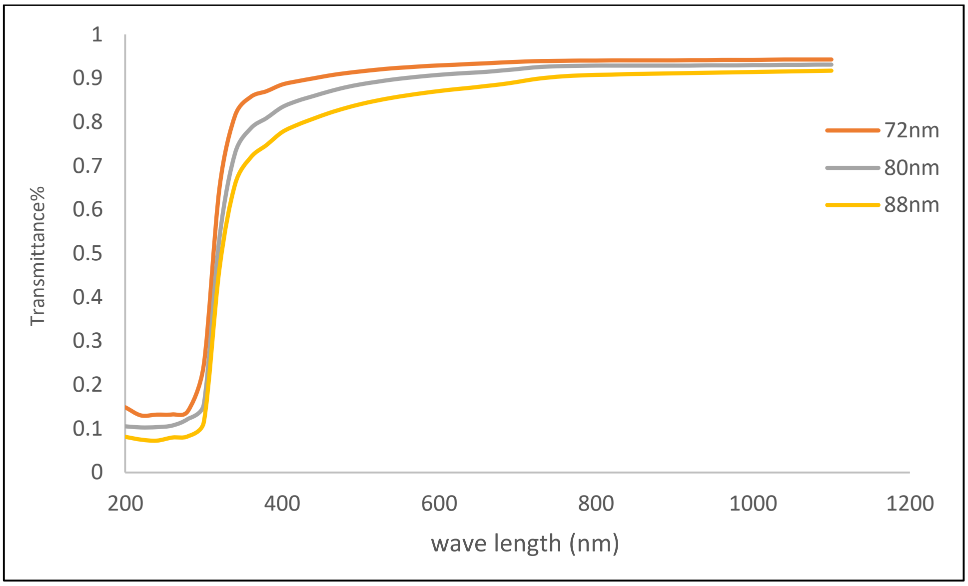

Fig 9. Transmittance versus of the wavelength of CdTe thin films with different thicknesses.

The wavelengths within the range of (200 to 1100 nm) were used to measure the optical absorbance spectra. The absorbance of these films increased as their thickness increased up to (1150 nm), as seen in Fig 10. The reduction in scattering loss due to improvements in crystallinity caused the absorbance to increase in correlation with the size of the CdTe films' crystallites. Previous studies have shown that the films have high absorbance in the near-infrared region [25,26].

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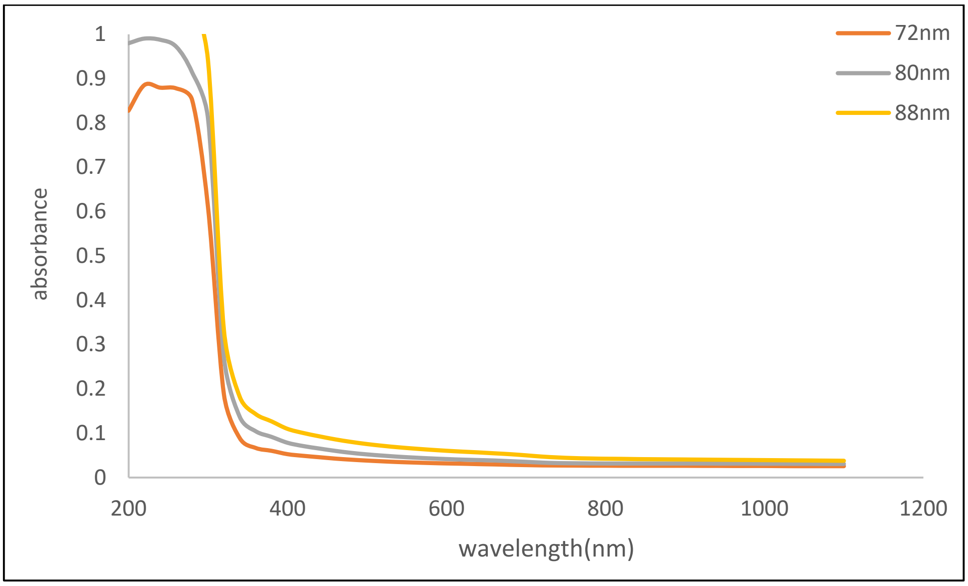

Fig 10. Absorbance spectra as a function of the wavelength of CdTe thin films with various thicknesses.

The absorbance spectra can be used to determine the absorption coefficient of the films using the formula [27]:

$$\alpha = \frac{2.303\,A}{t} \qquad (2)$$

where α: absorption coefficient, A: is the absorption, and t: is the thickness of the film.

By the Tauc equation, the optical energy gap (Eg) values of CdTe films created using the thermal evaporation process were calculated from the area of high absorption at these films basic absorption edge. The optical band gap of the films can be identified for direct band transition by examining the correlation between the absorption coefficient (α) and photon energy (hυ) as in the relationship (3):

$$\alpha h\nu = A\,(\,h\nu - E_g\,)^n \qquad (3)$$

The relation's value of n ($n = \frac{1}{2}$) for a direct transition and (n = 2) for an indirect transition determines the type of transition. In this instance, it was found that the plot of $(ahv)^2$ vs (hv) was linear, indicating that the bandgap is direct. By stretching the limiting of the chart to meet the x-axis, the value of the energy bandgap was determined.

It is obvious that as the film thickness increases, optical energy gaps of CdTe thin films grow smaller. The optical energy gap for CdTe thin films is reduced as a result of the vacancies' effect on the depth of donor levels, which is what is responsible for this. When the film thickness increased from (72 to 88 nm), the optical energy gap's value changed from (3.60 to 3.42 eV). The findings are displayed in Table (3). Fig. 11 shows the variation of the energy gap with the thickness.

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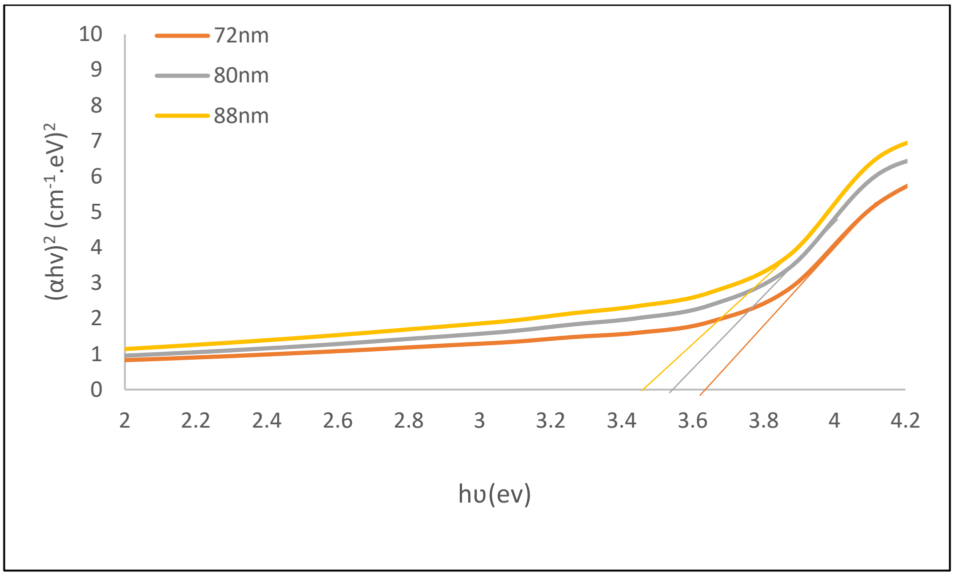

Fig 11. The allowed energy gap estimated from the relation between $(\alpha h\upsilon)^2$ and photon energy (hυ) of CdTe thin films with different thicknesses.

Table 2. The energy gap values of the permissible direct transition in CdTe thin films with varying thicknesses.

Thickness of CdTe	Optical energy gap (eV)
72	3.60
80	3.50
88	3.42

The difference of the extinction coefficient with film thickness is one of the most important factors to take into account in the creation of thin films. Understanding thin films' extinction coefficient is essential for improving their efficiency and improving their features for a variety of applications [28]. A thin film extinction coefficient tends to increase as its thickness increases also. the phenomenon may be explained by the reality that as thickness increases, the probability of photon interaction within the bulk material increases. Therefore, in order to produce thin films with appropriate optical and electrical characteristics to suit the requirements of certain applications, regulating the film thickness is important.

The connection was employed to ascertain the extinction coefficient of the CdTe thin films. [29] :

$$k_o = \alpha\lambda/4\pi \qquad (4)$$

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Figure 12 illustrates the relationship between the extinction coefficient and the thickness of the coating.

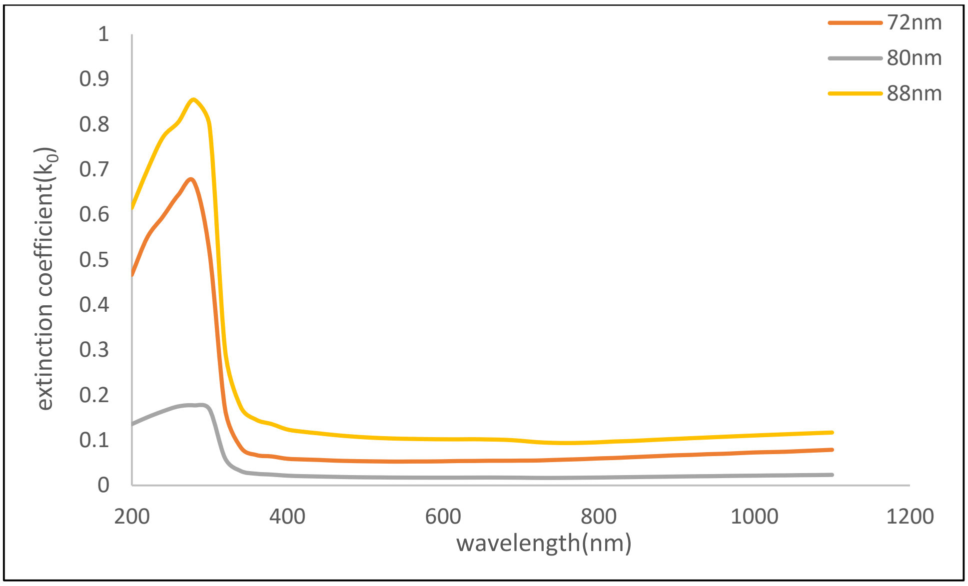

Fig 12. Extinction coefficient of CdTe thin films with different thicknesses vs wavelength.

From Fig. 13, The investigation focused on examining the connection amid the refractive index and the wavelength in thin films of CdTe with varying thickness. The findings indicated a positive correlation between the thickness and wavelength of the CdTe films and their refractive index (n). This phenomenon can be attributed to the rise in the quantity of atoms present in the films, along with the wavelength-dependent characteristics of the material's optical properties. The films had a notable wavelength-dependent refractive index in the near-infrared region, consistent with the observations made by previous researchers [29]. The refractive index (n) for CdTe thin films is determined by using the equation [30]:

$$n = \frac{(R+1)}{(R-1)} + \left(\frac{4R}{(1-R)^2} - k^2\right)^{1/2} \qquad (5)$$

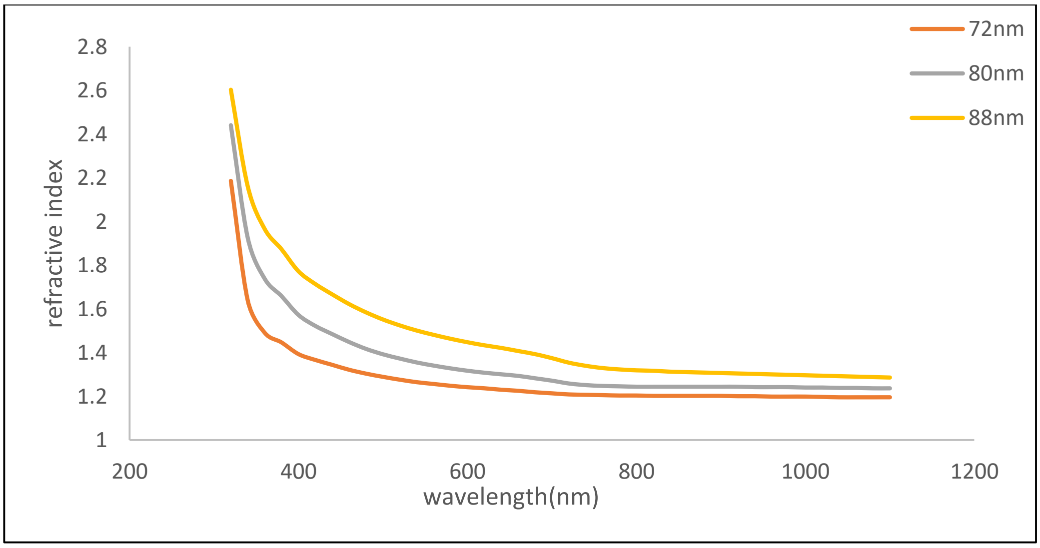

Fig 13. Refractive index of CdTe thin films with different thicknesses vs wavelength.

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The real ($\mathcal{E}_r$) and imaginary ($\mathcal{E}_i$) parts of the dielectric constant of CdTe films were determined by using the equations [31]:

$$\mathcal{E}_r = n^2 - k^2 \quad (6)$$

$$\mathcal{E}_i = 2nk \quad (7)$$

Figures 14 and 15 show the connection between the real and imaginary dielectric constants of CdTe nanofilms with different thicknesses. It is clear from the figures that the $\mathcal{E}_r$ and $\mathcal{E}_i$ values increase as the thickness increased.

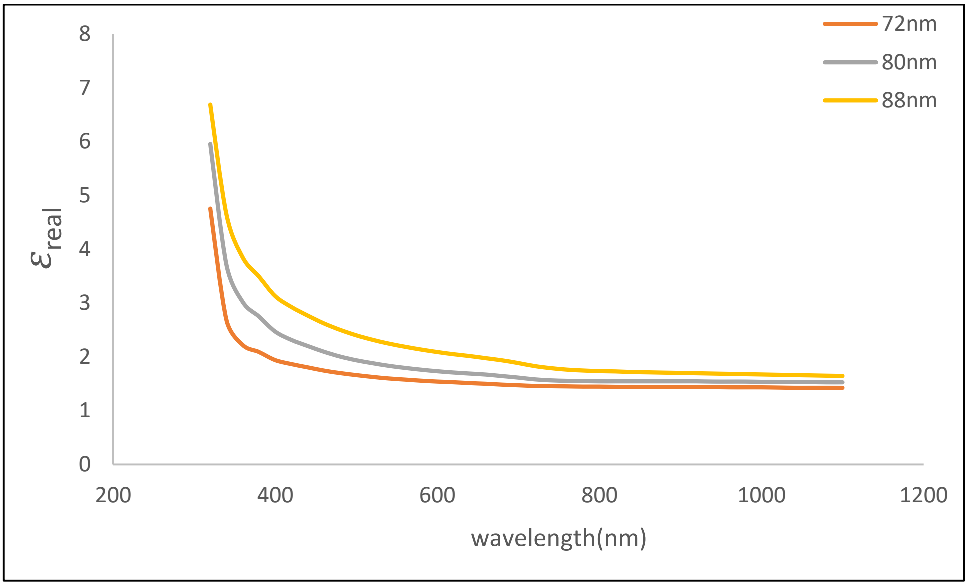

Fig 14. CdTe thin film thickness-dependent constant dielectric real.

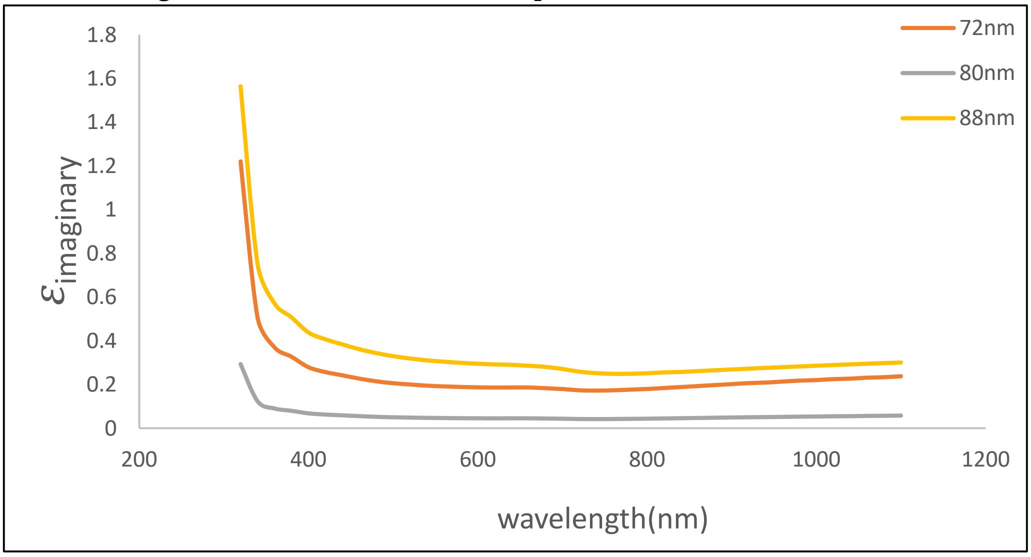

Fig 15. Imaginary dielectric constants of CdTe thin films with different thicknesses vs. wavelength.

The function of energy loss is a crucial element that may be used to illustrate the optical transitions of electrons in thin-film materials. According to the absorption energy, many or solitary free-carrier transitions through the material can be used to explain the energy loss process. These single or multiple carriers lose the light energy they have absorbed either

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through the volume or the surface of the material. The corresponding energy loss is referred to as (ELF) and is divided into surface energy (SELF) and volume energy loss function (VELF). The SELF and VELF are obtained from the complex dielectric constants given by [32]:

$$\text{SELF} = \frac{\varepsilon_r}{(\varepsilon_r + 1)^2 + \varepsilon_i^2} \quad (8)$$

$$\text{VELF} = \frac{\varepsilon_i}{\varepsilon_r^2 + \varepsilon_i^2} \quad (9)$$

The figures presented in Figures 16 and 17 illustrate the relationship between wavelength and the behavior of CdTe thin films. Based on the data acquired, it is evident that both the SELF and VELF exhibited an increase as the thickness rose. The findings indicate that the manufactured films exhibit sub-critical thickness, resulting in optimal film characteristics. Additionally, the films demonstrate layer-by-layer growth with a highly homogeneous surface.

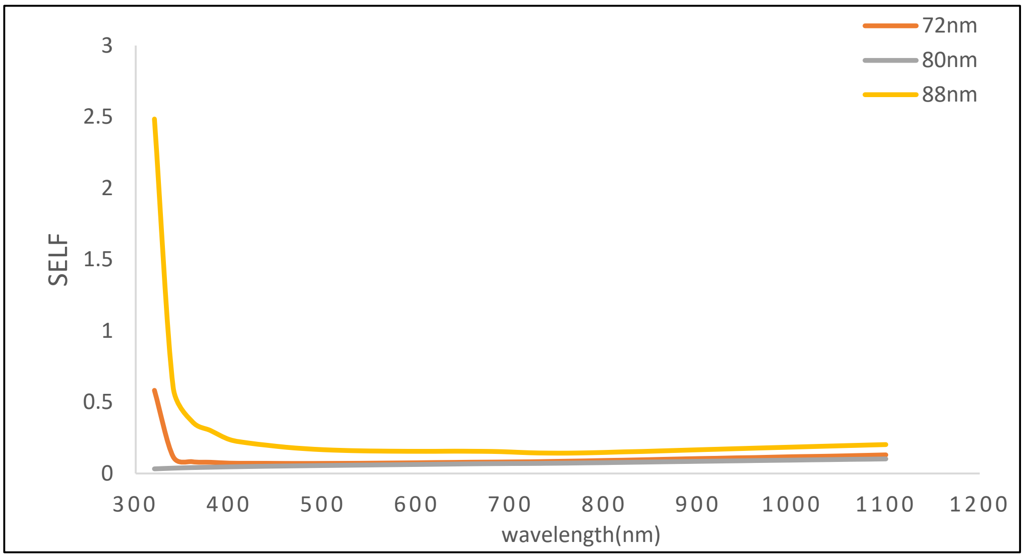

Fig 16. Surface energy loss function versus the wavelength of CdTe thin films (SELF).

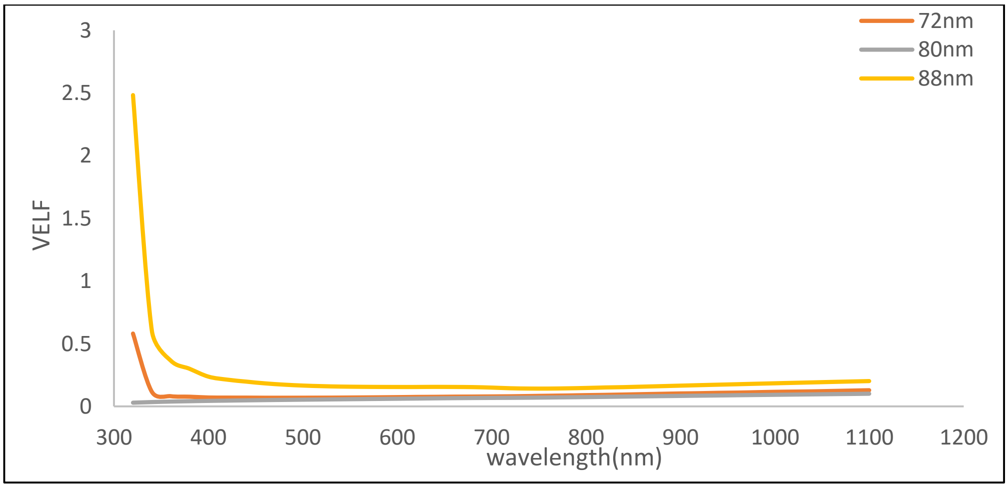

Fig 16. Volume energy loss function versus the wavelength of CdTe thin films (VELF).

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CONCLUSIONS

The deposition of cadmium telluride (CdTe) thin films of varying thicknesses was carried out on glass substrates using the thermal evaporation process. The X-ray diffraction (XRD) analysis revealed that the CdTe films exhibited a polycrystalline nature, characterized by a cubic crystal structure. A noticeable enhancement in the crystal structure was noticed as the thickness increased. The clear result of the scanning electronic microscopy is that homogeneously distributed crystal grain morphology was observed. The inference of SEM is consistent with the result of the XRD measurement. The morphology of the film grown had a good homogeneous surface and smoothy. With increased thickness, the absorption increased, while the direct energy bandgap of the films decreased. The obtained results of the refractive index, extinction coefficient, and real and imaginary dielectric constants indicate a significant influence of layer thickness on the optical parameters. The investigation of the surface energy loss function (SELF) and volume energy loss function (VELF) revealed a positive correlation between their values and the thickness of the material being researched.

Conflict of interests.

There are non-conflicts of interest.

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الخلاصة

مقدمة:

هناك العديد من الاستخدامات الكهروضوئية للأغشية الرقيقة من أشباه الموصلات II–VI. إحدى هذه المواد التي أثبتت فعاليتها في إنشاء الخلايا الشمسية وأجهزة الكشف الضوئية وتطبيقات الأجهزة الضوئية الأخرى هي تيلوريد الكادميوم

طرق العمل:

تم انشاء اغشية الكادميوم تيلوريد في فراغ عالٍ وترسيبها على ركائز زجاجية بسماكات مختلفة (72 ، 80 ، 88 نانومتر) بواسطة تقنية التبخير الحراري.

النتائج:

وفقًا لنتائج اختبار XRD ، فإن أغشية CdTe المبخرة حرارياً لها هيكل مكعب لوجود زاوية مميزة تقابل معامل ميلر (111). مع زيادة السمك ، لوحظ تحسن كبير في التبلور . يتم استخدام مجهر القوة الذرية (AFM) لتقييم شكل الفيلم الذي يوضح السطح المتجانس الجيد للأغشية التي تم إنتاجها. تمت دراسة القياسات الضوئية للأغشية بواسطة مقياس الطيف الضوئي المرئي فوق البنفسجي. عندما يزداد السمك، يزداد الامتصاص ، بينما تقل النفاذية. تشير قيم فجوة الطاقة المباشرة المحسوبة من علاقة Tauc إلى تأثير التكميم وانخفضت من (3.60 إلى 3.42) فولت مع زيادة السمك. وجد أن النفاذية (T) والامتصاصية (A) وفجوة النطاق البصري تعتمد بشكل ملحوظ على سمك الفيلم. أظهرت النتائج التي تم الحصول عليها من معامل الانكسار ومعامل الخمود وثوابت العزل الحقيقي والخيالي أن سمك الفيلم يؤثر بشدة على المعلمات الضوئية. تعتبر وظيفة فقدان الطاقة السطحية (SELF) ووظيفة فقدان الطاقة بالحجم (VELF) مهمة للدراسة بسبب التأثير الكمي. تشير الاختبارات الهيكلية وقيم فجوة الطاقة إلى حجم الجسيمات الدقيقة وسطح الأغشية المحضرة ويمكن أن تكون مرشحة للتطبيقات الإلكترونية الضوئية

الاستنتاجات:

تم الكشف عن علاقة بين السمك والخصائص المورفولوجية والتركيبية في هذه الدراسة كذلك علاقة السمك مع الثوابت البصرية ومعاملات التشتت ووجد انها تزداد بزيادة السمك.

الكلمات المفتاحية : الكادميوم تيلوريد , التبخير الحراري , مورفولوجية , حجم حبيبي.